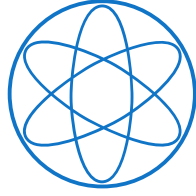


1  
PHYSIK-DEPARTMENT



3 **Exploring the Strange-Meson Spectrum**  
4 **with COMPASS in the Reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$**

5 **Dissertation**

6 Stefan Wallner

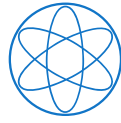


8 TECHNISCHE UNIVERSITÄT MÜNCHEN





Technische Universität München



Fakultät für Physik

**Exploring the Strange-Meson Spectrum  
with COMPASS in the Reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$**

Stefan Wallner

Vollständiger Abdruck der von der Fakultät für Physik der Technischen Universität München zur Erlangung des akademischen Grades eines

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## Abstract

In the naïve quark-model picture, strange mesons consist of a strange and an up or down (anti)quark, which are bound by the strong interaction. Although strange mesons have been studied since more than 70 years, many parts of their excitation spectrum are still unexplored.

The COMPASS experiment at CERN collected the so far world's largest sample of 720 494 exclusive events for the diffractive-scattering reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . This sample allows us to study strange mesons decaying into the  $K^- \pi^- \pi^+$  final state. In this thesis, we present the analysis of this data sample, starting from the event selection, up to an elaborate partial-wave analysis (PWA), with which we extract the strange-meson resonances. We develop a novel method for the identification of beam kaons using the full experimentally available information, which doubles the efficiency for kaon identification compared to the previously used method. We extend the classical PWA approach by employing model-selection techniques in order to construct the partial-wave model, and by applying Bootstrapping techniques in order to improve the parameter and uncertainty estimates. Furthermore, we develop a novel approach to treat incoherent background contributions to our  $K^- \pi^- \pi^+$  sample in the PWA. We perform extensive systematic studies as well as Monte Carlo studies in order to validate the analysis results. Finally, we perform a first study of the amplitudes of light mesons appearing in the  $\pi^- \pi^+$  and  $K^- \pi^+$  subsystems of the  $K^- \pi^- \pi^+$  final state.

Our analysis yields the so far most complete picture of the strange-meson spectrum coming from a single analysis. In total, we study 14 strange mesons. We find signals from well-known strange mesons, as well as indications for states that are not yet established. For example, we find indications for the  $K_2(2250)$ ,  $K_3(2320)$ , and  $K_4(2500)$  for the first time in a PWA of a final state other than  $\Lambda \bar{p}$  or  $\bar{\Lambda} p$ . In addition, we find indications for three excited pseudoscalar kaons; i.e. the  $K(1460)$ , the  $K(1630)$ , and the  $K(1830)$ ; while quark-model calculations predict only two excited states in this mass region. This hints towards an exotic nature of one of these three states. Our estimates for the masses and widths of the 14 strange mesons mostly agree with previous measurements and with quark-model calculations. Our uncertainties for most of the measured masses and widths are competitive with the corresponding so far best measurements of these parameters by previous measurements.



## Kurzzusammenfassung

Entsprechend dem Quarkmodell bestehen leichte Mesonen mit Strangeness aus einem Strange und einem Up (Anti-)Quark, welche durch die starke Wechselwirkung gebunden sind. Seit mehr als 70 Jahren werden diese Mesonen studiert und dennoch sind Teile ihres Anregungsspektrums bis heute unbekannt.

Das COMPASS Experiment am CERN hat den bisher weltweit größten Datensatz für die diffraktive Streureaktion  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , bestehend aus 720 494 exklusiven Ereignissen gemessen. Dieser Datensatz erlaubt es, leichte Mesonen mit Strangeness in deren Zerfall in den  $K^- \pi^- \pi^+$  Endzustand zu studieren. In dieser Arbeit präsentieren wir die zugehörige Analyse, von der Ereignisauswahl bis hin zu einer umfangreichen Partialwellenanalyse (PWA). Hierfür entwickeln wir eine neuartige Methode zur Identifikation von Kaonen im Strahl, die eine doppelt so hohe Effizienz verglichen mit der zuvor verwendete Methode aufweist. Zudem erweitern wir den klassischen PWA Ansatz um eine Methode zur systematischen Konstruktion des Partialwellenmodells mittels Modellselektionsverfahren, sowie um Bootstrapping-Verfahren zur Verbesserung der Parameter- und Unsicherheitsbestimmung. Des Weiteren entwickeln wir einen neuartigen Ansatz zur Modellierung inkohärenter Untergründe und führen weitreichende systematische sowie Monte Carlo Studien zur Verifizierung unserer Ergebnisse durch. Abschließend messen wir erstmals die quantenmechanischen Amplituden von leichten Mesonen in den  $\pi^- \pi^+$  und  $K^- \pi^+$  Subsystemen des  $K^- \pi^- \pi^+$  Endzustandes.

In dieser Arbeit präsentieren wir das bisher umfassendste Bild des Spektrums leichter Mesonen mit Strangeness, welches aus einer einzigen Analyse stammt. Wir studieren insgesamt 14 leichte Mesonen mit Strangeness, wobei wir sowohl Signale von wohlbekanntem Zuständen, als auch Anzeichen für bisher nicht etablierte Zustände finden. Beispielsweise beobachten wir Anzeichen für die Zustände  $K_2(2250)$ ,  $K_3(2320)$  und  $K_4(2500)$ . In dieser Arbeit werden sie das erste Mal in einer PWA in einem anderen Endzustand als  $\Lambda \bar{p}$  oder  $\bar{\Lambda} p$  beobachtet. Des Weiteren finden wir Anzeichen für drei pseudoskalare Kaonen. Da das Quarkmodell nur zwei Zustände in dieser Massenregion vorhersagt, deuten unsere Beobachtungen auf eine exotische Natur eines dieser Zustände hin. Unsere Messung der Massen und Breiten der 14 Zustände stimmt mit vorherigen Messungen überein. Die Unsicherheiten unserer Messung sind meist ähnlich gut, wie die Unsicherheiten der bisher besten Messungen dieser Parameter.





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<sup>177</sup> **List of Todos**

DRAFT



# 1 Introduction

179 Our current understanding of nature is that there are four fundamental interactions: (i) gravitation,  
 180 which, e.g., binds planets and stars to solar systems and solar systems together with other  
 181 components to galaxies; (ii) the electromagnetic interaction, which, e.g., binds electrons and  
 182 nuclei to atoms and atoms to molecules; (iii) the strong interaction, which, e.g., binds quarks to  
 183 hadrons, such as strange mesons, and hadrons to nuclei; and (iv) the weak interaction, which,  
 184 e.g., is responsible for radioactive decays of nuclei.<sup>[a]</sup> Often, the study of bound systems  
 185 allows us to gain more knowledge about the respective interaction. For example, the high-  
 186 precision measurements of the fine and hyper-fine structure of the hydrogen atom, one of the  
 187 simplest electromagnetically bound systems, contributed greatly to the development of Quantum  
 188 Electrodynamics (QED), the fundamental theory of the electromagnetic interaction [1, 2]. For  
 189 certain bound systems, their composition is not completely known, but the study of the properties  
 190 of such bound systems gives access to their composition. For example, the density of dark  
 191 matter in galaxies can be studied based on observations of the distribution and movement of the  
 192 visible matter [3–5]. Similarly, the composition of strongly bound systems, i.e. hadrons, is not  
 193 completely understood as we cannot study the individual components of hadrons separately due  
 194 to the confinement. In the same spirit as the studies of systems bound by the electromagnetic  
 195 interaction or gravitation, the goal of hadron spectroscopy programs, such as the strange-meson  
 196 spectroscopy program at COMPASS, is to gain a better understanding of the strong interaction  
 197 and its fundamental theory the Quantum Chromodynamics (QCD) by studying strongly bound  
 198 systems.

199 In the naïve quark-model picture [6–8], mesons are states build up from a constituent quark and  
 200 antiquark pair ( $q\bar{q}'$ ). Hence, they are the simplest strongly bound system. Light mesons are build  
 201 up from up, down, or strange (anti)quarks. Strange mesons are light mesons with strangeness  $\pm 1$ ,  
 202 i.e. they are build up from a strange (anti)quark and an up or down (anti)quark.

203 Important properties of light mesons are their quantum numbers, i.e. their isospin  $I$ , their total  
 204 spin  $J$ , and their parity  $P$ . The latter two are often written as  $J^P$ .<sup>[b]</sup> In the quark model, light  
 205 mesons form for each  $J^P$  a SU(3) flavor nonet. Each nonet consists of two isoscalar mesons with  
 206  $I = 0$ , three isovector mesons with  $I = 1$ , and four strange mesons with  $I = 1/2$ .

<sup>[a]</sup> We list the four fundamental interactions as they appear after electroweak symmetry breaking.

<sup>[b]</sup> In addition, neutral non-strange light mesons are characterized by their charge parity quantum number  $C$ . By convention, the  $C$  parity of a neutral meson is often also assigned to its charged partners. Furthermore, one can extend the idea of charge conjugation to charged mesons by introducing the  $G$  parity. Strange mesons are not eigenstates of the  $C$ - or  $G$ -parity operators and hence do not have  $C$ - or  $G$ -parity quantum numbers.

207 In the quark-model picture, the total spin  $J$  of the meson is given by the coupling of the total  
 208 intrinsic spin  $S_{q\bar{q}'}$  of the  $q\bar{q}'$  system and the relative orbital angular momentum  $L_{q\bar{q}'}$  between the  
 209 two constituent quarks. The half-integer spins of the two quarks can couple to a total intrinsic  
 210 spin of

$$S_{q\bar{q}'} = 0 \text{ or } 1. \quad (1.1)$$

211 The relative orbital angular momentum can take values of

$$L_{q\bar{q}'} = 0, 1, 2, \dots \quad (1.2)$$

212 The total spin of the meson is in the range

$$|S_{q\bar{q}'} - L_{q\bar{q}'}| \leq J \leq (S_{q\bar{q}'} + L_{q\bar{q}'}). \quad (1.3)$$

213 The parity of the meson can be expressed as

$$P = (-1)^{L_{q\bar{q}'}+1}. \quad (1.4)$$

214 Finally, the so-called naturality of the meson is defined as

$$\eta \equiv (-1)^J P = (-1)^{J+L_{q\bar{q}'}+1}. \quad (1.5)$$

215 Strange mesons are grouped into two families: (i) states with positive naturality called  $K_J^*$  and  
 216 (ii) states with negative naturality called  $K_J$ .<sup>[c]</sup>

217 Besides their quantum numbers, another important property of mesons is their mass. For light  
 218 mesons, a large fraction of the meson mass is dynamically generated by the strong interaction.  
 219 Hence, understanding the emergence of the meson masses by measuring the masses of a wide  
 220 variety of mesons and comparing them to theory predictions leads to a better understanding of  
 221 the strong interaction and its fundamental theory QCD. Furthermore, all strange mesons, except  
 222 for the lightest strange meson, i.e. the kaon, quickly decay via the strong interaction to final-state  
 223 hadrons such as pions, kaons, protons, or lambda baryons.<sup>[d]</sup> Hence, they have an extremely  
 224 short lifetime and thus appear as resonances in the final states. The width of these resonances  
 225 is another important property. Measuring the masses and widths of mesons is a major task of  
 226 meson spectroscopy.

227 For fixed  $J^P$ , there are  $K_J^*$  states with  $L_{q\bar{q}'} = J - 1$  and with  $L_{q\bar{q}'} = J + 1$ .  $K_J$  states always have  
 228  $L_{q\bar{q}'} = J$ .<sup>[e]</sup> In addition, there are radial excitations of the  $q\bar{q}'$  system. Hence, there is not only  
 229 one state for a given  $J^P$ , but we expect from angular and radial excitations a whole excitation

---

<sup>[c]</sup> There are two exceptions to this naming scheme. The pseudoscalar mesons with  $J^P = 0^-$ , which would be called  $K_0$ , are actually called  $K$ . The vector mesons with  $J^P = 1^-$ , which would be called  $K_1^*$ , are actually called  $K^*$ .

<sup>[d]</sup> These final-state particles are stable with respect to the strong and electromagnetic interaction, but can decay via the weak interaction. However, weak decays proceed more slowly. Thus, these final-state particles are considered as stable. The only exception is the  $\pi^0$ , which can electromagnetically decay, but which has still a comparably long lifetime of  $(8.43 \pm 0.13) \times 10^{-17}$  s [9] and hence can also be considered as stable.

<sup>[e]</sup> Because of equation (1.5),  $J + L_{q\bar{q}'}$  has to be even for a negative naturality state. This is possible only for  $L_{q\bar{q}'} = J$  as  $S_{q\bar{q}'} \leq 1$  [see equation (1.3)].



---

230 spectrum of states with increasing masses.<sup>[f]</sup> While  $K_J^*$  states have always  $S_{q\bar{q}'} = 1$ ,<sup>[g]</sup>  $K_J$  states  
231 can have  $S_{q\bar{q}'} = 0$  or  $S_{q\bar{q}'} = 1$ . Thus, for a given  $J^P$ ,  $L_{q\bar{q}'}$ , and radial excitation there are two states  
232  $K_{J,a}$  and  $K_{J,b}$  with different  $S_{q\bar{q}'}$ , which cannot be distinguished by their  $J^P$  quantum numbers and  
233 which are close in mass. These two states can mix. Thus, the two physical states, for example  
234 the  $K_1(1270)$  and the  $K_1(1400)$ , are actually a mixture of  $K_{J,a}$  and  $K_{J,b}$ .

235 So far, we mainly discussed strange mesons in the context of the quark-model. However, QCD  
236 in principle allows for more than just constituent quark-model states, which are build up from  
237 a  $q\bar{q}'$  pair. For example, there could be states with four constituent quarks called molecules  
238 or tetraquarks. Also, so-called hybrids could exist, which have an excited gluon-field that  
239 contributes to their quantum numbers. Historically, states beyond the constituent quark-model  
240 are called exotics. In the non-strange light-meson sector, a candidate for such an exotic state is  
241 the  $\pi_1(1600)$  [11], which has quantum numbers that are forbidden for a  $q\bar{q}'$  state. In order to  
242 establish exotic states, it is important to find their strange partners in the corresponding SU(3)  
243 flavor multiplet. In the strange-meson sector, exotic states have the same quantum numbers  
244 as ordinary quark-model states. Therefore, such exotic states are also called crypto-exotic.  
245 They appear only as supernumerary states in addition to the ordinary states of the quark-model  
246 SU(3) flavor nonets. Establishing exotic strange mesons hence requires to completely map out  
247 the strange meson spectrum and to compare it to quark-model predictions in order to identify  
248 supernumerary states.

249 At the low energies of the light-meson masses, QCD cannot be solved perturbatively. The  
250 only available first-principles approach is lattice QCD, i.e. the numerical simulation of QCD  
251 on a discrete space-time lattice. This approach has recently made significant progress [12, 13].  
252 However, most lattice QCD calculations for hadron spectroscopy still need to be performed  
253 at unphysically high quark masses. This makes an extrapolation down to the physical point  
254 necessary and introduces additional uncertainties to the lattice QCD predictions. Nevertheless,  
255 lattice QCD provides important insight into the spectrum of mesons including the existence  
256 of potential exotic states. With improved methods and computing power, lattice QCD also  
257 started to study the strong decays of meson resonances, such as the  $K^*(892)$  [14–16]. This  
258 opens the possibility to compare first-principle QCD predictions for hadron resonances with  
259 experimental observations. However, such a comparison requires a complete and precise picture  
260 of the strange-meson spectrum from experiments.

261 Strange mesons also appear as resonances in multi-body decays of heavy mesons or  $\tau$  leptons  
262 with kaons in the final state. Hence, a complete understanding of such decays typically requires  
263 incorporating all appearing strange mesons in an amplitude analysis. This is a challenge especially  
264 in rare decays, because even with the largest data sets currently available, the precision is typically  
265 not high enough to determine all appearing mesons from the data set itself. Thus, also for these  
266 analyses a precise knowledge of the complete strange meson spectrum is mandatory as an input.  
267 Such rare decays of  $B$  and  $D$  mesons are studied, e.g., in searches for  $CP$  violation and in

---

[f] Side note: According to the quark model calculation in ref. [10], the first radial excitation of a  $K_J^*$  ground state, which has  $L_{q\bar{q}'} = J - 1$ , is close in mass to the angular excitation, which has  $L_{q\bar{q}'} = J + 1$ .

[g] Because of equation (1.5), a positive naturality state must have  $L_{q\bar{q}'} \neq J$ , which can only be satisfied for  $S_{q\bar{q}'} = 1$  [see equation (1.3)].

268 the measurements of the angles of the unitarity triangle of the CKM matrix performed at the  
 269 Belle [17], LHCb [18], and BaBar [19] experiments. Strange mesons also play a role in the search  
 270 for new physics, e.g. in the decay  $B^0 \rightarrow K^+ \pi^- l^+ l^-$ ,<sup>[h]</sup> where a complete understanding of all  
 271 strange-meson contributions to the  $K^+ \pi^-$  system is mandatory [20, 21]. These requirements on a  
 272 precise and complete picture of the strange meson spectrum will become even more demanding  
 273 with upcoming high-precision data from experiments such as Belle II and LHCb. Therefore,  
 274 strange-meson spectroscopy not only allows us to study QCD, but gives also important input to  
 275 other fields of fundamental physics.

276 At experiments, strange mesons can be produced in various ways in order to study them. At fixed-  
 277 target experiments such as LASS at SLAC [22], and WA3 [23] and the  $\Omega$  spectrometer [24] at  
 278 CERN, strange mesons were produced in the scattering of high-energy kaon beams off stationary  
 279 targets. In this process, the beam kaon is excited to  $K_J^*$  and  $K_J$  states. The produced excited  
 280 strange mesons were then observed in their decays to various final states such as  $K\pi$  or  $K\pi\pi$ .  
 281 Strange mesons can also be produced in the scattering of high-energy photon beams. Such  
 282 photoproduction reactions are currently studied at the GlueX experiment at Jefferson Lab [25].  
 283 Yet another way to access the strange meson spectrum is in multi-body decays of heavy mesons  
 284 such as  $D^0 \rightarrow K^\mp \pi^\pm \pi^\pm \pi^\mp$  [26],  $B^+ \rightarrow J/\psi K^+ \pi^+ \pi^-$  [27], or  $J/\psi \rightarrow K^+ K^- \pi^0$  [28]; or in  $\tau$  decays  
 285 such as  $\tau^- \rightarrow K^- \pi^+ \pi^- \nu_\tau$  [29]. Here, the strange mesons appear in subsystems of the multi-body  
 286 final states such as the  $K\pi$  and  $K\pi\pi$  subsystems. These studies of strange mesons were performed  
 287 or are still ongoing at experiments such as LHCb, Belle (II), BESIII, and CLEO.

288 Figure 1.1 shows the current status of our knowledge about the strange-meson spectrum. At  
 289 the moment, the PDG [9] lists 25 strange mesons. Only 16 of them are considered as estab-  
 290 lished states (blue data points). The remaining 9 states still need further confirmation (orange  
 291 data points). The black horizontal lines in figure 1.1 represent the result of the quark-model  
 292 calculation from ref. [10]. Many of the predicted states were not yet observed experimentally.  
 293 Especially, in the high-mass region above about  $1.8 \text{ GeV}/c^2$ , many of the predicted states still  
 294 lack experimental evidence and most of the states listed in the PDG, e.g. the  $K_3(2320)$  [30, 31]  
 295 and the  $K_4(2500)$  [31], were seen by only a few or even only a single experiment. A reason for  
 296 this is that it is experimentally more challenging to find resonances in the high-mass region, due  
 297 to the large overlap between the states given by the high density of states (see figure 1.1) and  
 298 their typically large widths. Not only are many parts of the strange meson sector still unexplored  
 299 after more than 70 years of experimental searches [32], but also most of the experimental studies  
 300 of the strange-meson spectrum were performed more than 30 years ago. Only four additional  
 301 strange mesons have been included in the PDG listening since 1990 [33]. Most of the more  
 302 recent studies were performed based on large data samples of heavy-meson or  $\tau$  decays from  
 303 experiments such as Belle [27], BESIII [28], and LHCb [34]. However, even with these large  
 304 data samples they could often study only a limited set of  $J^P$  sectors and only limited mass ranges.  
 305 In general, most of the previous measurements of strange mesons were focused only on limited  
 306 mass ranges and only on limited sets of  $J^P$  sectors, thereby neglecting the contributions of states  
 307 outside these limits. For example, the two ground state  $K_2(1770)$  and  $K_2(1820)$  [34, 35] and  
 308 the excited  $K_2(2250)$  [31, 36, 37] were studied so far in completely separate sets of analyses,

<sup>[h]</sup>  $l$  stands for lepton.

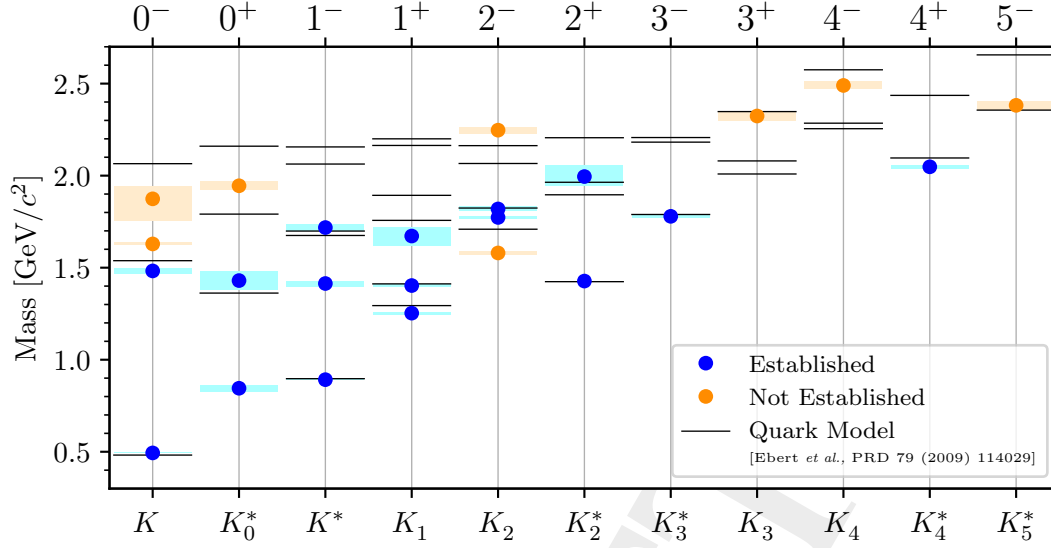


Figure 1.1: Spectrum of strange mesons, i.e. nominal masses of strange mesons grouped by their  $J^P$  quantum numbers. The blue data points show the masses of established states, the orange data points those of not established states as listed by the PDG [9]. The similarly colored boxes represent the corresponding uncertainties. The black horizontal lines show the masses of states as predicted by the quark-model calculation in ref. [10]. As we show only masses below  $2.7 \text{ GeV}/c^2$  for a better visualization, the not-established  $K(3100)$  is omitted here.

309 although the  $K_2(2250)$  partly overlaps with the ground states. A more complete analysis covering  
 310 a wide mass range and considering many  $J^P$  sectors simultaneously is still missing and would  
 311 give a more complete and realistic picture of the strange-meson spectrum.

312 The main goal of the spectroscopy program at the COMPASS experiment at CERN is to obtain a  
 313 more complete picture of the non-strange and strange light-meson spectrum. Using the dominant  
 314  $\pi^-$  contribution in the beam, COMPASS performed a detailed high-precision measurement of the  
 315 isovector light-meson spectrum. COMPASS measured the largest data sample for the decay to  
 316 the  $\pi^- \pi^- \pi^+$  final state in the reaction  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$ . The COMPASS  $\pi^- \pi^- \pi^+$  analysis  
 317 is the so-far most comprehensive analysis of this reaction, where novel analysis techniques were  
 318 applied [11, 38–42]. An even more detailed analysis of the  $\pi^- \pi^- \pi^+$  final state at COMPASS is  
 319 currently ongoing [43].

320 The goal of this thesis is to obtain a more complete picture of the strange-meson spectrum by  
 321 mapping out the spectrum of strange mesons similarly to the measurement of the isovector  
 322 light-meson spectrum by COMPASS. Therefore, we used the  $K^-$  contribution in the high-energy  
 323 hadron beam at COMPASS and studied strange mesons in their decay to the  $K^- \pi^- \pi^+$  final state  
 324 in the diffractive scattering reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , which is similar to the reaction  
 325  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  used for isovector-meson spectroscopy. Based on a first analysis of only  
 326 a subset of the COMPASS data [44], we aimed to extend and improve the event selection in  
 327 order to obtain a large data sample of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . In order to search  
 328 for strange mesons in this data sample, our goal was to perform the so far most comprehensive

329 partial-wave analysis (PWA) of the  $K^- \pi^- \pi^+$  final state, which is split into two stages. In the first  
330 stage called partial-wave decomposition (PWD), the data are decomposed into contributions  
331 from various  $J^P$  sectors. We aimed to develop and apply models and analyses techniques that go  
332 beyond what was used in previous analyses of the  $K^- \pi^- \pi^+$  final state. To this end, much of the  
333 experience gained in the COMPASS  $\pi^- \pi^- \pi^+$  analysis entered our analysis and was developed  
334 further, and some methods applied in our analysis were developed in close collaboration with  
335 the currently ongoing COMPASS  $\pi^- \pi^- \pi^+$  analysis. In the second stage of our analysis called  
336 resonance-model fit (RMF), strange-meson resonances are extracted and their masses and widths  
337 are measured. Here, our goal was to study a large variety for strange mesons from many  $J^P$   
338 sectors and from a wide mass range simultaneously in a single analysis. Finally, we intended  
339 to scrutinize our analysis methods and results in extensive systematic studies and Monte Carlo  
340 input-output studies.

341 In chapter 2, we discuss the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  and briefly introduce the COMPASS  
342 experimental setup. In chapter 3, we discuss improvements in the identification of beam kaons  
343 at COMPASS and the performance of the final-state particle identification, which were major  
344 challenges of our analysis. In chapter 4, we describe the event selection and present kinematic  
345 distributions of the  $K^- \pi^- \pi^+$  final state. In chapter 5, we describe the partial-wave decomposition.  
346 We also provide a first glimpse on the results of the PWD, and we discuss extensive studies to  
347 scrutinize the PWD. In chapter 6, we describe the resonance-model fit. We also provide a first  
348 glimpse on the results of the RMF, and we discuss extensive studies to scrutinize the RMF. In  
349 chapter 7, we discuss the major physics results of our analysis and compare them to previous  
350 measurements and to theory predictions. In chapter 8, we present a first attempt to also study  
351 mesons appearing in the  $K^- \pi^+$  and  $\pi^- \pi^+$  subsystems of the  $K^- \pi^- \pi^+$  final state using the so-called  
352 freed-isobar approach. Finally, in chapter 9, we conclude our results and present further prospects  
353 for strange-meson spectroscopy at COMPASS and at other experiments. Technical details of  
354 our analysis and additional results are given in appendices A to H. Important expressions and  
355 terminology specific to this analysis are underlined in the text and summarized in the [glossary](#).

## 2 Strange-Meson Spectroscopy at the COMPASS Experiment

### 2.1 The Studied Process: Diffractive Production of $K^- \pi^- \pi^+$

Our goal is to explore the strange meson-spectrum with COMPASS by studying the diffractive<sup>[a]</sup> scattering of a  $K^-$  beam off a liquid-hydrogen target. At high center-of-momentum energies of the  $K^-_{\text{beam}} p_{\text{target}}$  system, like at COMPASS, the scattering process is dominated by the  $t$ -channel exchange of a Pomeron  $\mathbb{P}$ . Pomeron exchange is an effective description of the underlying strong-interaction processes using Regge theory [45, 46]. In the reaction of interest, the target proton remains intact, whereas the beam  $K^-$  gets excited into an intermediate state  $X^-$  with mass  $m_X$ .<sup>[b]</sup> Here,  $X^-$  represents the excited strange mesons that we aim to study. In this way, we can produce all  $K_J^*$  and  $K_J$  states, except for  $K_0^*$  states.<sup>[c]</sup> Finally, we observe these strange mesons in their decays to final state particles. In this work, we focus on the decay to the  $K^- \pi^- \pi^+$  final state. The reaction is depicted in figure 2.1.

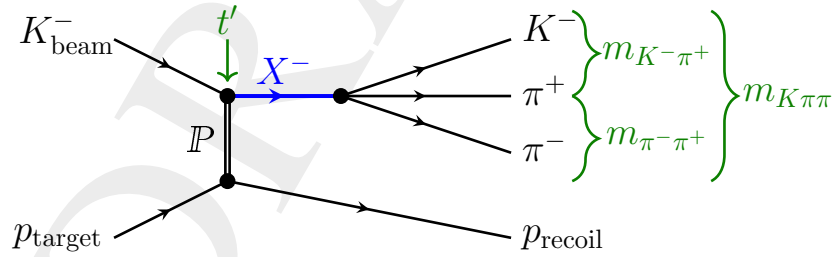


Figure 2.1: Schematic view of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ .

<sup>[a]</sup> Diffractive scattering reactions are inelastic scattering reactions, where the energy transfer between the two hadrons is comparably small and where one or both hadrons dissociate into a multi-particle final state. Diffractive scattering reactions are analogous to scattering off a gray disk in optics.

<sup>[b]</sup> In principle, there can be also excitations of the target proton. However, in our analysis excitations of the target proton are experimentally suppressed by the event selection section 4.1.

<sup>[c]</sup> As the beam  $K^-$  is a  $J^P = 0^-$  state, the relative orbital angular momentum  $L_{K\mathbb{P}}$  of the  $K^-_{\text{beam}} \mathbb{P}$  system has to be equal to the spin  $J_{\mathbb{P}}$  of the exchange particle in order to produce a  $J = 0$  system. The  $\mathbb{P}$  has positive naturality, which means that it has a parity of  $(-1)^{J_{\mathbb{P}}}$ . Hence, the parity of the  $K^-_{\text{beam}} \mathbb{P}$  system with  $J = 0$ , i.e. the parity of  $X^-$  with  $J = 0$ , is  $(-1)^{1+J_{\mathbb{P}}+L_{K\mathbb{P}}} = (-1)^{1+2J_{\mathbb{P}}} = -1$ . Thus, only  $K$  states with  $J^P = 0^-$  can be produced in diffractive kaon scattering, but no  $K_0^*$  states with  $J^P = 0^+$ .

369 In addition to the center-of-momentum energy, the invariant mass  $m_{K\pi\pi}$  of the  $K^-\pi^-\pi^+$  system,  
 370 and the invariant masses  $m_{K^-\pi^+}$  and  $m_{\pi^-\pi^+}$  of the  $K^-\pi^+$  and  $\pi^-\pi^+$  subsystems, respectively, the  
 371 reaction is characterized by the Mandelstam variable  $t$ , which is the squared four-momentum  
 372 transfer between the beam  $K^-$  and the target proton. It is always negative and given by

$$t = (p_{\text{beam}} - p_X)^2 = m_{\text{beam}}^2 + m_X^2 - 2(E_{\text{beam}}E_X - |\vec{p}_{\text{beam}}| |\vec{p}_X| \cos \theta). \quad (2.1)$$

373 Here,  $p_{\text{beam}}$  is the four-momentum of the beam particle,  $p_X$  is the four-momentum of the  $X^-$ ,  $E_i$   
 374 are the corresponding energies,  $|\vec{p}_i|$  are the corresponding magnitudes of the three-momenta, and  
 375  $\theta$  is the scattering angle, i.e. the angle between the  $X^-$  and the beam  $K^-$  momenta. It is more  
 376 convenient to use the reduced squared four-momentum transfer

$$t' \equiv |t| - |t|_{\text{min}}, \quad (2.2)$$

377 which takes into account the minimal squared four-momentum transfer,

$$|t|_{\text{min}} = -m_{\text{beam}}^2 - m_X^2 + 2(E_{\text{beam}}^{\text{CoM}}E_X^{\text{CoM}} - |\vec{p}_{\text{beam}}^{\text{CoM}}| |\vec{p}_X^{\text{CoM}}|), \quad (2.3)$$

378 necessary to produce an excited state with mass  $m_X$ . Here, the energies  $E_i^{\text{CoM}}$  and momenta  
 379  $|\vec{p}_i^{\text{CoM}}|$  are given in the overall center-of-momentum frame of the  $K_{\text{beam}}^- p_{\text{target}}$  system.<sup>[d]</sup> For the  
 380 kinematic region analyzed in this work,  $|t|_{\text{min}} \ll |t|$  and hence  $t' \approx |t|$ .

### 381 2.1.1 Non-Resonant Production of the $K^-\pi^-\pi^+$ Final State

382 In addition to the reaction depicted in figure 2.1, there can be other processes that also end up in  
 383 the  $K^-\pi^-\pi^+$  final state. However, these reactions do not proceed via intermediate resonances  $X^-$   
 384 in the  $K^-\pi^-\pi^+$  system. Hence, they are called non-resonant processes.

385 One class of such non-resonant processes are the so-called Deck-like reactions [47] depicted in  
 386 figure 2.2. The dominant graph, where a virtual pion is exchanged and rescatters off the target  
 387 proton, is shown in figure 2.2a. In forward direction in the laboratory frame, a fast intermediate  
 388 resonance  $\xi$  is produced, which then decay into  $K^-\pi^+$ . Figure 2.2b shows another possible graph,  
 389 where a virtual kaon is exchanged and a forward going  $\pi^-\pi^+$  system is produced. Due to the  
 390 higher mass of the kaon, this process is suppressed with respect to the pion-exchange process.

391 Further possible non-resonant processes are central-production reactions shown in figure 2.3. In  
 392 the dominant graph shown in figure 2.3a, both the target proton and the beam  $K^-$  emit a Pomeron.  
 393 The two Pomerons fuse and centrally<sup>[e]</sup> produce an intermediate resonance  $\xi$ , which then decays

<sup>[d]</sup> In general,  $E_i$  and  $|\vec{p}_i|$  depend on  $\theta$ . However, in the overall center-of-momentum frame, the energies  $E_i^{\text{CoM}}$  equal to the two-body breakup energies and the momenta  $|\vec{p}_i^{\text{CoM}}|$  equal to the two-body breakup momenta. This means  $E_i^{\text{CoM}}$  and  $|\vec{p}_i^{\text{CoM}}|$  are independent of  $\theta$ . Hence, in this frame, equation (2.1) has a maximum for  $\cos \theta = 1$ , which is a minimum of  $|t|$ .

<sup>[e]</sup> Here, ‘‘centrally’’ means that the intermediate  $\pi\pi$  resonance  $\xi$  is approximately at rest in the overall  $K_{\text{beam}}^- p_{\text{target}}$  center-of-momentum frame.

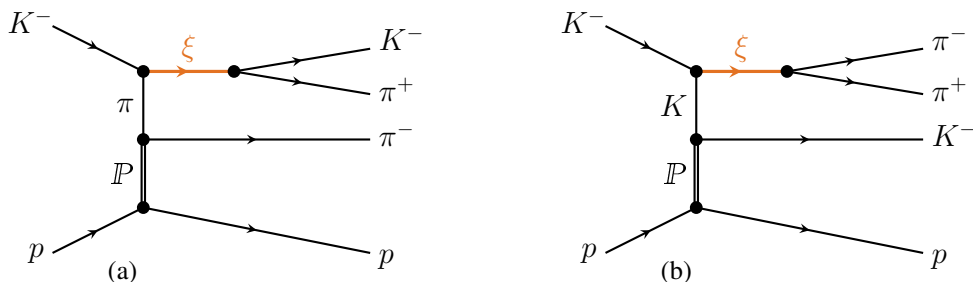


Figure 2.2: Schematic view of Deck-like reactions with (a) pion exchange and (b) kaon exchange.

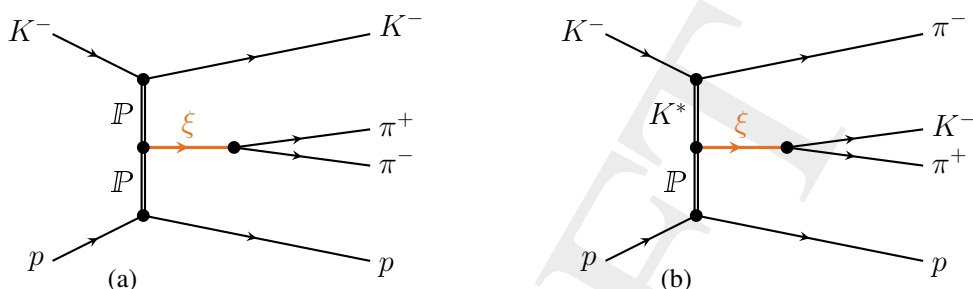


Figure 2.3: Schematic view of central-production reactions for a centrally produced  $\pi^- \pi^+$  (a) or  $K^- \pi^+$  (b) subsystem.

394 into  $\pi^- \pi^+$ . Alternatively, a virtual  $K^*$  can be exchanged at the top vertex in order to centrally  
 395 produce an intermediate resonance  $\xi$ , which decays into  $K^- \pi^+$  as shown in figure 2.3b. Further  
 396 exchanges in addition to  $\mathbb{P}$  and  $K^*$  are in principle also possible.

397 The main goal of this thesis is to study strange-meson resonances in the  $K^- \pi^- \pi^+$  system. Here,  
 398 non-resonant processes are considered as background. We discuss the treatment of these back-  
 399 grounds in section 6.1.2. However, studies of non-resonant processes, as done by JPAC based on  
 400 COMPASS data on the  $\eta\pi$  and  $\eta'\pi$  final states [48], are an interesting topic for themselves.

## 401 2.2 The COMPASS Experiment at CERN

402 COMPASS (COmmon Muon Proton Apparatus for Structure and Spectroscopy) is a very ver-  
 403 satile experiment designed to study QCD in the low-energy regime. It was used to study  
 404 the internal structure of hadrons by measuring, for example, the polarizability of pions [50]  
 405 or the contribution of the transverse quark spins to the nucleon spin [51]. The 2008 and  
 406 2009 diffraction data-taking campaigns at COMPASS were mainly devoted to light-meson spec-  
 407 troscopy. In the following, we briefly introduce the COMPASS experimental setup as it was used  
 408 during 2008 and 2009. A detailed description can be found in refs. [49, 52].

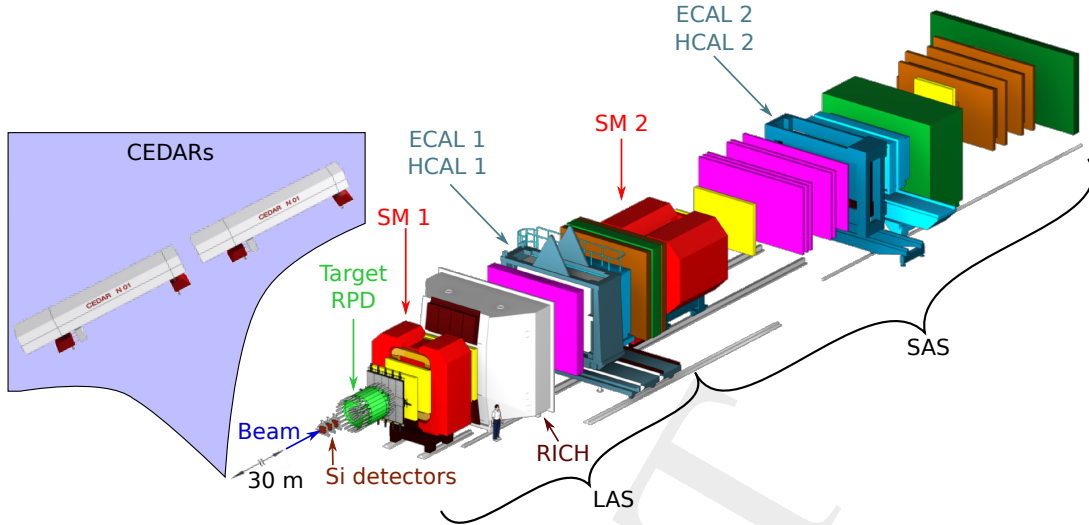


Figure 2.4: Schematic view of the COMPASS setup for measurements with hadron beams. The beam (blue arrow) is entering the target region surrounded by the RPD (green) from the left side. The final-state particles are measured with the COMPASS Large-Angle (LAS) and Small-Angle (SAS) magnetic Spectrometer. Different detector types are represented by different colors. The CEDAR detectors placed upstream of the COMPASS target are shown as an inset. The figure was taken from ref. [49] and adjusted.

409 COMPASS is a fixed-target experiment located at the M2 beam line at the CERN accelerator  
 410 laboratory. The setup is shown in figure 2.4. Protons from the Super Proton Synchrotron (SPS)  
 411 accelerator with a momentum of about  $400 \text{ GeV}/c$  impinge on a Beryllium production target (not  
 412 shown), where showers of secondary hadrons; mainly pions, kaons, and protons; are produced  
 413 with a large momentum spread. Then, particles in the desired momentum range are selected by a  
 414 series of magnets and collimators along the about 1 km long beam line. For the diffraction data  
 415 taking, we used a  $190 \text{ GeV}/c$  negative hadron beam, which corresponds to a center-of-momentum  
 416 energy of about  $19 \text{ GeV}/c^2$  for the reaction shown in figure 2.1. This beam has a high nominal  
 417 intensity of  $5 \times 10^6 \text{ s}^{-1}$  with a low momentum spread of about 1 % [49]. It is mainly composed  
 418 out of  $\pi^-$  (96.8 %), with smaller contributions from  $K^-$  (2.4 %) and  $\bar{p}$  (0.8 %) [49]. To distinguish  
 419 the beam-particle species, two alike CEDAR detectors (ChErenkov Differential counters with  
 420 Achromatic Ring focus) are positioned approximately 30 m upstream of the COMPASS target.

421 The negative hadron beam impinges on a cylindrical liquid-hydrogen target with a diameter of  
 422 35 mm and a length of 400 mm. The latter corresponds to about 5.5 % of the nuclear interaction  
 423 length [49]. Silicon microstrip detectors are placed upstream and downstream of the target to  
 424 measure the tracks of charged beam and final-state particles with high precision. This allows us  
 425 to reliably find and precisely reconstruct the interaction point of the beam particle with the target  
 426 proton. Furthermore, the target is surrounded by a barrel-shaped recoil-proton detector (RPD),  
 427 which measures the track of the recoiling proton. Detecting the recoil protons requires them to  
 428 have a minimal kinetic energy, which imposes a lower limit on  $t'$  of about  $0.1 \text{ GeV}/c^2$ .<sup>[†]</sup>

[†] For  $t' < 0.1 \text{ GeV}/c^2$ , the RPD acceptance quickly drops and becomes practically zero for  $t' < 0.07 \text{ GeV}/c^2$ .



429 The momenta of the forward-going charged final-state particles are measured by a two-stage  
430 magnetic spectrometer. The first stage called Large-Angle Spectrometer (LAS) covers polar  
431 angles of the final-state particles of up to 180 mrad [49]. It is followed by the Small-Angle  
432 Spectrometer (SAS), which extends the experimental acceptance to particles going in very  
433 forward direction with small polar angles in the range  $\pm 30$  mrad [52]. Each of the two stages  
434 consists of a bending magnet (SM 1/2) surrounded by multiple layers of tracking detectors. For  
435 a high-precision measurement of tracks close to the beam axis micropattern gaseous detectors  
436 are used namely Gas Electron Multipliers (GEM) and micromesh gaseous structure detectors  
437 (micromegas), as well as Scintillating Fibre counter (SciFi). To cover larger areas up to 12 m<sup>2</sup>  
438 further away from the beam axis, wire-based gas detectors are used such as Drift Chambers  
439 (DC), Multi-Wire Proportional Chambers (MWPC), and straw-tube chambers. Final-state particle  
440 identification is performed by the Ring-Imaging Cherenkov detector (RICH), which distinguishes  
441 pions, kaons and (anti)protons. Furthermore, each spectrometer stage is equipped with an  
442 Electromagnetic CALorimeter (ECAL) used to measure high-energy photons and electrons and a  
443 Hadronic CALorimeter (HCAL). The calorimeters were not used in our analysis.

444 Events are recorded only if they fulfill certain trigger criteria. The so-called Diffractive Trigger  
445 (DT0) was designed to perselect diffractive scattering events studied in this analysis. It requires  
446 coincidence of three signals: (i) an incoming beam particle is measured by two scintillator-based  
447 beam-trigger detectors placed upstream of the COMPASS target; (ii) a recoil proton is measured  
448 by the RPD; (iii) there is no signal from the veto system, which rejects events with beam particles  
449 that enter the setup outside the target region, events with final-state particles outside the LAS  
450 acceptance, or events with non-interacting beam particles. The DT0 trigger was designed to have  
451 a minimal bias on the selected events. For data management, the recorded data were grouped  
452 into up to approximately 2 hour long periods in time, the so-called runs. Finally, the recorded  
453 data were processed by the COMPASS reconstruction and analysis software CORAL [53].

454 The setups for 2008 and 2009 were nearby identical, with only minor changes. For example,  
455 between 2008 and 2009 one additional tracking detector was installed for detector testing and  
456 during 2009 the position of one of the beam trigger detectors was shifted, because a small part  
457 of the sensitive area of this detector was not working anymore. These effects had only a minor  
458 influence on the detector performance. Nonetheless, we take into account these changes in the  
459 partial-wave decomposition discussed in chapter 5 by splitting the total data set into three subsets  
460 labeled by: (i) 2008, (ii) 2009 W2X, (iii) 2009 W35.

461 Due to its two-stage layout, COMPASS has a large experimental acceptance for charged particles,  
462 which uniformly covers a wide kinematic range. Furthermore, COMPASS has a high resolution  
463 for the measurement of the momenta of charged particles. The CEDAR and RICH detectors  
464 allow us to identify events with kaons in the initial and final state, which is important for the  
465 studied reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  studied. Hence, COMPASS is perfectly suited for  
466 strange-meson spectroscopy, which requires applying partial-wave analysis techniques that rely  
467 on a precise knowledge of the involved particles and their momenta.



## 3 Particle Identification

One of the main experimental challenges in analyzing the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  is the identification of the particle species of the beam and final-state particles. Beam kaons have to be separated from the about 36 times larger pion content of the beam. In order to achieve a high efficiency of beam-kaon identification, while maintaining a sufficiently low pion contamination of the kaon-beam sample, we developed a novel likelihood approach using the information from two Cherenkov differential counters (CEDARs) [54], which is presented in section 3.1. Applying this method, we gained a factor two in beam-particle identification efficiency over a previously used method. The main task of the final-state particle identification is to distinguish the  $K^-$  from the  $\pi^-$  in the  $K^- \pi^- \pi^+$  final state. In section 3.2 we briefly introduce the method used to identify charged particles in the final state using information from the ring-imagine Cherenkov detector (RICH). In addition, we present in sections 3.1 and 3.2 performance studies of the applied methods, which were performed separately for the 2008 and 2009 diffraction data set. The results of the performance studies are discussed exemplary for the 2008 diffraction data set. The 2009 diffraction data set shows similar results.

### 3.1 Beam-Particle Identification

#### 3.1.1 The CEDAR Detectors

The negatively charged hadron beam at COMPASS is mainly composed out of pions (96.8 %), with smaller contributions from kaons (2.4 %) and antiprotons (0.8 %) [49]. To distinguish these particle species, two alike CEDAR detectors [55, 56] are positioned 30 m upstream of the COMPASS target. The central part of each CEDAR is a 6 m long vessel containing pressurized helium gas. Beam particles traverse the CEDAR approximately parallel to its optical axis, which is represented by the dashed line in figure 3.1. Since they move faster than the speed of light in the helium gas, they emit Cherenkov light, which is focused by a concave mirror and a system of lenses. Using a diaphragm, Cherenkov light that is emitted in a narrow angular range with respect to the optical axis is selected. Finally, the Cherenkov photons are detected by eight photomultipliers (PMTs) arranged on a ring around the optical axis. The momentum as defined by the beam optics is approximately the same for all beam particles. Therefore, the angle under which the Cherenkov light is emitted is the same for beam particles of the same species, but different for beam pions, kaons, or antiprotons. Each CEDAR detector can be tuned to identify a certain particle species, by selecting the pressure of the helium gas and the opening of the

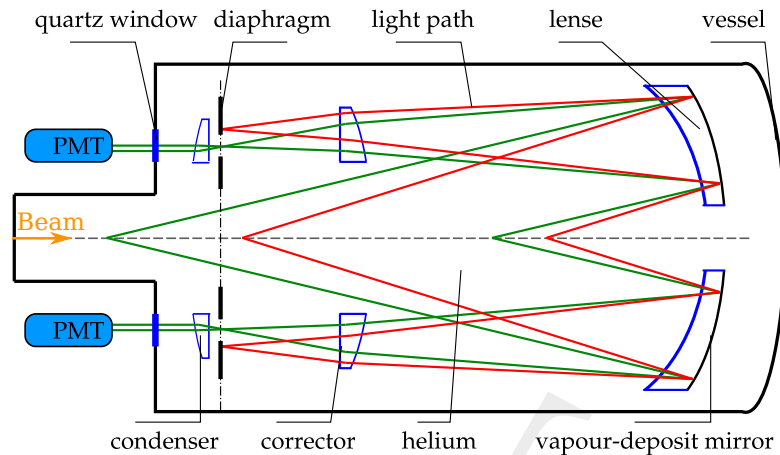


Figure 3.1: Basic operation principle of a CEDAR detector. The dashed line represents the optical axis of the detector, which coincides with the direction of the beam. The green and red lines represent the paths of Cherenkov light, which is emitted under different angles. Taken from ref. [49] and modified.

499 diaphragm, such that the Cherenkov ring of the selected species is focused on the PMTs (green  
 500 lines in figure 3.1), while the Cherenkov rings of the other species are shielded by the diaphragm  
 501 (red lines in figure 3.1).

502 For the diffraction data taking, both CEDARs were tuned to identify kaons. This means that the  
 503 kaon Cherenkov ring was focused on the PMTs. Thus, a beam kaon should generate signals in  
 504 the PMTs, while a beam pion or antiproton should not.

### 505 3.1.2 Challenges of the CEDAR Beam-Particle Identification

506 In previous analyses [44, 57], beam kaons were identified by requiring signals in the PMTs in  
 507 coincidence with the incoming beam particle. Taking into account the imperfect efficiency of the  
 508 PMTs, a signal in at least six out of the eight PMTs of one of the two CEDARs was required.

509 Unfortunately, this so-called majority method has a low efficiency of only 40 to 50 % [44]. The  
 510 main reason is the finite spread in the inclination of the beam particles with respect to the optical  
 511 axis of the CEDAR detectors. This beam divergence is about  $200\ \mu\text{rad}$  and thus of the same  
 512 order of magnitude as the difference between the kaon and pion Cherenkov angles, which is  
 513 around  $130\ \mu\text{rad}$  for the CEDAR parameters used in the diffraction data taking. For particles  
 514 traversing the CEDAR parallel to its optical axis (figure 3.2a), the Cherenkov ring of a kaon  
 515 (green ring) is in the sensitive area covered by the PMTs (gray circular area) and the Cherenkov  
 516 ring of a pion (red ring) is outside of the PMTs' acceptance. However, if the beam particle has  
 517 some finite inclination with respect to the optical axis its Cherenkov ring is shifted with respect  
 518 to the diaphragm aperture. In the example shown in figure 3.2b, the Cherenkov light of a kaon  
 519 would no longer hit the topmost three and bottommost three PMTs and only the leftmost and  
 520 rightmost PMT would have a signal, while for a pion with the same inclination the topmost

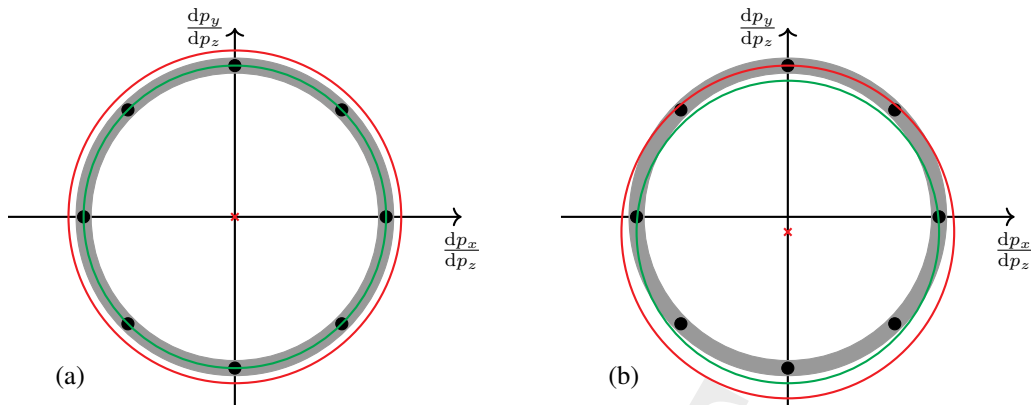


Figure 3.2: Illustration of the Cherenkov rings in the inclination space of beam particles represented by the red crosses. The green ring represents a beam-kaon Cherenkov ring. The red ring represents a beam-pion Cherenkov ring. The gray band represents the acceptance for Cherenkov photons defined by the diaphragm of the CEDAR. The black dots represent the position of the eight PMTs. (a) illustrates kaons and pions that traverse the CEDAR parallel to its optical axis. (b) illustrates kaons and pions that have some finite inclination in  $y$ -direction with respect to the optical axis.

521 PMTs would now give a signal. Therefore, for larger beam-kaon inclinations, fewer PMTs give a  
 522 signal leading to the low efficiency of the majority method. However, figure 3.2 also shows that a  
 523 certain hit pattern in the eight PMTs (i.e. which of the PMTs give a signal) is characteristic for a  
 524 certain particle species at a given inclination. We exploit this to formulate a likelihood ansatz in  
 525 section 3.1.3.

526 In a previous analysis of the Primakoff reactions measured in a different COMPASS data-taking  
 527 campaign; Friedrich J., et al. developed in ref. [58] already a likelihood-based approach for the  
 528 beam-particle identification. In ref. [59], a first attempt to formulate another likelihood-based  
 529 approach for the 2008 diffraction data set was developed. Both approaches have in common,  
 530 that they use independent parameterizations for the likelihood of beam kaons and pions with  
 531 independent sets of parameters. Therefore, both methods rely on large calibration samples of  
 532 pure beam kaons and pure beam pions.

533 In addition, the CEDAR parameters exhibit large modulations with time. For example, the helium  
 534 gas density varied (see figure 3.5), caused by small gas leaks, which made a daily refilling of  
 535 the gas vessel necessary. Also, the temperature of the CEDARs was not stable enough. These  
 536 variations considerably effected the position of the Cherenkov rings making a time-dependent  
 537 calibration mandatory. This exacerbates the requirement on the size of the calibration samples.

538 For the diffraction data set, the size of such beam samples, especially of a pure kaon-beam  
 539 sample, is very limited, as shown in section 3.1.6. Therefore, pure kaon-beam and pure pion-  
 540 beam samples that are sufficiently large to perform a time-dependent calibration of the CEDARs  
 541 could not be obtained from the diffraction data sets. The goal of the likelihood ansatz developed  
 542 in the following section is to not rely on pure kaon and pion-beam samples, but to extract the  
 543 calibration from a mixed sample of beam kaons and pions.

544 **3.1.3 Likelihood Method**

545 The main difference between particle species  $S$ , e.g. kaons or pions, traversing the CEDAR  
546 detectors is their different Cherenkov angle<sup>[a]</sup>

$$\cos \theta_{\text{Ch}}^S = \frac{1}{n\beta} = \frac{1}{n} \sqrt{1 + \left(\frac{m_S}{|\vec{p}|}\right)^2}. \quad (3.1)$$

547 The known beam momentum  $|\vec{p}|$ <sup>[b]</sup> and the refraction index of the helium gas  $n$  are the same for  
548 all particle species. The only particle-species specific quantity is the particle mass  $m_S$ , which is  
549 known [9]. The CEDARs are designed to accept light emitted in a certain angular range with  
550 respect to their optical axis. The emission angle is determined by the value of the Cherenkov  
551 angle and by the inclination of the beam-particle's trajectory with respect to the optical axis  
552 of CEDAR  $k$ . The inclination is defined by the beam particle momentum<sup>[c]</sup> in the small-angle  
553 approximation<sup>[d]</sup> as

$$\left(\frac{dp_x}{dp_z}\right)_{\text{Beam}}^k \equiv {}^k\vartheta_x \quad \text{and} \quad \left(\frac{dp_y}{dp_z}\right)_{\text{Beam}}^k \equiv {}^k\vartheta_y. \quad (3.2)$$

554 **Coordinate System**

555 The CEDAR response on a Cherenkov photon only depends on its emission angle with respect  
556 to the CEDARs optical axis. For a given emission angle, the response is independent of the  
557 particle species. Thus, the response of the individual PMTs can be parameterized uniformly for  
558 all particle species. As we did not measure the emission angle of individual photons, we first  
559 had to define a suitable coordinate system to parameterize the response of a PMT. Therefore,  
560 we find for a certain particle species all possible beam particle inclinations (red/orange points  
561 in figure 3.3a), where the corresponding Cherenkov rings (red/orange rings in figure 3.3a) hit  
562 the PMT centrally. In the inclination space, these beam particles lie on a circle around the PMT  
563 with radius given by the Cherenkov angle (dashed green circle in figures 3.3a and 3.3b). For a  
564 beam particle of species  $S$  with an arbitrary inclination, e.g. the magenta point in figure 3.3b, the  
565 probability for a signal in PMT  $j$ <sup>[e]</sup> mainly depends on the distance, to the ideal inclination that

<sup>[a]</sup> The difference in the number of emitted Cherenkov photons (see equation 34.43 in ref. [9]) is about 1 % and hence negligible.

<sup>[b]</sup> The beam-momentum spread is less than 1 % [49] and hence has a negligible effect on the Cherenkov angle compared to the difference in  $m_S$ .

<sup>[c]</sup> The beam particle inclination was measured by the silicon beam telescope near the target position with high precision. From this, the inclination at the CEDAR position was calculated using a transport matrix determined from the known beam optics [60]. The inclinations of the beam particle with respect to optical axes were calculated, taking into account the CEDARs' tildes with respect to the laboratory frame.

<sup>[d]</sup> The small beam inclinations of about 200  $\mu\text{rad}$  allows to use the small-angle approximation, i.e.  $\sin \vartheta \approx \vartheta$

<sup>[e]</sup> The index,  $j$ , uniquely identifies each PMT in the two CEDARs. Therefore,  $j = 0, \dots, 15$ .

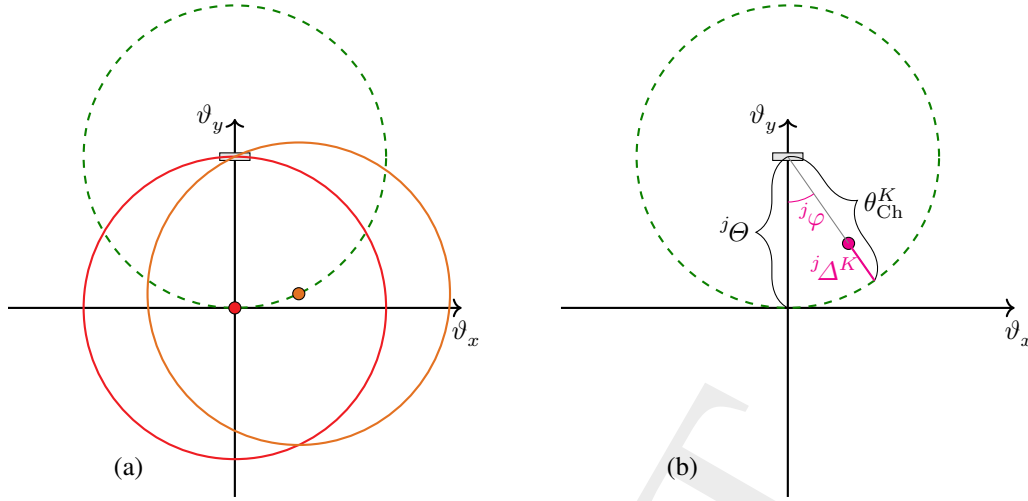


Figure 3.3: Two-dimensional inclination space of a beam particle with respect to the CEDARs optical axis. The gray box represents the center of the sensitive region of a PMT defined by the diaphragm. For illustration, the coordinate system was rotated such that the center of the PMT is on the vertical axis. (a) shows two exemplary beam inclinations (red/orange points), where the corresponding Cherenkov rings for kaons (red/orange circles) and the PMT's sensitive region intersect. The green dash circle shows all inclinations that fulfill this constraint. (b) shows a beam particle with arbitrary inclination (magenta point).

566 yields a signal in the PMT:

$$j\Delta^S(k\vartheta_x, k\vartheta_y) = \theta_{Ch}^S - \left\| \begin{pmatrix} k\vartheta_x \\ k\vartheta_y \end{pmatrix} - \begin{pmatrix} j\Theta \cos j\Phi \\ j\Theta \sin j\Phi \end{pmatrix} \right\|. \quad (3.3)$$

567 Here,  $j\Theta$  and  $j\Phi$  are the PMT's "position" in the inclination space, i.e. the direction in which  
 568 a photon has to be emitted in order to hit the PMT centrally. As the CEDARs were tuned to  
 569 beam-kaon identification,  $j\Theta \approx \theta_{Ch}^K$ .

570 The PMT response depends also on the angle  $j\varphi$ , which corresponds to the tilt of the Cherenkov  
 571 ring with respect to the sensitive area of the PMT defined by the diaphragm. It is calculated from  
 572 the measured inclination and the PMT position as

$$\sin [j\varphi(k\vartheta_x, k\vartheta_y)] = \frac{k\vartheta_x j\Theta \sin j\Phi - k\vartheta_y j\Theta \cos j\Phi}{\sqrt{(k\vartheta_x)^2 + (k\vartheta_y)^2 + (j\Theta)^2 - 2(k\vartheta_x j\Theta \cos j\Phi - k\vartheta_y j\Theta \sin j\Phi) j\Theta}}. \quad (3.4)$$

573 Equations (3.3) and (3.4) define the coordinate transformation from  $(k\vartheta_x, k\vartheta_y)$  to  $(j\Delta^S, j\varphi)$ , which  
 574 is different for each PMT  $j$  and each particle species  $S$ .

575 **Parameterization of the Likelihood**

576 The probability of a signal in PMT  $j$ , called hit probability  ${}^jP_{\text{PMT}}(\text{Hit} | {}^j\mathcal{A}^S, {}^j\varphi)$ , is a detector  
 577 property given by the PMT response to a Cherenkov photon. Its functional dependence on  
 578  ${}^j\mathcal{A}^S$  and  ${}^j\varphi$  is the same for all particle species. Thus, we could model it with one uniform  
 579 parameterization using the same parameters for all particle species. The hit probability consist  
 580 of a signal part and background part that accounts for hits, uncorrelated to the incoming beam  
 581 particle. The  ${}^j\mathcal{A}^S$  dependence of the signal, which we discuss first, is dominated by the diaphragm,  
 582 which selects a range in  ${}^j\mathcal{A}^S$ . We modeled this range by a rectangular function with a width  
 583 of  $2{}^j\Gamma$ . This rectangular function was smeared out e.g. by the uncertainty of the measured  
 584 beam inclination or by chromatic aberration of the CEDAR optics. We took this into account  
 585 by convoluting the rectangular function with a Gaussian function of width  ${}^j\sigma$ . This equals to a  
 586 difference of two error functions

$$\text{Signal}({}^j\mathcal{A}^S, {}^j\varphi) = \text{Erf}\left(\frac{{}^j\mathcal{A}^S + {}^j\Gamma({}^j\varphi)}{{}^j\sigma({}^j\varphi)}\right) - \text{Erf}\left(\frac{{}^j\mathcal{A}^S - {}^j\Gamma({}^j\varphi)}{{}^j\sigma({}^j\varphi)}\right). \quad (3.5)$$

587 To obtain the total hit probability, we added a constant background term  ${}^j\text{Bkg}$  to this signal. The  
 588 sum was normalized to its maximum at  ${}^j\mathcal{A}^S = 0$  and multiplied by an amplitude parameter  ${}^j\mathcal{A}$ ,  
 589 which takes into account the efficiency of the PMT. The final parameterization for a hit and for  
 590 no hit in the PMT reads

$${}^jP_{\text{PMT}}(\text{Hit} | {}^j\mathcal{A}^S, {}^j\varphi) = {}^j\mathcal{A}({}^j\varphi) \frac{\text{Signal}({}^j\mathcal{A}^S, {}^j\varphi) + {}^j\text{Bkg}}{\text{Signal}(0 \text{ rad}, {}^j\varphi) + {}^j\text{Bkg}}, \text{ and} \quad (3.6)$$

$${}^jP_{\text{PMT}}(\overline{\text{Hit}} | {}^j\mathcal{A}^S, {}^j\varphi) = 1 - {}^jP_{\text{PMT}}(\text{Hit} | {}^j\mathcal{A}^S, {}^j\varphi), \quad (3.7)$$

591 respectively. We expected the hit probability to be only weakly modulated within the small range  
 592 in  ${}^j\varphi$  of about 10 mrad covered by the beam divergence.<sup>[1]</sup> This modulation was modeled by a  
 593 quadratic dependence of the  ${}^j\mathcal{A}$ ,  ${}^j\Gamma$ , and  ${}^j\sigma$  parameters on  ${}^j\varphi$ :

$${}^j\mathcal{A}({}^j\varphi) = {}^j c_0^{\mathcal{A}} + {}^j c_2^{\mathcal{A}} \cdot ({}^j\varphi)^2 \quad (3.8)$$

$${}^j\Gamma({}^j\varphi) = {}^j c_0^{\Gamma} + {}^j c_2^{\Gamma} \cdot ({}^j\varphi)^2 \quad (3.9)$$

$${}^j\sigma({}^j\varphi) = {}^j c_0^{\sigma} + {}^j c_2^{\sigma} \cdot ({}^j\varphi)^2 \quad (3.10)$$

594 In total, the parameterization in equation (3.6) contains seven free parameters.

595 Assuming, that the hit probabilities for the eight PMTs are independent, the total probability to  
 596 see a certain hit pattern in CEDAR  $k$  for a given particle species and particle inclination is

$${}^kP_{\text{C}}(\text{Hit pattern} | S; {}^k\vartheta_x, {}^k\vartheta_y) = \prod_{j \in \text{CEDAR } k} {}^jP_{\text{PMT}}(\text{Hit pattern} | S; {}^k\vartheta_x, {}^k\vartheta_y), \quad (3.11)$$

[1] The beam divergence of about 200  $\mu\text{rad}$  translates to a range in  ${}^j\varphi$  of  $\pm 10$  mrad in the inclination space.



597 where

$${}^jP_{\text{PMT}}(\text{Hit pattern} | S; {}^k\vartheta_x, {}^k\vartheta_y) = \begin{cases} {}^jP_{\text{PMT}}(\text{Hit} | {}^j\Delta^S, {}^j\varphi) & \text{if PMT } j \text{ is hit} \\ {}^jP_{\text{PMT}}(\overline{\text{Hit}} | {}^j\Delta^S, {}^j\varphi) & \text{if PMT } j \text{ is not hit} \end{cases}. \quad (3.12)$$

598 Equation (3.11) is the likelihood function that the beam particle is of species  $S$  using the  
599 information from CEDAR  $k$

$${}^k\mathcal{L}_C(S; \text{Hit pattern}, {}^k\vartheta_x, {}^k\vartheta_y) = {}^kP_C(\text{Hit pattern} | S; {}^k\vartheta_x, {}^k\vartheta_y). \quad (3.13)$$

600 For the coordinate transformations  $({}^k\vartheta_x, {}^k\vartheta_y) \rightarrow ({}^j\Delta^S, {}^j\varphi)$ , the positions of PMTs in the inclination  
601 space has to be known, which gives two additional free parameters per PMT. We used the  
602 difference,  ${}^j\Delta\theta = {}^j\theta - \theta_{\text{Ch}}^K$ , of the PMT positions,  ${}^j\theta$ , to the expected position of the kaon  
603 Cherenkov ring at  $\theta_{\text{Ch}}^K$  as free parameter in the fit, which reduced the correlation among the  
604 fit parameters and therefore lead to a more robust fit. Also, the refraction index of the helium  
605 gas has to be known, which is one further parameter common for all PMTs of one CEDAR.  
606 Therefore, the employed likelihood parameterization for a single CEDAR detector has in total  
607  $8(7 + 2) + 1 = 73$  free parameters to be determined by from data. All of them are detector specific  
608 parameters, which are independent of the particle species.

609 Finally, the information of both CEDARs was combined in a single likelihood

$$\mathcal{L}(S; \text{Hit pattern}, \vartheta_x, \vartheta_y) = {}^1\mathcal{L}_C(S; \text{Hit pattern}, {}^1\vartheta_x, {}^1\vartheta_y) \cdot {}^2\mathcal{L}_C(S; \text{Hit pattern}, {}^2\vartheta_x, {}^2\vartheta_y). \quad (3.14)$$

610 Based on this likelihood, two particle hypotheses can be compared by calculating the log-  
611 likelihood difference of hypotheses  $S$  and  $S'$ :

$$\mathcal{D}_C(S, S') = \log_{10} \left[ \mathcal{L}(S; \text{Hit pattern}, \vartheta_x, \vartheta_y) \right] - \log_{10} \left[ \mathcal{L}(S'; \text{Hit pattern}, \vartheta_x, \vartheta_y) \right], \quad (3.15)$$

612 which is the same as the  $\log_{10}$  of the likelihood-ratio. We assumed a beam particle to be of species  
613  $S$  if  $\mathcal{D}_C(S, S')$  was above a chosen threshold  $\mathcal{T}_C(S)$  using the information of the CEDARs.<sup>[g]</sup>

#### 614 3.1.4 Likelihood Calibration

615 In the section above, we formulated in equation (3.13) a likelihood for each CEDAR detector.  
616 Therefore, we could calibrate the two detectors separately. In order to account for the time  
617 dependence of the CEDAR parameters, we performed the calibration independently in up to 2  
618 hour long periods in time, the so-called runs.<sup>[h]</sup>

<sup>[g]</sup> We used the  $\log_{10}$  as the likelihoods cover a wide dynamic range.

<sup>[h]</sup> In studies, we performed calibrations in time periods shorter than a run and compared the resulting likelihood parameters. From these studies we concluded, that a run-by-run calibration is sufficient to resolve the time evolution of the CEDAR parameters.

619 Before calibrating the likelihood parameters, we determined the tilt of the CEDAR detectors with  
 620 respect to the nominal beam axis in the laboratory frame and the time resolution of the PMTs,  
 621 which determines when a signal in a PMT is associated to the event and considered to be a hit.  
 622 The time resolution of the PMTs is about 0.13 ns and the tilt of the CEDARs is about 70  $\mu\text{rad}$ .  
 623 Details can be found in ref. [54].

624 All 73 free parameters of the likelihood function in equation (3.13) are detector specific param-  
 625 eters that are independent of the particle species hypothesis. Therefore, any sufficiently large data  
 626 sample with a mixture of particle species can be used to calibrate the likelihood. The precision of  
 627 the measured beam-particle inclination is higher for a larger number of final-state particles.<sup>[i]</sup> In  
 628 order to obtain a calibration sample that has a similar beam-inclination precision as the  $K^- \pi^- \pi^+$   
 629 sample analyzed in this work, but is much larger than the  $K^- \pi^- \pi^+$  sample, we used events with  
 630 three charged hadrons in the final state for calibration. The applied event selection is explained  
 631 in detail in appendix A.1.1. The number of calibration events per run is in the range of  $1 \times 10^4$  to  
 632  $7 \times 10^5$  events, which is sufficient to perform an independent calibration in each run. In total, the  
 633 calibration sample consists of  $1.5 \times 10^8$  events for the 2008 and  $1.3 \times 10^8$  events for the 2009  
 634 diffraction data set.

635 For calibrating the likelihood, we take into account only the pion and kaon hypothesis. Muons  
 636 and electrons in the beam have almost the same Cherenkov angle as pions,<sup>[j]</sup> and thus cannot be  
 637 separated from pions. Antiprotons in the beam have a Cherenkov angle much smaller than that  
 638 of kaons.<sup>[k]</sup> Therefore, the vast majority of antiprotons will not produce a hit in any of the PMTs,  
 639 similar to the majority of pions. This means, also antiprotons are indistinguishable from pions.  
 640 Given the much larger pion fraction in the beam; electrons, muons, and antiprotons do not bias  
 641 the result of the likelihood calibration.<sup>[l]</sup>

642 The admixture of beam pions and kaons in the calibration sample is taken into account in the  
 643 formulation of the probability for seeing a certain hit pattern in CEDAR detector  $k$ :

$$\begin{aligned} {}^k P_C(\text{Hit pattern} | {}^k \vartheta_x, {}^k \vartheta_y) &= {}^k P_C(\text{Hit pattern} | \pi; {}^k \vartheta_x, {}^k \vartheta_y) [1 - P(K)] \\ &+ {}^k P_C(\text{Hit pattern} | K; {}^k \vartheta_x, {}^k \vartheta_y) P(K). \end{aligned} \quad (3.16)$$

644 This approach adds only one additional free parameter, which is the probability  $P(K)$  to find a  
 645 kaon in the beam. The probabilities  ${}^k P_C(\text{Hit pattern} | \pi; {}^k \vartheta_x, {}^k \vartheta_y)$  and  ${}^k P_C(\text{Hit pattern} | K; {}^k \vartheta_x, {}^k \vartheta_y)$   
 646 share the same set of 73 likelihood parameters used to parameterize the CEDAR response. Their

<sup>[i]</sup> The precision of the measured position of the beam particle in the target is given by the precision of the interaction-vertex reconstruction. It is higher for a larger number of final-state particles, because more information entered the vertex reconstruction. As the beam-particle inclination at the CEDAR position is related to its position in the target region by the beam optics, the vertex reconstruction also determines the precision of the beam-particle inclination.

<sup>[j]</sup> Muons have almost the same mass as pions. The Cherenkov angle of electrons is only 10  $\mu\text{rad}$  larger than the one of pions for the helium pressure of the CEDARs.

<sup>[k]</sup> For the CEDAR parameters during the diffraction data taking, the Cherenkov angle of antiprotons is approximately 350  $\mu\text{rad}$  smaller than the Cherenkov angle of kaons, which is a large difference compared to the beam divergence of about 200  $\mu\text{rad}$ .

<sup>[l]</sup> In a study, we tried to include the antiproton hypothesis in the likelihood calibration. This led to very unstable and partly unrealistic results.

647 only difference is the different transformation  $({}^k\vartheta_x, {}^k\vartheta_y) \rightarrow ({}^j\Delta^S, {}^j\varphi)$ , which requires only the  
 648 known particle masses. Finally, the likelihood function that is maximized in an unbinned  
 649 maximum-likelihood fit to determine the 74 free parameters,  $\{p_C\}$ , reads

$$\mathcal{L}_{\text{Fit}}(\{p_C\}) = \prod_{\zeta=1}^{N_{\text{Events}}} {}^kP_C(\text{Hit pattern}^{(\zeta)} | {}^k\vartheta_x^{(\zeta)}, {}^k\vartheta_y^{(\zeta)}, \{p_C\}). \quad (3.17)$$

### 650 3.1.5 Agreement of the Likelihood Parameterization with the Calibration 651 Sample

652 To illustrate the results of the likelihood calibration, a single run<sup>[m]</sup> is used as an example. The hit  
 653 probability for PMT0 of CEDAR1, i.e. the ratio of events with a PMT hit to the total number of  
 654 events (data points in figure 3.4), is reproduced well by the result of the calibration fit (red dashed  
 655 curves). In the central  ${}^0\varphi$  region shown in figure 3.4a, the hit probability distribution exhibits a  
 656 clear peak at  ${}^0\Delta^K \approx -130 \mu\text{rad}$ , which is dominantly described by the pion contribution (orange  
 657 curve below the red curve). Furthermore, the data show a slight shoulder around  ${}^0\Delta^K = 0 \mu\text{rad}$ ,  
 658 which is described by the kaon contribution (green curve). As we chose to use the coordinate  
 659 transformation for the kaon hypothesis ( ${}^0\Delta^K$ ) to show the data, it is expected that the kaon peak  
 660 is at  ${}^0\Delta^K = 0 \mu\text{rad}$  and that the distance between the kaon and the pion peak corresponds to the  
 661 difference between their Cherenkov angle, which is about  $130 \mu\text{rad}$ . Also, the  ${}^0\varphi$  dependence of  
 662 the hit probability is described well by the calibrated likelihood, as shown by the hit probability  
 663 distribution in the outer  ${}^0\varphi$  region in figures 3.4a and 3.4b. Due to the limited beam spread,  
 664 only half of the pion peak can be accessed in the outer  ${}^0\varphi$  region. Overall, the agreement of the  
 665 calibrated likelihood function with the calibration sample is similarly good for all PMTs and  
 666 runs of the diffraction data taking. Therefore, we can conclude, that the employed likelihood  
 667 parameterization of equation (3.13) is able to describe the CEDAR response and that we are able  
 668 to reliably determine its parameters from data.

### 669 Time Evolution of the Likelihood Parameters

670 In the following, the time dependence of the CEDAR likelihood parameters is discussed based  
 671 on selected examples of the parameters of PMT0 in CEDAR1 during the 2008 diffraction data  
 672 taking. The time evolution of the refraction index parameter is stable within small fluctuations  
 673 on the  $10^{-5}$  level, except for the last few days of the data taking (see black line with blue band  
 674 in figure 3.5). However, it is not proportional to the measured density of the helium gas (red  
 675 dots) as it would be expected. Despite, the positions  ${}^j\theta$  of the PMTs in the inclination space,  
 676 which are also free parameters, exhibit a clear correlation with the helium density, as shown  
 677 exemplarily for PMT0 in CEDAR1 by the black line with blue band in figure 3.6. The reason  
 678 is an approximate ambiguity in the likelihood function between the refraction-index parameter

<sup>[m]</sup> We use the data from run number 70450.

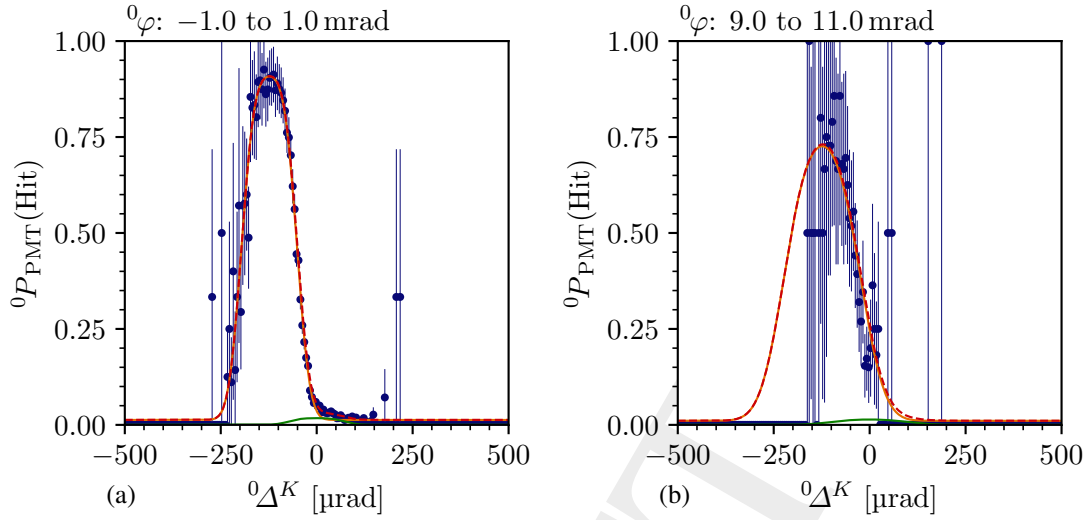


Figure 3.4: Hit probability distribution for PMT0 of CEDAR1 as a function of the distance  ${}^0\Delta^K$  to the nominal kaon ring for (a) the central and (b) an outer  ${}^j\varphi$  region. The points represent the data. The red dashed curve is the result of the maximum-likelihood fit. The orange curve represents the pion and the green curve the kaon contribution according to equation (3.6).<sup>[m]</sup>

679 and the PMT-position parameters.<sup>[n]</sup> As the refraction-index parameter cannot be determined  
 680 precisely in the likelihood calibration, we obtained a roughly constant refraction-index parameter.  
 681 The true variation of the refraction index of the helium gas is effectively accounted for by the  
 682 PMT-position parameters.<sup>[o]</sup>

683 The time evolution of the width parameter  ${}^j c_0^r$  of the rectangular function of the hit-probability  
 684 parameterization in equation (3.6) exhibits two clear steps as shown in figure 3.7. These steps  
 685 coincide with the narrowing and widening of the diaphragm aperture during data taking. The  
 686 determined value of  ${}^j c_0^r$  is approximately directly proportional to the measured aperture, as  
 687 expected. Except for these steps, the parameter is stable. The width  ${}^j c_0^\sigma$  of the Gaussian smearing  
 688 of the rectangular function is also stable with time (not shown) and is not affected by the changes  
 689 of the diaphragm aperture.

<sup>[n]</sup> The reason for this ambiguity is, that the position of the peaks in the hit probability distribution in  ${}^j\Delta^S$  (see figure 3.4) is given by two parameters [see equation (3.3)]. First, the peak positions depend on the predicted Cherenkov angle,  $\theta_{\text{Ch}}^S$ , and thereby on the refraction-index parameter. Second, the peak positions can be shifted by adjusting the PMT-position parameters  ${}^j\theta$ . The PMT-position parameters cannot be determined from other constraints. The refraction-index parameter could in principle be determined from two other constraints. Either from the radius of the Cherenkov ring, i.e. the green dashed line in figure 3.3b. However, the beam illuminates only a very small segment of this circle, which is insufficient to determine the refraction index. Or by the difference between the pion and the kaon Cherenkov angle, given by the difference of the peak positions. However, this difference is less sensitive on the refraction index than the absolute Cherenkov angle. Therefore, it is also insufficient to determine the refraction index.

<sup>[o]</sup> The refraction index could not be calculated from the measured helium density, because it was not measured for the full diffraction data taking.

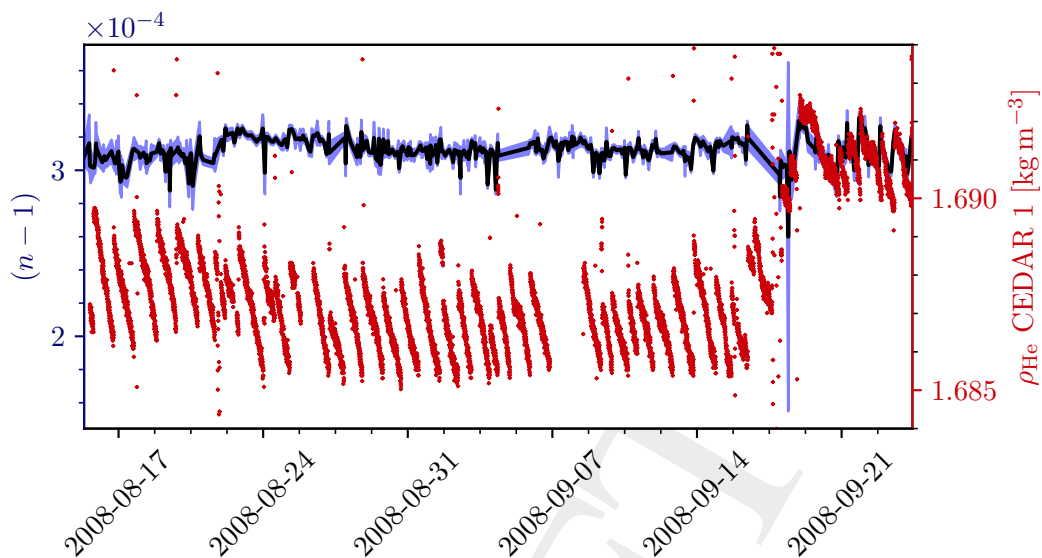


Figure 3.5: Time evolution of the refraction index  $n$  of the He gas in CEDAR1. The black line represents the central values and the blue band the statistical uncertainties of the refraction index as determined by the likelihood calibration fit. The red dots represent the density  $\rho_{\text{He}}$  in CEDAR1 as measured during the data taking. The CEDAR1 density was not measured continuously.

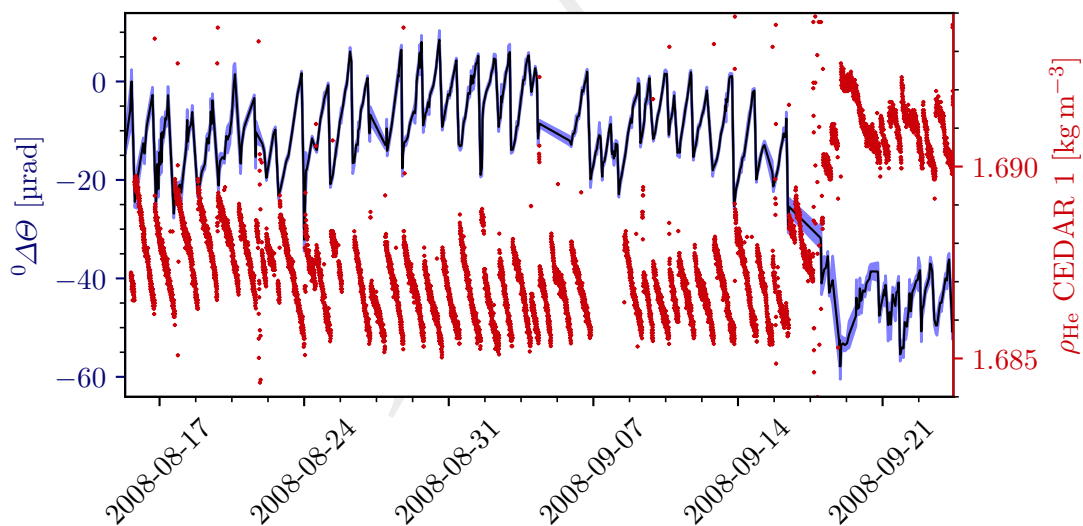


Figure 3.6: Time evolution of the  $^j\theta$ -position of PMT0 in CEDAR1. The black line represents the central value and the blue band the statistical uncertainty of the difference between the PMT  $^j\theta$ -position with respect to the kaon Cherenkov ring as determined by the likelihood calibration fit. The red dots represent the density in CEDAR1 as recorded during the data taking. The CEDAR1 density was not measured continuously.

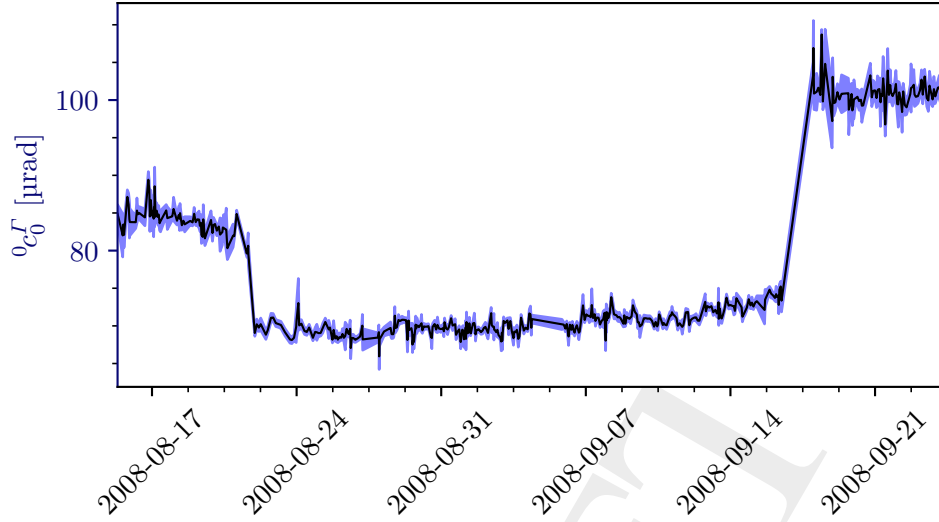


Figure 3.7: Time evolution of the width parameter  ${}^0c_0^\sigma$  of PMT0 in CEDAR1. The black line represents the central values and the blue band the statistical uncertainties of the width parameter as determined by the likelihood calibration fit.

690 Overall, we were able to determine all likelihood parameters reliably. Some parameters such  
 691 as  ${}^j c_0^F$  follow the physical quantities they represent. Other parameters such as the refraction  
 692 index and the PMT positions act as an effective parameterization of the corresponding physical  
 693 quantities. This shows, that the likelihood parameterization is able to reproduce the physical  
 694 properties of the CEDARs.

### 695 3.1.6 Estimation of Particle Identification Performance

696 As was shown in section 3.1.5, the likelihood parameterization in equation (3.17) is able to repro-  
 697 duce the calibration sample and the obtained parameters correlate with the physical quantities of  
 698 the CEDAR detectors, as expected. However, we still have to verify, that the likelihood-based  
 699 beam-particle identification is able to separate kaons from pions. The efficiency of the particle  
 700 identification, i.e. the fraction beam particles of species  $S$  that are identified as  $S$ , and its impurity,  
 701 i.e. the fraction of beam particles of another species contained in a data set where the beam  
 702 particle species was identified as  $S$ , has to be determined. This requires pure pion-beam and  
 703 kaon-beam validation samples. In contrast to the calibration sample, the size of the validation  
 704 samples may be significantly smaller. However, it must still be sufficiently large in order to be  
 705 able to study the CEDAR performance for the 2008 and 2009 diffraction data set separately.

706 To obtain a clean pion-beam sample, we selected events of the reaction  $\pi^- + p \rightarrow \pi^- \pi^0 \pi^0 + p$ ,  
 707 where we identified all final-state particles. Thereby, we ensure that the beam particle is a pion

without using the CEDAR information.<sup>[p]</sup> The pion-beam sample consist of about  $10^6$  events each for the 2008 and 2009 diffraction data set. In order to obtain a pure kaon-beam sample, we selected decays of beam kaons into different final states:  $K^- \rightarrow \mu^- \bar{\nu}_\mu$ ,  $K^- \rightarrow \pi^- \pi^- \pi^+$ , and  $K^- \rightarrow \pi^- \pi^0$ ; with about  $80 \times 10^3$ ,  $15 \times 10^3$ , and  $7 \times 10^3$  events; respectively; each for the 2008 and 2009 diffraction data set. The  $K^- \rightarrow \pi^- \pi^- \pi^+$  and  $K^- \rightarrow \pi^- \pi^0$  samples show non-negligible background, which is accounted for by performing a statistical background subtraction. The event selections for the calibration samples are explained in detail in appendix A.1.2.

### Likelihood Distributions and Particle Identification Cuts

We verified the calibrated likelihood in equation (3.13) by identifying beam particles in the pion- and kaon-beam<sup>[q]</sup> samples selected from the 2008 diffraction data set using the information of only CEDAR1. The distribution of the log-likelihood difference is shown in figure 3.8a as a function of the beam-particle inclination,<sup>[r]</sup>

$${}^1\vartheta = \sqrt{({}^1\vartheta_x)^2 + ({}^1\vartheta_y)^2}, \quad (3.18)$$

for the pion-beam sample. As expected, the distribution concentrates mainly in the region where the log-likelihood difference is below 1, i.e. where the pion hypothesis is the more likely one. Likewise, the log-likelihood difference distribution for the kaon-beam sample (see figure 3.8b) is concentrated in the region where the log-likelihood difference is above 1, i.e. where the kaon hypothesis is the more likely one. With increasing beam-particle inclination, both distributions approach the central region where pion and kaon hypothesis become similar and therefore harder to distinguish (dashed line).

Both distributions in figures 3.8a and 3.8b show clear bands. To understand their origin, we study the log-likelihood difference distribution of events with a certain number of hits in the PMTs of CEDAR1. Requiring hits in all eight PMTs projects out the topmost band of the log-likelihood difference distribution in the kaon-beam sample (see figure 3.8d), while the pion-beam sample contains practically no events with eight PMT hits (see figure 3.8c). Here, the discrimination between kaons and pions works best, which is exploited in the majority method (see section 3.1.2). However, figure 3.8d also shows, that the inclination for beam particles with eight PMT hits is limited to be below about  $100 \mu\text{rad}$ . For larger inclinations, the kaon Cherenkov ring moves out of the PMTs' acceptance defined by the diaphragm aperture. The validation data show similar limitations of the  ${}^1\vartheta$  range for events with seven or six PMT hits. Therefore, the majority method is able to distinguish beam pions from kaons only in a limited inclination range, which explains its low efficiency. Beam pions and kaons with hits in only four

<sup>[p]</sup> By ensuring that the final state consists only of pions, we ensured that the beam particle was also a pion and not a kaon or antiproton, because of strangeness and baryon number conservation in diffractive scattering reactions.

<sup>[q]</sup> Here, we use only the  $K^- \rightarrow \mu^- \bar{\nu}_\mu$  sample. It is the only one that is nearly background free and sufficiently large.

<sup>[r]</sup> The beam-particle inclination with respect to the optical axis of CEDAR  $k$ ,  ${}^k\vartheta$ , is different from the beam inclination in the laboratory frame due to the finite tilt of the CEDAR detectors of about  $70 \mu\text{rad}$ , which is similar for both CEDAR detectors. We chose to use  ${}^1\vartheta$  to show the data.

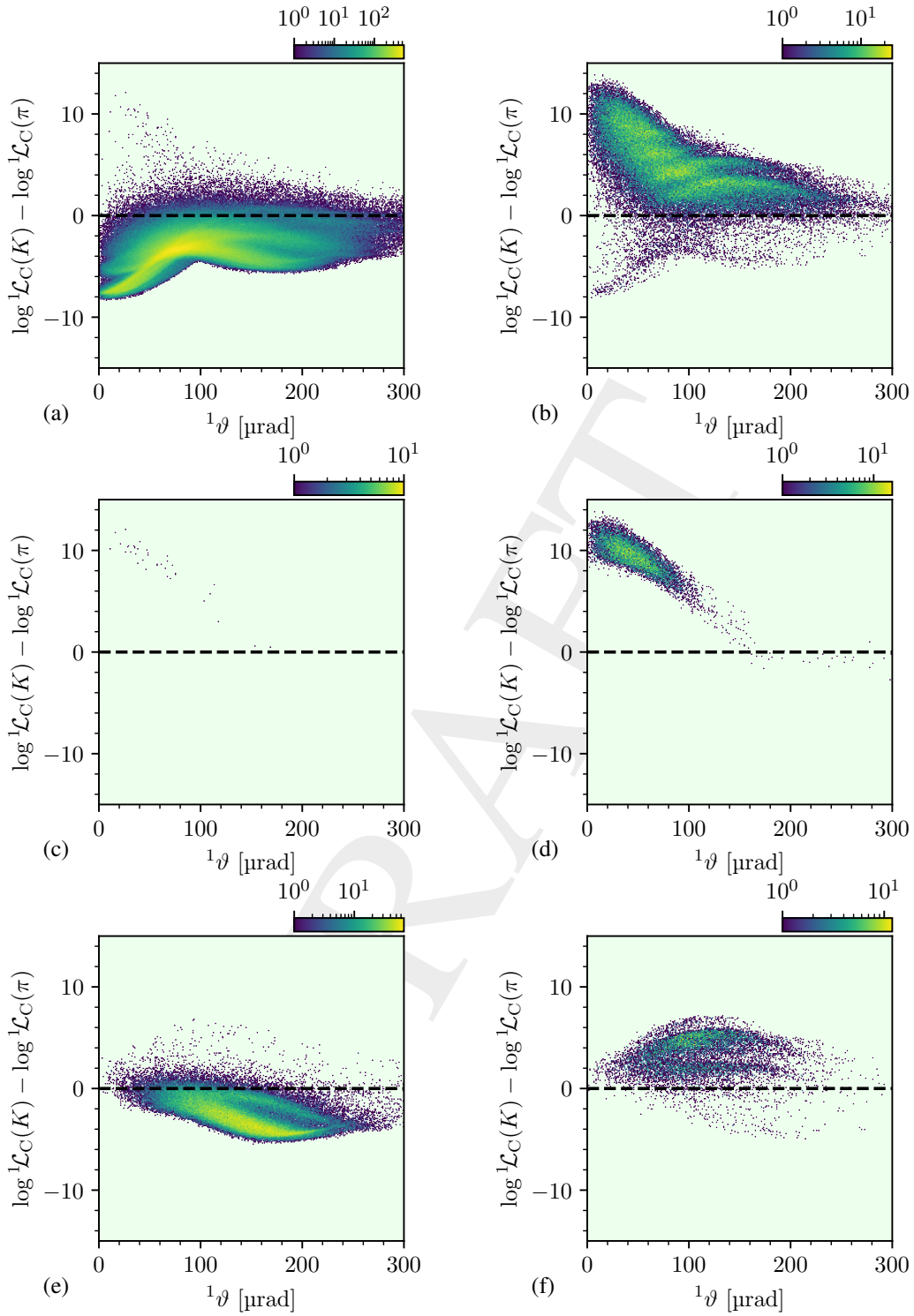


Figure 3.8: Difference of the kaon and pion log-likelihood for CEDAR1 as a function of the beam inclination angle  ${}^1\vartheta$  defined in equation (3.18). The left column shows the pion-beam sample, the right column shows the kaon-beam sample. The first row shows all events, the second row shows events with hits in all eight PMTs, and the last row shows events with hits in four PMTs. Histogram cells with zero events are shown in light green.



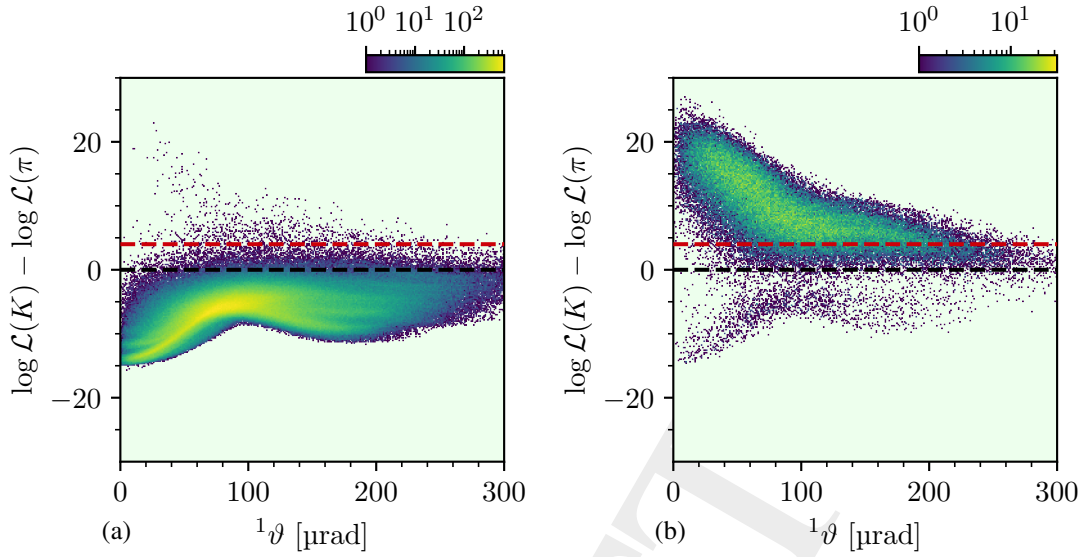


Figure 3.9: Difference of the kaon and pion log-likelihood for both CEDARs as defined in equation (3.15). We chose the beam inclination angle,  ${}^1\vartheta$ , with respect to the optical axis of CEDAR1 as coordinate system. The left column shows the pion-beam sample, the right column shows the kaon-beam sample. The dashed red line represents the threshold,  $\mathcal{T}_C(K) = 4.0$ , in log-likelihood difference for kaon identification. Histogram cells with zero events are shown in light green.

739 PMTs cannot be discriminated using the majority method. However, the log-likelihood difference  
 740 discrimination clearly favors the pion hypothesis for the pion-beam sample (see figure 3.8e) and  
 741 the kaon hypotheses for the kaon-beam sample (see figure 3.8f). This improved discrimination  
 742 power of the likelihood-based method compared to the multiplicity method arises from taking  
 743 into account the difference in the hit patterns for pions and kaons, even for a small number of  
 744 PMT hits. Hence, the likelihood-based method allows separating beam kaons from pions also for  
 745 larger inclinations beyond 100  $\mu\text{rad}$ .

746 For the final decision about the beam-particle species, the likelihood of both CEDARs was com-  
 747 bined into a single likelihood for a given particle-species hypothesis according to equation (3.14).  
 748 The distribution of the combined log-likelihood difference again exhibits bands as shown in  
 749 figure 3.9. Due to the combination of the information from both CEDARs, the bands are smeared  
 750 out compared to the log-likelihood difference distribution of a single CEDAR discussed above.  
 751 Comparing the log-likelihood difference distribution for the kaon- and pion-beam samples, a  
 752 clear separation between kaons and pions in the likelihood space is observed. To identify a beam  
 753 particle as a kaon, we required the log-likelihood difference in equation (3.15) to be above a  
 754 certain threshold  $\mathcal{T}_C(K)$  (red dashed lines in figure 3.9). To identify a beam particle as a pion,  
 755 we required the log-likelihood difference to be below another threshold  $\mathcal{T}_C(\pi)$ .

756 **Efficiency and Purity**

757 Efficiency and impurity of this method depend on the choice of the thresholds  $\mathcal{T}_C(\pi)$  and  $\mathcal{T}_C(K)$   
 758 in log-likelihood difference. For an optimum choice of these thresholds we determined estimates  
 759 for efficiency and impurity as a function of the threshold. Therefore, we compared the number of  
 760 pions or kaons before and after applying the CEDAR likelihood method to the pion or kaon beam  
 761 validation samples, respectively. Details can be found in appendix A.1.3. As determining a single  
 762 number for the efficiency or impurity implies averaging over the beam-particle inclinations, the  
 763 distribution of the beam particles in the validation samples should be similar to the one in the  
 764  $K^- \pi^- \pi^+$  sample analyzed in this work. This holds approximately for the pion-beam sample. The  
 765 inclination distributions of the three kaon-beam samples however differ slightly from the ones  
 766 in the  $K^- \pi^- \pi^+$  sample (see figure A.1). To estimate the corresponding systematic effect, we  
 767 determined efficiency and impurity from all three samples.  $\mathcal{T}_C(K)$  and  $\mathcal{T}_C(\pi)$  were optimized  
 768 using the kaon-beam sample from  $K^- \rightarrow \pi^- \pi^- \pi^+$  decays of the 2008 diffraction data set.

769 For the beam kaon identification, the dependence of efficiency and impurity on  $\mathcal{T}_C(K)$  is shown  
 770 in figure 3.10a. To achieve a small impurity, but still maintain a high efficiency, we have chosen  
 771 a threshold for the kaon identification of  $\mathcal{T}_C(K) = 4.0$ . Table 3.1 summarizes the results for all  
 772 three kaon-beam samples and for the 2008 and 2009 diffraction data. The various kaon-beam  
 773 samples give slightly different results, which provides a measure the systematic uncertainty on  
 774 the measured efficiency and impurity. Overall, we obtained a kaon-identification efficiency of  
 775 about 85 % at an impurity of about 3 %. The impurity of the identified-kaon sample due to the  
 776 antiprotons in the beam is expected to be negligible.<sup>[s]</sup>

777 For the beam pion identification, which is important in other analyses[43, 61, 62], the dependence  
 778 of efficiency and impurity on  $\mathcal{T}_C(\pi)$  is shown in figure 3.10b. As the impurity is already very  
 779 small for all considered thresholds, we chose a pion identification threshold of  $\mathcal{T}_C(\pi) = 0$   
 780 to achieve a high efficiency of about 98 % with a low impurity of about 0.05 % as listed in  
 781 table 3.2.<sup>[t]</sup> The impurity of the identified-pion due to the antiproton fraction in the beam cannot  
 782 be larger than the overall antiproton fraction in the beam of about 1 % [63].

783 In summary, the likelihood-based method developed in this work identifies the species of beam  
 784 particles with high efficiency, while maintaining a low impurity from other species. The method  
 785 provides a similar performance as the likelihood method developed in ref. [58] for the COMPASS  
 786 Primakoff data set.<sup>[u]</sup> Using the fact, that the CEDAR response on Cherenkov photons emitted  
 787 under a certain angle with respect to the CEDAR's optical axis is independent of the particle

<sup>[s]</sup> With the approach used here, we cannot make quantitative statements on the impurity of an identified-kaon sample due to the antiprotons in the beam. However, as the antiprotons should mainly be tagged as pions (see section 3.1.4), we expect a similar suppression for antiprotons and pions of about  $10^{-3}$ . Since the antiproton fraction in the beam is small, the antiproton impurity of a kaon-identified sample is a negligible effect.

<sup>[t]</sup> We suspect, that the reason for the large impurity value from  $K^- \rightarrow \pi^- \pi^0$  kaon-beam sample is that it is not clean enough to obtain a reasonable value for the misidentification probability  $P(K \rightarrow \pi)$  from it. The two other validation samples give consistent results for the impurity value.

<sup>[u]</sup> To directly compare the results of both methods, we applied our method and the method from ref. [58] to a small fraction of the Primakoff data. Both methods yielded similar results.

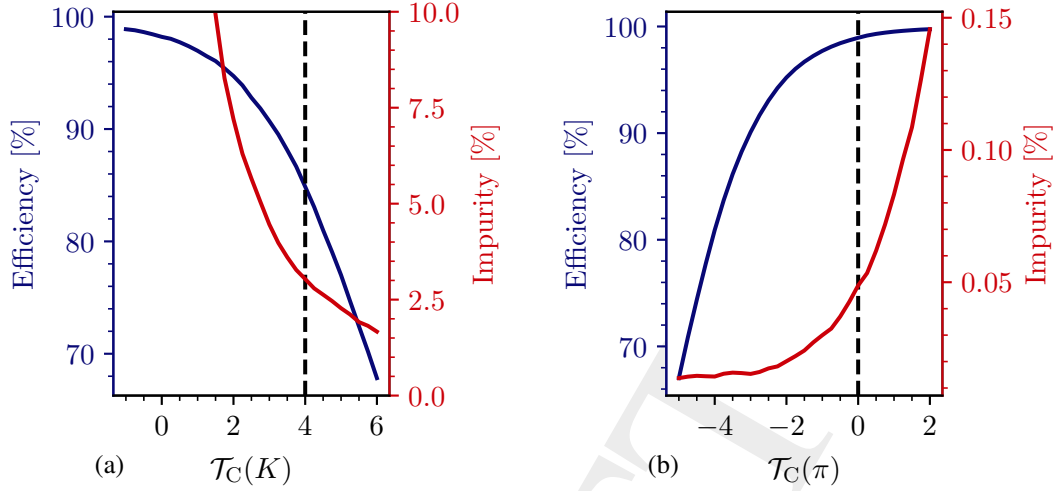


Figure 3.10: Efficiency (blue) and impurity (red) for (a) kaon and (b) pion particle identification as a function of the thresholds  $\mathcal{T}_C(K)$  and  $\mathcal{T}_C(\pi)$ , respectively, applied to the log-likelihood difference. The black dashed lines shows the chosen threshold values. The pion-beam sample is used to determine the efficiency of the pion identification and the impurity an identified-kaon sample. The  $K^- \rightarrow \pi^- \pi^- \pi^+$  sample is used to determine the efficiency of the kaon identification and the impurity of an identified-pion sample.

Table 3.1: Efficiency and impurity of the beam-kaon identification. The efficiency was obtained either from the  $K^- \rightarrow \pi^- \pi^- \pi^+$ , the  $K^- \rightarrow \pi^- \pi^0$ , or from the  $K^- \rightarrow \mu^- \bar{\nu}_\mu$  sample. The misidentification probability was obtained from the pion-beam sample. The table lists the central values and statistical uncertainties.

		$K^- \rightarrow \pi^- \pi^- \pi^+$	$K^- \rightarrow \pi^- \pi^0$	$K^- \rightarrow \mu^- \bar{\nu}_\mu$
Efficiency ( $K \rightarrow K$ )	2008 [%]	$84.9 \pm 1.0$	$88.9 \pm 2.0$	$89.2 \pm 0.5$
	2009 [%]	$83.2 \pm 1.0$	$84.4 \pm 2.0$	$86.3 \pm 0.6$
Impurity ( $\pi \rightarrow K$ )	2008 [%]	$3.04 \pm 0.13$	$2.90 \pm 0.14$	$2.89 \pm 0.12$
	2009 [%]	$2.89 \pm 0.13$	$2.85 \pm 0.14$	$2.79 \pm 0.12$

Table 3.2: Efficiency and impurity of the beam-pion identification. The efficiency was obtained from the pion-beam sample. The misidentification probability was obtained either from the  $K^- \rightarrow \pi^- \pi^- \pi^+$ , the  $K^- \rightarrow \pi^- \pi^0$ , or from the  $K^- \rightarrow \mu^- \bar{\nu}_\mu$  sample. The table lists the central values and statistical uncertainties. The value of the efficiency is independent of the used kaon-beam sample and therefore given only once.

		$K^- \rightarrow \pi^- \pi^- \pi^+$	$K^- \rightarrow \pi^- \pi^0$	$K^- \rightarrow \mu^- \bar{\nu}_\mu$
Efficiency ( $\pi \rightarrow \pi$ )	2008 [%]	$98.94 \pm 0.13$		
	2009 [%]	$97.56 \pm 0.13$		
Impurity ( $K \rightarrow \pi$ )	2008 [%]	$0.049 \pm 0.003$	$0.18 \pm 0.05$	$0.038 \pm 0.003$
	2009 [%]	$0.050 \pm 0.003$	$0.14 \pm 0.05$	$0.044 \pm 0.003$

788 species, the calibration of the likelihood method developed here does not require pure kaon-beam  
789 and pion-beam samples. This is a major advantage over the methods developed in refs. [58,  
790 59] and allowed us to perform a time-dependent calibration. Compared to the majority method  
791 used in previous analyses [44, 57], our method achieves a two times larger kaon-identification  
792 efficiency, mainly by being able to identify beam kaons also at larger inclinations.

## 793 3.2 Final-State Particle Identification

794 Final-state particles of various species are produced in the interaction of the high-energy hadron  
795 beam with the liquid-hydrogen target. In the analysis presented here, we are interested only  
796 in charged final-state particles. The charged final-state particles that are measured with the  
797 COMPASS spectrometer are electrons, muons, pions, kaons, or protons. These particle species  
798 are distinguished by employing the information from Cherenkov photons measured in the ring-  
799 imaging Cherenkov detector (RICH).

### 800 3.2.1 Particle Identification using the RICH Detector

801 High-energy final-state particles produce Cherenkov photons while traversing the 3 m long RICH  
802 vessel, which is filled with  $C_4F_{10}$  as a radiator gas [49]. The Cherenkov photons are focused by a  
803 system of mirrors onto two arrays of position-sensitive photon detectors, <sup>[v]</sup> where they form  
804 rings. Measuring the radius of these rings allows to determine the Cherenkov angle defined in  
805 equation (3.1) under which the Cherenkov photons were emitted.

806 The Cherenkov angle is directly related to the particle species by its mass, its measured momen-  
807 tum, and the known refraction index of the gas in the RICH volume. In contrast to beam particles,  
808 which have approximately the same momentum, final-state particles have a broad momentum  
809 distribution leading to a broad distribution of their Cherenkov angles. Therefore, the value of the  
810 Cherenkov angle is measured for each final-state particle and is compared to predictions for the  
811 various particle-species hypotheses to identify the particle.

812 Figure 3.11 shows the distribution of the measured Cherenkov angles as a function of the  
813 particle momentum. This distribution exhibits clear bands from pions, kaons, and protons for  
814 momenta above about 2.5, 9, and 17 GeV/c, respectively. These lower limits are determined by  
815 the corresponding Cherenkov threshold, <sup>[w]</sup> which is given by the particle mass. Above about  
816 50 GeV/c, the Cherenkov angles of kaons and pions become similar, which limits the kaon-pion  
817 separation to lower momenta. Similarly, proton identification is limited to momenta below about

---

<sup>[v]</sup> In the peripheral regions, multiwire proportional chambers with solid-state CsI photocathodes are used. In the central region with higher background, multi-anode photomultiplier tubes are used.

<sup>[w]</sup> In order to reconstruct the Cherenkov ring and determine the Cherenkov angle, a minimum of four measured Cherenkov photons is required. This translates so a minimal Cherenkov angle of about 20 mrad.

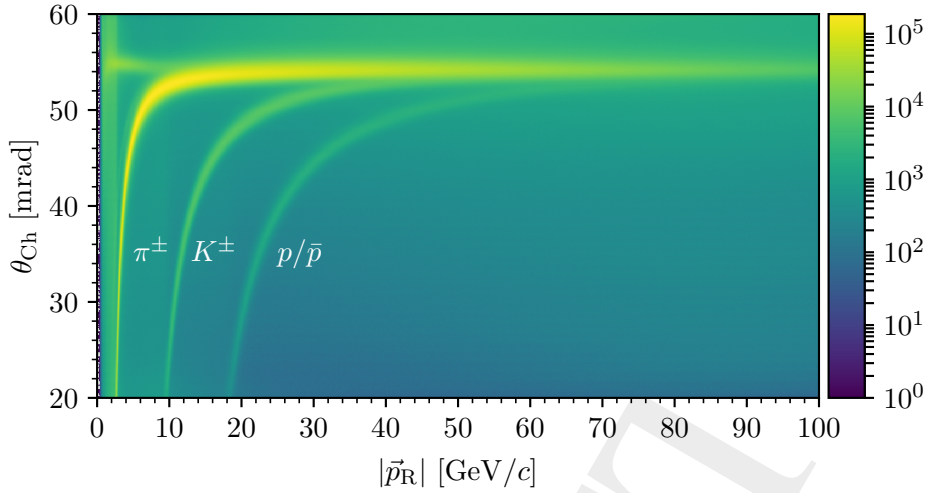


Figure 3.11: Distribution of the measured Cherenkov angles as a function of the final-state particle momentum,  $|\vec{p}_R|$ , at the RICH position. We show the data sample with three charged particles per event obtained by applying the preselection criteria (see section 4.1) to the 2008 diffraction data set.

818 80 GeV/c, because for higher momenta the Cherenkov angle of protons becomes similar to  
 819 the angles of kaons and pions. Muons cannot be separated well from pions for most of the  
 820 momentum range, due to their similar mass. Electrons have  $\beta \approx 1$  for most of the momentum  
 821 range and therefore end up in the upper horizontal band at about 55 mrad. As we study hadronic  
 822 reactions in this work, there is only a small contribution of electrons and muons in the final state  
 823 from background reactions. Therefore, they play only a minor role in the final-state particle  
 824 identification.

825 The likelihood for a given final-state particle hypothesis  $S$  is formulated in terms of the probability  
 826 of the measured hit pattern of individual Cherenkov photons in the RICH detector. Details can  
 827 be found in appendix A.2.1 and in ref. [64]. Using this approach, we obtained for each final-state  
 828 particle a likelihood  $\mathcal{L}(S)$  for each particle-species hypothesis  $S$ . In order to compare several  
 829 hypotheses we calculated the likelihood ratio

$$\mathcal{R}_R(S) = \frac{\mathcal{L}(S)}{\max_{S' \neq S} \mathcal{L}(S')}, \quad (3.19)$$

830 where  $\max_{S' \neq S} \mathcal{L}(S')$  is the largest likelihood of all other particle hypothesis  $S'$  different from  $S$ . In  
 831 order to assign a particle hypothesis  $S$  to a final-state particle, we required the likelihood ratio for  
 832  $S$  to be above a certain threshold,<sup>[x]</sup> i.e.  $\mathcal{R}_R(S) > \mathcal{T}_R$ , where  $\mathcal{T}_R$  is the so-called RICH threshold.  
 833 Thereby, we implicitly required, that we can distinguish hypothesis  $S$  from all other hypotheses  
 834 that were taken into account in order to assign  $S$  to a final-state particle. We took into account

[x] We used the same threshold for all particle-species hypotheses, which was optimized for a high efficiency and a low misidentification probability.

835 the hypotheses pion, kaon, proton, and background.<sup>[y]</sup> The background hypothesis represents  
 836 Cherenkov photons that are uncorrelated to the final-state particle. If the background hypothesis  
 837 was assigned to a particle, we treated this as if no hypothesis could have been assigned to it.

838 A steel pipe of 5 cm radius around the nominal beam axis separates non-interacting beam particles  
 839 from the RICH gas vessel, in order to avoid background. However, also final-state particles  
 840 can traverse the RICH detector within this steel pipe volume. Such particles do not produce  
 841 Cherenkov light within the RICH gas volume. Therefore, we did not assign a particle hypothesis  
 842 to final-state particles that traverse the RICH within this steel pipe, i.e. if the distance of the  
 843 particle position from the nominal beam axis at the RICH entrance window is smaller than  
 844 5 cm.

#### 845 3.2.2 Final-State Particle Identification Performance

846 In order to estimate the performance of the RICH particle identification; i.e. the efficiency to  
 847 identify a particle,  $P(S \rightarrow S)$ , and the misidentification probability,  $P(S \rightarrow S')$ , to assign the  
 848 wrong particle hypothesis  $S'$ , validation samples of final-state particles are required. These  
 849 samples need to contain particles that were identified without using the RICH information. Such  
 850 samples were obtained by selecting decays of known particles into daughter particles of a specific  
 851 species. Following ref. [64], we used the decay  $K_S^0 \rightarrow \pi^- \pi^+$  as a source of pions, the decay  
 852  $\phi(1020) \rightarrow K^- K^+$  as a source of kaons, and the decay  $\bar{\Lambda} \rightarrow \pi^\pm \bar{p}$  as a source of (anti)protons.<sup>[z]</sup>  
 853 Details can be found in appendix A.2.2.

854 The efficiency and misidentification probability can depend on the particles charge on its kine-  
 855 matics at the position of the RICH detector, especially on its momentum  $|\vec{p}_R|$  and on the angle  
 856  $\theta_R$  of its trajectory with respect to the beam axis.<sup>[aa]</sup> We took this into account by determining  
 857 the efficiency and misidentification probability independently in cells of  $(|\vec{p}_R|, \sqrt{\theta_R})$ <sup>[ab]</sup> and  
 858 separately for positive and negative particles.

859 Negative pions are identified efficiently for momenta above about 3 GeV/c (see figure 3.12a).  
 860 Most of the pions below this limit are attributed to the background hypothesis or are unidentified.  
 861 The maximum momentum for which pions can be identified efficiently is about 40 GeV/c. Above  
 862 this limit, most of the pions are not identified, because they cannot be separated from kaons. The  
 863 pion identification efficiency shows only a weak dependence on the angle of the particle track. In  
 864 the center of the distribution, it is about 95 %.

<sup>[y]</sup> We did not consider the muon and electron particle hypotheses, because they cannot be distinguished from pions for momenta above about 10 GeV/c.

<sup>[z]</sup> Instead of  $\bar{\Lambda}$  decays, we used  $K_S^0$  decays as a pion source, because they cover a broader kinematic range. This is important, because this data sample is also used to model the RICH acceptance (see appendix C.2.3).

<sup>[aa]</sup> The particle kinematics  $(|\vec{p}_R|, \theta_R)$  at the position of the RICH detector are in general different from its kinematics at the interaction vertex in the target region. We used the kinematics at the RICH entrance window for the characterization of the RICH performance.

<sup>[ab]</sup> We use  $\sqrt{\theta_R}$  instead of  $\theta_R$ , because the former better maps out the region in which the efficiency changes (see figure 3.12b).

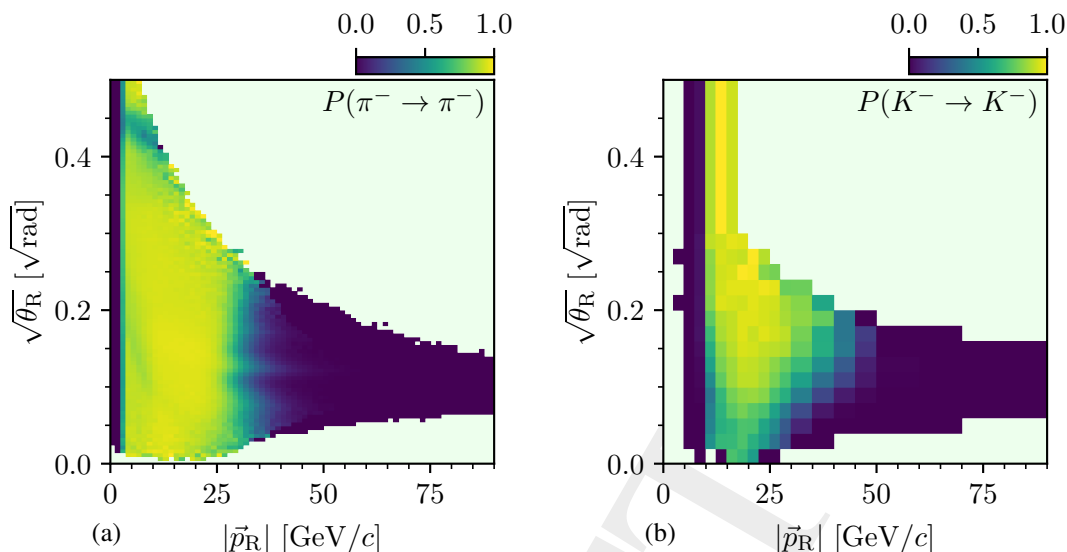


Figure 3.12: RICH efficiency for the identification of (a) negative pions and (b) negative kaons in cells of the particle momentum  $|\vec{p}_R|$  and the square-root of the track angle  $\theta_R$  at the position of the RICH detector. The plots show the 2008 diffraction data set for a likelihood-ratio threshold value of  $\mathcal{T}_R = 1.15$ . Regions without calibration data are drawn in light green.

865 Due to the larger kaon mass, the minimum momentum necessary to identify a negative kaon of  
 866 about 10 GeV/c is larger than for the identification of pions (see figure 3.12b). The maximum  
 867 momentum for which kaons can be identified efficiently, depends on the angle of the particle  
 868 track. For small angles, we can identify kaons only up to about 30 GeV/c, while for larger  
 869 angles, kaon identification is possible up to about 50 GeV/c.<sup>[ac]</sup> In the central kinematic region  
 870 we achieve a high efficiency of about 90 %.

871 Figure 3.13 shows that the efficiencies and misidentification probabilities for the RICH final-state  
 872 particle identification depend strongly on the choice of the likelihood-ratio threshold  $\mathcal{T}_R$ . The  
 873 maximum efficiency for pion identification does not strongly depend on the choice of  $\mathcal{T}_R$  (see  
 874 figure 3.13a). The lower momentum limit is not sensitive to  $\mathcal{T}_R$ , because it is given by the  
 875 Cherenkov threshold. As expected, the drop in efficiency for high momenta strongly depends on  
 876  $\mathcal{T}_R$ . While for  $\mathcal{T}_R = 1.00$ , the efficiency to identify a pion is above 20 % also for momenta above  
 877 50 GeV/c, it drops quickly in the region around 30 GeV/c when applying larger likelihood-ratio  
 878 thresholds. However, for  $\mathcal{T}_R = 1.00$ , the misidentification probability increases drastically  
 879 above 30 GeV/c (see figure 3.13b), while for  $\mathcal{T}_R = 1.15$ , it stays below 2 %. A likelihood-ratio  
 880 threshold of  $\mathcal{T}_R = 1.00$  means that we always assign the hypothesis with the largest likelihood.  
 881 At high momenta, kaons cannot be separated from pions. Therefore, their likelihoods become  
 882 similar and, for  $\mathcal{T}_R = 1.00$ , we almost randomly assign the pion or kaon hypothesis. This explains  
 883 the comparably high misidentification probability and also the high efficiency above 20 %. For a

<sup>[ac]</sup> The maximum momentum up to which the particle species can be identified is higher for kaons than for pions. The reason for this is, that the Cherenkov angle of identified pions has an upper limit for  $\beta \rightarrow 1$  and a lower limit given by the kaon hypothesis, while the Cherenkov angle of identified kaons has only an upper limit given by the pion hypotheses (see figure 3.11).

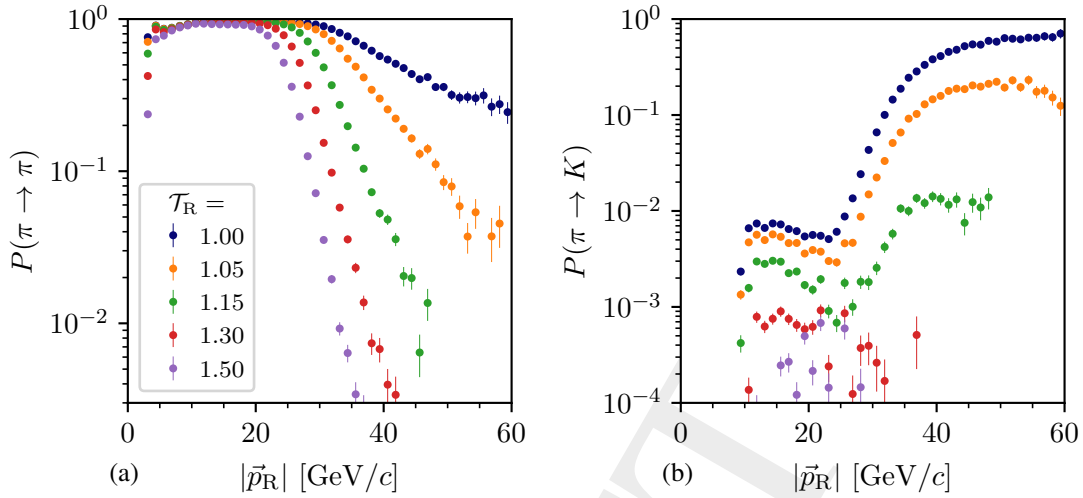


Figure 3.13: (a) RICH efficiency to identify a negative pion and (b) probability to misidentify a negative pion as a kaon as a function of the particle momentum at a track angle of about  $\sqrt{\theta_R} = 0.15 \sqrt{\text{rad}}$  for the 2008 diffraction data set. The different colors represent different RICH likelihood-ratio thresholds.

884 reliable identification of final-state particles of species  $S$  it is important to require a significantly  
 885 larger likelihood for the hypothesis  $S$ , i.e. it is important to use a likelihood-ratio threshold  
 886 greater than one. More details on the RICH performance can be found in appendix A.2.3.

### 887 3.2.3 RICH Threshold Optimization for the $K^- \pi^- \pi^+$ Final State

888 As discussed in the previous section, the performance of the final-state particle identification  
 889 depends on the kinematic distribution of the final-state particles. Therefore, the final choice of  
 890  $\mathcal{T}_R$  depends on the analyzed final state, which is  $K^- \pi^- \pi^+$  in this work, and must be optimized  
 891 to achieve high efficiency purity. Here, the purity is the fraction of events where the  $K^-$  and  
 892  $\pi^-$  hypothesis were assigned correctly. Figure 3.14 shows how both quantities depend on  
 893 the likelihood-ratio threshold. Details on how we estimated these numbers can be found in  
 894 appendix A.2.4.

895 As expected, the efficiency continuously decreases with increasing  $\mathcal{T}_R$ . In contrast, the purity  
 896 rises steeply with increasing  $\mathcal{T}_R$  and saturates at about  $\mathcal{T}_R = 1.2$ . In order to achieve a high purity,  
 897 while maintaining a high efficiency, we chose a likelihood-ratio threshold of  $\mathcal{T}_R = 1.15$ . Using  
 898 this threshold, the  $K^-$  and  $\pi^-$  were identified correctly by the RICH for 98.1 % of the selected  
 899  $K^- \pi^- \pi^+$  events, while efficiency remains sufficiently high as the relative efficiency is 67.3 %.



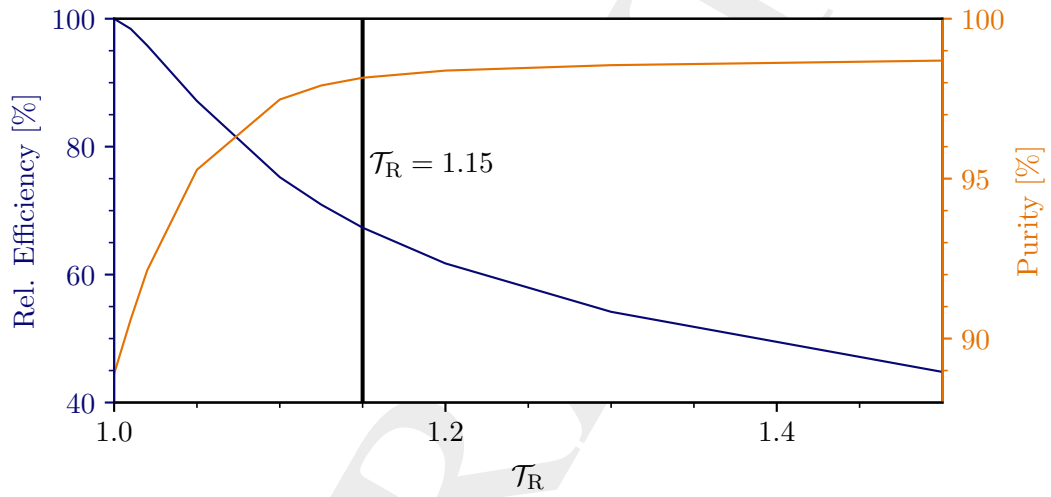


Figure 3.14: Efficiency to identify the  $K^-\pi^-\pi^+$  final state relative to the efficiency for a likelihood-ratio threshold of  $\mathcal{T}_R = 1.0$  (blue curve). The orange curve represents the purity, i.e. fraction of events where the  $K^-$  and  $\pi^-$  were correctly identified. Details on how we estimated these numbers can be found in appendix A.2.4.



## 4 Event Selection

COMPASS collected data of various reactions during the data taking campaign in the years 2008 and 2009. The main task of the event selection discussed in section 4.1 is to extract a clean sample of the diffractive dissociation reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  from the total data set. An additional challenge of the event selection of this reaction is to determine which of the three final-state particles belongs to which species.

Unless stated differently, all plots in this section show the final  $K^- \pi^- \pi^+$  sample of the combined 2008 and 2009 diffraction data set. The probability to measure a produced event, the so-called acceptance, is non-uniform in the kinematic variables of the  $K^- \pi^- \pi^+$  final state. Thus, the shapes of the measured kinematic distributions shown in this chapter are distorted with respect to the physical distributions. However, the measured distributions still exhibit qualitatively the main features of the physical distributions. Due to the high dimensionality of the kinematic distributions of the  $K^- \pi^- \pi^+$  final state and the complex dependence of the acceptance on these distributions, a correction of these acceptance effects is feasible only at the level of the partial-wave decomposition discussed in chapter 5.

### 4.1 Selection of the $K^- \pi^- \pi^+$ Final State

In order to select the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , we applied a series of selection criteria, called cuts, to the diffraction data set. They can be grouped into six stages: (i) preselection cuts to select events with three charged final-state particles, (ii) cuts on the event topology, (iii) cuts on the initial- and final-state particle species, (iv) cuts to ensure energy and momentum conservation, (v) cuts to suppress non-diffractive reactions that lead to the same final state, and (vi) cuts that limit the data sample to the kinematic region of interest. Figure 4.1 gives an overview over the number of events after the cuts for the 2008 and 2009 diffraction data set.

The event selection was inspired by previous analyses of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  [44] and other reactions [39] that were performed on a subset of the COMPASS diffraction data set. We improved and extended them, and we optimized their parameters in order to increase the size of the data sample and to improve the quality of the data.

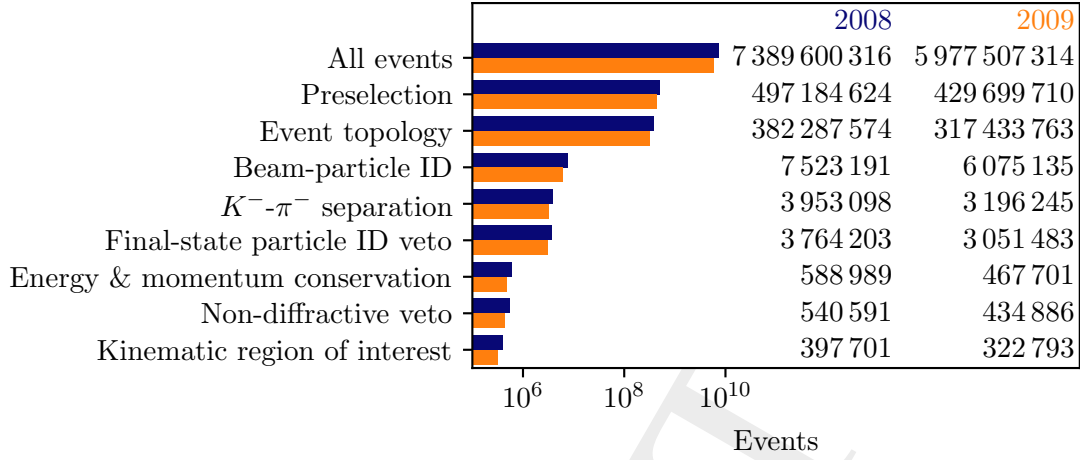


Figure 4.1: Number of selected events after applying the six stages of selection cuts for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . The cuts on the initial- and final-state particle identification [stage (iii)] are listed separately. The blue bars and the numbers in the first column show the results for the 2008 diffraction data set. The orange bars and the numbers in the second column show the results for the 2009 diffraction data set. The cuts are explained in the text.

## 927 Preselection Cuts

928 Diffractive scattering of pion or kaon beams can produce a whole family of final states that  
 929 consists of three charged particles. The first stage of the event selection aims to select a sample of  
 930 event candidates of this generic type. This sample is used also in the analyses of other diffractive  
 931 reactions such as  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  [43],  $\pi^- + p \rightarrow \pi^- K^- K^+ + p$  [65],  $\pi^- + p \rightarrow \pi^- \pi^0 \omega + p$   
 932 with  $\omega \rightarrow \pi^- \pi^+ \pi^0$  [62],  $\pi^- + p \rightarrow \pi^- \eta + p$  with  $\eta \rightarrow \pi^- \pi^+ \pi^0$  [66], and  $\pi^- + p \rightarrow \pi^- \eta' + p$  with  
 933  $\eta' \rightarrow \pi^- \pi^+ \eta$  [66].

934 First, we required that at least one interaction point of a beam particle with a target proton, a  
 935 so-called interaction vertex, was reconstructed in the target area.<sup>[a]</sup> Next, we required that three  
 936 charged particles leave the interaction vertex.<sup>[b]</sup> As the beam particle is negatively charged, we  
 937 required the charge sum of these three final-state particles to be minus one. Finally, we checked  
 938 the stability of the data taking by studying the time evolution of various kinematic distributions  
 939 of the reactions  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  and  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  (see appendix B.4). We  
 940 removed data that show clear outliers in one of the studied kinematic variables.<sup>[c]</sup>

<sup>[a]</sup> We required the interaction-vertex position  $Z_{\text{vtx}}$  along the beam direction to be within  $-200 \leq Z_{\text{vtx}} < 160$  cm, which includes the liquid-hydrogen target cell and additionally about 130 cm before and after the target.

<sup>[b]</sup> If more than one interaction vertex was reconstructed in the event, we chose the “best” vertex candidate, which is the one with most associated particles and with the smallest  $\chi^2$  value from the vertex reconstruction fit.

<sup>[c]</sup> First, we studied the time evolution of kinematic distributions after applying all event-selection cuts, except for this cut on the time stability. Then, in a second iteration of the event-selection, we removed data that show clear outliers.

941 From the 13.4 billion events in the diffraction data set, we pre-selected 931 million event  
942 candidates of the generic type with three charged final-state particles. Roughly 54 % of the events  
943 were collected in 2008, the remaining 46 % were collected in 2009.

#### 944 Cuts on Event Topology

945 The so-called DT0 trigger was designed to include diffractive scattering reactions with minimal  
946 bias as described in section 2.2. Therefore, we selected only events that were triggered by a DT0  
947 signal.

948 Due to the high intensity of the hadron beam, it infrequently happened that two or more beam  
949 particles enter the experimental setup during the time window that defines an event. In cases  
950 where two or more beam particles interact with the target, we reconstruct multiple interaction  
951 vertices. To remove such events, we rejected events with more than one interaction vertex. In  
952 cases where we reconstruct only one interaction vertex, e.g. if only one of the beam particles  
953 interacts with the target, we ensured that we associated the correct beam particle with the  
954 interaction vertex. This is done by requiring a coincidence in time between the trigger signal and  
955 the measurement of the beam particle,<sup>[d]</sup> in addition to the spatial constraints, imposed by the  
956 interaction vertex reconstruction.

957 Beam particles do not only interact with the protons in the liquid-hydrogen target, but may  
958 interact with any material on their path. This can be seen in figure 4.2a, which shows the  
959 distribution of interaction vertices along the direction of the beam. In addition to the plateau  
960 from about  $-65$  to  $-25$  cm, which corresponds to interactions within the 40 cm long target cell,  
961 the distribution exhibits a peak at about  $-68$  cm. This peak arises from beam particles interacting  
962 with the cooling pipe of the target [57]. In the plane transverse to the beam axis, the hadron beam  
963 is well focused on the liquid-hydrogen target as shown in figure 4.2b. Still, some vertices lie  
964 outside the target cylinder indicated by the gray circle. To select only events where the beam  
965 particle interacts with a proton of the target, we required the interaction vertex position to be  
966 within  $-65 \leq Z_{\text{Vtx}} < -30$  cm along the beam axis and within a radial distance of  $R_{\text{Vtx}} < 1.5$  cm  
967 in the plane transversal to the nominal beam axis.

#### 968 Cuts on Particle Species

969 In order to separate the kaon component in the beam from the about 36 times larger pion  
970 component, we applied a novel likelihood approach, which employs the full information provided  
971 by both CEDAR detectors (see section 3.1 for details). Using a log-likelihood difference threshold

---

<sup>[d]</sup> Coincidence in time of the trigger signal and the beam particle was enforced by selecting events only if the time of the beam particle was within  $\pm 3\sigma_t$  around the trigger signal, where  $\sigma_t$  is the time resolution. The time of the beam particle was calculated from the measured hit times in the tracking detectors.

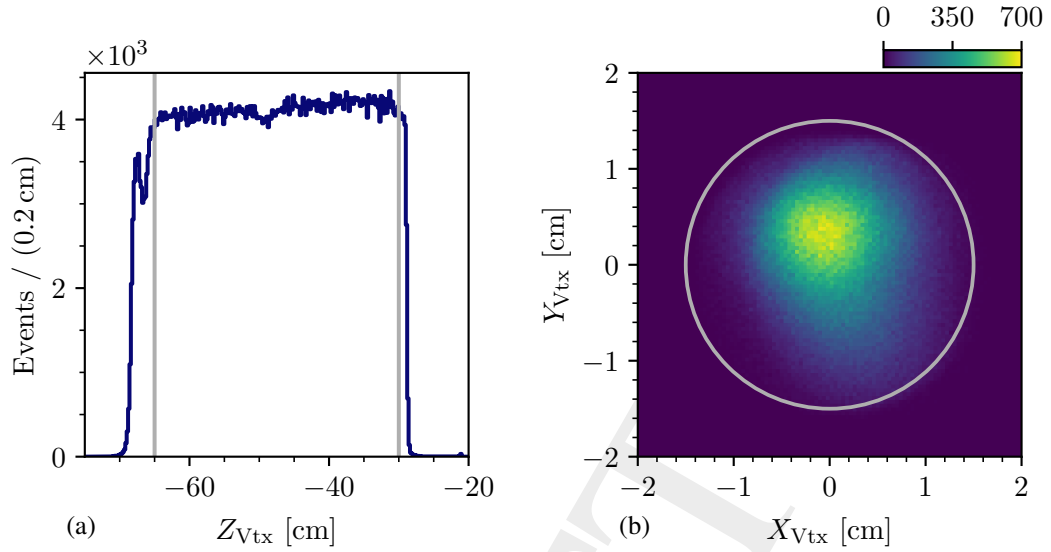


Figure 4.2: Spatial distribution of the interaction-vertex position. (a) shows the position along the beam axis, without the cut on the vertex  $Z$ -position. (b) shows the position in the plane transverse to the beam axis, without the cut on the vertex  $R$ -position. The gray lines represent the cuts on  $Z$ - and  $R$ -position, respectively.

972 of  $\mathcal{T}_C(K) = 4.0$  for the selection, we achieved a high kaon-identification efficiency of about  
 973 85 %.

974 The  $K^-\pi^-\pi^+$  final state has two negative particles of different species. To distinguish them, we  
 975 employed the information from the RICH detector (see section 3.2.3). Particles can be identified  
 976 as pions, kaons, protons, muons, electrons; or they can be not identified. We identified all three  
 977 final-state particles separately, using a likelihood-ratio threshold of  $\mathcal{T}_R = 1.15$  and limiting the  
 978 particle identification to the momentum range where the RICH identification works with a high  
 979 purity, and where we can describe the effects imposed by the RICH particle identification in the  
 980 detector Monte Carlo simulation discussed in appendix C.2.3.<sup>[e]</sup>

981 As discussed in section 3.2.2, the final-state particle identification works efficiently only up to  
 982 about 50 GeV/ $c$ . However, the final-state particles have momenta up to the beam momentum  
 983 of about 190 GeV/ $c$ . Therefore, we cannot identify all three particles in the final state using the  
 984 RICH detector. Therefore, we assumed that the data set contains only events of the  $K^-\pi^-\pi^+$   
 985 final state, because we were able to select beam kaons with high purity using the CEDARs and the  
 986  $K^-\pi^-\pi^+$  final state it is the dominant final state for kaon diffraction into three charged particles.  
 987 Under this assumption, the positive particle was assumed to be a pion and the main task of the  
 988 final-state particle identifications is to separate the  $K^-$  from the  $\pi^-$ . We either identified both  
 989 negative particles accordingly or we identified only one of the negative particles as a kaon or a  
 990 pion and assumed for the not-identified particle the other particle species, respectively. If none of

<sup>[e]</sup> The momentum ranges for particle identification are  $3 \leq |\vec{p}_\pi^+| < 60$  GeV/ $c$  for pions,  $10 \leq |\vec{p}_K^-| < 60$  GeV/ $c$  for kaons and  $18 \leq |\vec{p}_p^+| < 100$  GeV/ $c$  for protons.

991 the negative particles was identified or if the negative particles were identified to be both pions or  
 992 both kaons, the event was rejected.

993 To suppress events where the three reconstructed particles do not belong to the  $K^- \pi^- \pi^+$  final  
 994 state, e.g. decays to  $K^- K^- K^+$ , we rejected events where the assigned particle species hypothesis  
 995 conflicts the  $K^- \pi^- \pi^+$  assumption, i.e. if the positive particle was identified as a kaon or if one  
 996 of the three final-state particles was identified as a (anti)proton. However, this suppresses only  
 997 a small fraction of the background, as the identification of the  $K^- \pi^-$  system requires one of  
 998 the negative particles to have a momentum below about 50 GeV/c, which is the region where  
 999 the RICH is efficient. Given the total beam momentum of about 190 GeV/c, the two remaining  
 1000 final-state particles therefore typically have momenta above 50 GeV/c, which is too large for the  
 1001 particles to be identified by the RICH. Thus, the final-state particle ID veto rejects only a small  
 1002 number of events (see figure 4.1).

1003 The limited momentum range of the final-state particle identification introduces large acceptance  
 1004 effects. They can be best seen in the momentum distribution of the final-state particles that  
 1005 have to be identified, i.e. the  $\pi^-$  and the  $K^-$ , shown in figure 4.3. We observe a horizontal and  
 1006 a vertical band. For events in the horizontal band, the  $K^-$  have momenta in the range of about  
 1007  $10 \leq |\vec{p}_{K^-}| < 50$  GeV/c, in which they are identified by the RICH. For events in the vertical band,  
 1008 the  $\pi^-$  have momenta in the range of about  $3 \leq |\vec{p}_{\pi^-}| < 50$  GeV/c, in which they are identified.  
 1009 We find more events in the vertical band where the  $\pi^-$  was identified. For events where both  
 1010 negative particles have momenta above about 50 GeV/c, we could not decide which of the two  
 1011 negative particles is which species. Therefore, we rejected those events. However, this leads to a  
 1012 region with zero experimental acceptance in the triangular region of the momentum distribution  
 1013 where both negative particles have momenta above about 50 GeV/c. This hole in the momentum  
 1014 distribution introduces a non-uniform acceptance also in many other kinematic variables, in  
 1015 particular in the mass spectra and angular distributions used in the partial-wave analysis. The  
 1016 treatment of this acceptance effect and its consequences are one of the major challenges of this  
 1017 analysis and will be a topic throughout this work.

## 1018 Cuts on Energy and Momentum Conservation

1019 The data set contains contamination from background events with more than three final-state  
 1020 particles, but where some of these final-state particles were not detected. For example, reactions  
 1021 of the type  $K^- + p \rightarrow K^- \pi^- \pi^+ \pi^0 + p$ , where the neutral  $\pi^0$  was not detected.<sup>[f]</sup> Such, so-called  
 1022 non-exclusive events can be suppressed in the event selection by requiring energy and momentum  
 1023 conservation of the measured energies and momenta of the initial- and final-state particles in the  
 1024 scattering process.

<sup>[f]</sup> In the event selection presented here, we did not use the information from the electromagnetic calorimeters to detect  $\pi^0$  and suppress events with  $\pi^0$  in the final state, as the electromagnetic calorimeters would require a computationally expensive and complicated treatment in the detector Monte Carlo simulation. However, we performed a study where we applied such a cut to suppress  $\pi^0$ . This cut had a negligible effect on the final event sample.

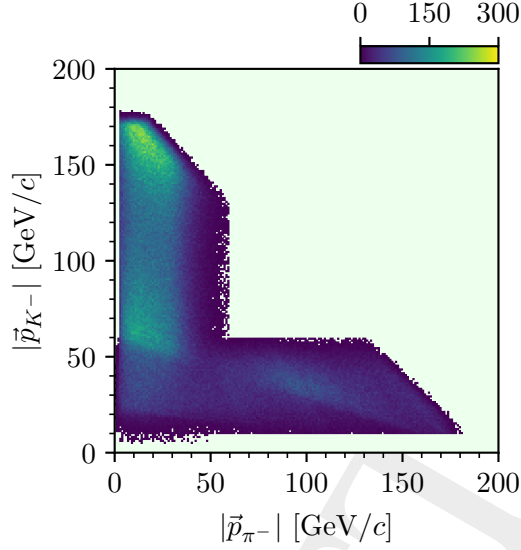


Figure 4.3: Distributions of the magnitudes of the reconstructed momenta of the identified  $K^- \pi^-$  subsystem in the  $K^- \pi^- \pi^+$  final state.

1025 Unfortunately, the energy of the individual beam particle was not measured by the experimental  
 1026 setup. However, the energy spread of the beam is only about 1% [49]. In addition, we can  
 1027 calculate the beam particle energy from the measured three-momenta of the  $K^- \pi^- \pi^+$  final-state  
 1028 particles and the measured inclination of the beam particle, which were both measured with high  
 1029 precision (see section 2.2), by applying energy conservation. The calculation can be found in  
 1030 appendix B.1. The distribution of the reconstructed beam-particle energy is shown in figure 4.4a  
 1031 and exhibits a clear exclusivity peak at 191.29 GeV, which corresponds to the nominal beam  
 1032 energy. We selected events if the reconstructed beam energy was within  $\pm 3\sigma_E$  around the peak  
 1033 center, where  $\sigma_E$  is the Gaussian width of the peak of about  $\sigma_E = 1.71$  GeV/c. [g]

1034 Due to momentum conservation, the projections of the total momentum of the  $K^- \pi^- \pi^+$  system  
 1035 and the momentum of the recoil proton in the plane perpendicular to the beam-particle track  
 1036 must be back-to-back for exclusive events. This means that the azimuthal angle between these  
 1037 two projections must be  $180^\circ$ . We employed this constraint to suppress non-exclusive events in  
 1038 our data by requiring that

$$\Delta\phi_{\text{recoil}} = 180^\circ - \angle(\vec{p}_{K^- \pi^- \pi^+}^\perp, \vec{p}_{\text{recoil}}^\perp) \quad (4.1)$$

1039 is compatible with zero within one standard deviation of the angular resolution of the RPD  
 1040 detector, with which the recoil proton was measured. [h]

[g] We fitted a single Gaussian function plus a third-order background polynomial to the peak region of  $182 \leq E_{\text{beam}} < 200$  GeV to determine the Gaussian width of the peak, i.e. the width of the Gaussian function.

[h] The angular resolution of the RPD detector depends on the hit pattern in the scintillator segments and can be either  $\pm 8.432^\circ$  or  $\pm 5.377^\circ$ . We applied cuts on  $\Delta\phi_{\text{recoil}}$  accordingly. See ref. [67] for details.



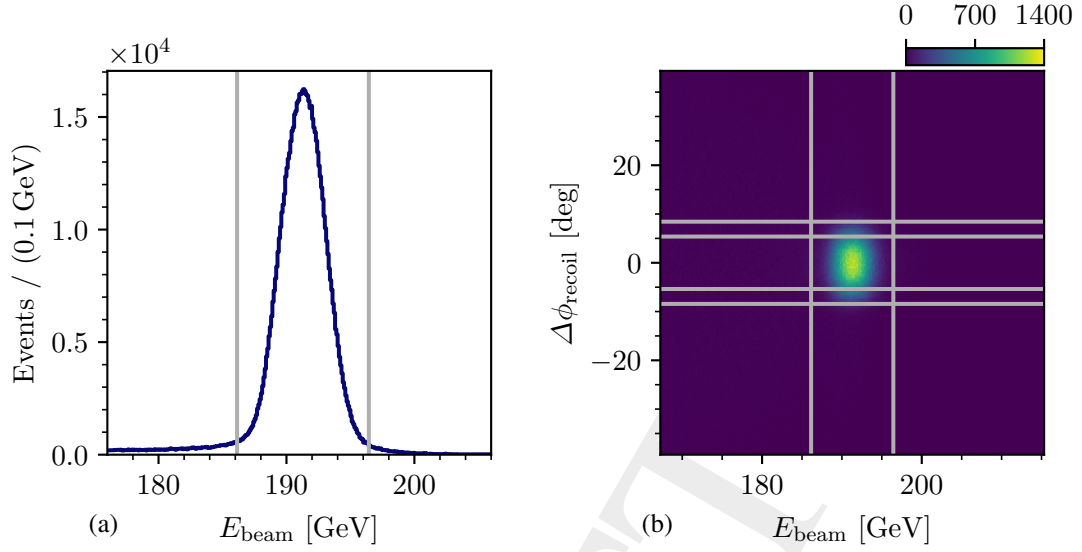


Figure 4.4: Distribution of the kinematic variables used to select exclusive events. (a) shows the distribution of the reconstructed beam energy after all cuts except for the cut on  $E_{\text{beam}}$ . (b) shows the distribution of  $\Delta\phi_{\text{recoil}}$ , which is a measure of momentum conservation (see text), versus the beam energy after all cuts, except for the cuts on  $\Delta\phi_{\text{recoil}}$  and  $E_{\text{beam}}$ . The gray lines represent the applied cuts.<sup>[h]</sup>

1041 We do not observe correlations between  $\Delta\phi_{\text{recoil}}$  and the beam energy (see figure 4.4b). This  
 1042 indicates, that both variables give independent information and applying both cuts helps to better  
 1043 separate exclusive from non-exclusive events. The non-exclusive background in the final  $K^- \pi^- \pi^+$   
 1044 sample was estimated to be only about  $(2 \pm 1 \text{ (sys.)})\%$ .<sup>[i]</sup>

#### 1045 Cuts to suppress Non-Diffractive Reactions

1046 In addition to diffractive scattering, there are other exclusive processes that lead also to the  
 1047  $K^- \pi^- \pi^+$  final state (see section 2.1.1). Thus, these processes cannot be separated from diffractive  
 1048 scattering in terms of their event topology, the particle species, or energy and momentum  
 1049 conservation. A special role play central-production reactions. The kinematic characteristic of  
 1050 central production is different from the one of diffractive scattering. In central production, the  
 1051 kaon scatters elastically of the centrally produced  $\pi^- \pi^+$  system. The scattered kaon goes mostly  
 1052 in very forward direction. To characterize this, the Feynman- $x$  variable of the final-state kaon is  
 1053 used, which can be approximated by [9]

$$x_F^K \approx \frac{2p_{\parallel}^{\text{cm}}}{\sqrt{s}}. \quad (4.2)$$

<sup>[i]</sup> As there is no model for the distribution of the reconstructed beam energy for non-exclusive contributions, this is only a rough estimate. See appendix B.2 for details.

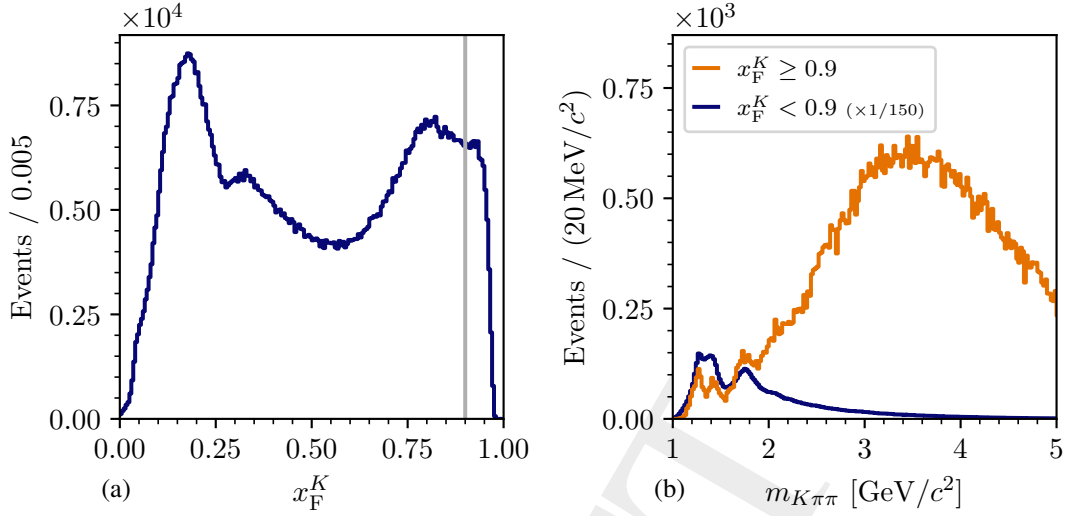


Figure 4.5: Kinematic distributions to study central-production reactions. (a) shows the distribution in  $x_F^K$ . The orange histogram in (b) shows the invariant mass spectrum of the  $K^-\pi^-\pi^+$  system for the subset of data with  $x_F^K \geq 0.9$ . The blue histogram in (b) shows the corresponding distribution for the complementary data set with  $x_F^K < 0.9$  scaled by a factor of  $1/150$ . For all distributions, the cuts on the  $t'$  and  $m_{K\pi\pi}$  region were not applied.

1054 Here,  $p_{\parallel}^{\text{cm}}$  is the momentum component of the final-state kaon in the direction of the incoming  
 1055 beam kaon in the  $K^-\pi^-\pi^+ + p$  center-of-momentum frame and  $\sqrt{s}$  is the center-of-momentum  
 1056 energy. We expect  $x_F^K \approx 1$  for the forward-scattered kaon of central-production reactions.  
 1057 Figure 4.5a shows the  $x_F^K$  distribution. As  $x_F^K$  is directly correlated with the momentum of the  
 1058 scattered kaon, most of the structures observed in this distribution arise from acceptance effects  
 1059 of the final-state particle identification shown in figure 4.3. In addition, a small peak at  $x_F^K \approx 0.92$   
 1060 is observed, which might be caused by central-production reactions. To suppress these events, we  
 1061 required  $x_F^K < 0.9$ . The  $m_{K\pi\pi}$  distribution of the central-production sample with  $x_F^K \geq 0.9$  (orange  
 1062 histogram in figure 4.5b) exhibits a broad bump at about  $3.5 \text{ GeV}/c^2$ , with a small low-mass  
 1063 tail leaking into the  $m_{K\pi\pi}$  region of interest below  $3 \text{ GeV}/c^2$ . A comparison with the selected  
 1064  $K^-\pi^-\pi^+$  sample (blue histogram in figure 4.5b) shows, that the central-production sample does  
 1065 not contribute dominantly to the  $m_{K\pi\pi}$  region of interest. In this low-mass tail, we observe  
 1066 structures on top of the continuous tail, similar to those of the selected  $K^-\pi^-\pi^+$  sample. This  
 1067 indicates, that by applying this cut, we also rejected a small fraction below 1% of diffractive  
 1068 scattering reactions.

1069 It should be noted, that first Monte Carlo studies based on simple models for central-production  
 1070 reactions [68, 69] also yielded a peak at large  $x_F^K$ , but with a dominant tail towards smaller values  
 1071 down to  $x_F^K \approx 0.5$  for  $m_{K\pi\pi} < 3 \text{ GeV}/c^2$ . This suggests, that the cut  $x_F^K < 0.9$  suppress only part  
 1072 of the central-production contribution to the  $K^-\pi^-\pi^+$  sample, which, however, is in general small  
 1073 for  $m_{K\pi\pi} < 3 \text{ GeV}/c^2$ .

## 1074 Cuts on the Kinematic Region of Interest

1075 As a last step, we defined the kinematic region of interest in  $t'$  and  $m_{K\pi\pi}$ . The lower limit of  
 1076  $t' = 0.1 \text{ (GeV}/c)^2$  is given by the minimal energy necessary for the recoil proton to produce a  
 1077 signal in the recoil-proton detector (see section 2.2). For  $t' > 1.0 \text{ (GeV}/c)^2$  or for  $K^-\pi^-\pi^+ <$   
 1078  $1.0 \text{ GeV}/c^2$ , an insufficient amount of data is available to perform a partial-wave analysis. Up to  
 1079 now, there are no well-known strange-meson resonances in the range  $m_{K\pi\pi} \gtrsim 2.5 \text{ GeV}/c^2$  [9].  
 1080 Therefore, we limited ourselves to the  $t'$  range of  $0.1 \leq t' < 1.0 \text{ (GeV}/c)^2$  and the  $m_{K\pi\pi}$  range of  
 1081  $1.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$ .

1082 Applying all cuts defined in this section, we obtained a final  $K^-\pi^-\pi^+$  sample of 307 701 events for  
 1083 the 2008 and 322 793 events for the 2009 diffraction data set, in the kinematic region of interest.  
 1084 In total, the COMPASS data sample for diffractive  $K^-\pi^-\pi^+$  production contains 720 494 events,  
 1085 which is about 2.7 times larger than the sample from a previous unpublished COMPASS analy-  
 1086 sis [44]. It is the so-far world's largest sample of this reaction and is 3.6 times larger compared  
 1087 to the previously world's largest sample measured by the WA3 experiment [23].

## 1088 4.2 Kinematic Distributions of the $K^-\pi^-\pi^+$ Sample

1089 In order to search for strange-meson resonances decaying into  $K^-\pi^-\pi^+$ , the most interesting  
 1090 kinematic variable to look at is the invariant mass spectrum of the  $K^-\pi^-\pi^+$  system shown in  
 1091 figure 4.6a. In the simplest case we expect resonances to appear as peaks in this spectrum. We  
 1092 observe clear peaks in the mass regions of the well-known  $K_1(1270)$ ,  $K_1(1400)$ , and  $K_2(1770)$   
 1093 resonances. These peaks sit on top of a broad spectrum starting at about  $1 \text{ GeV}/c^2$  and having a  
 1094 long tail beyond  $3 \text{ GeV}/c^2$ . In order to separate these signals and to also study weaker signals  
 1095 hidden in the broad spectrum, a comprehensive partial-wave analysis is mandatory. This will be  
 1096 discussed in chapters 5 to 8.

1097 An important property of the diffractive scattering process is its dependence on the squared four-  
 1098 momentum transfer  $t'$ . The  $t'$  spectrum shown in figure 4.6b falls approximately exponentially  
 1099 with  $t'$ . The slope becomes smaller for larger values of  $t'$ . In addition, the slope also changes  
 1100 with  $m_{K\pi\pi}$ . The extraction of the slope of the  $t'$  spectrum as a function of  $m_{K\pi\pi}$  is discussed  
 1101 in appendix B.3. The measured slope parameters are similar to those found in the COMPASS  
 1102  $\pi^-\pi^-\pi^+$  analysis [39]. Since both final states were produced in diffractive scattering reactions,  
 1103 this similarity demonstrates that the  $t'$  dependence is a property of the production mechanism.  
 1104 The observed approximately exponential  $t'$  dependence is also expected from Regge theory [46].  
 1105 However, the slope may be different for different  $K^-\pi^-\pi^+$  resonances. As the observed spectrum  
 1106 arises from various resonances and non-resonant contributions, its shape is the result of a  
 1107 superposition of many exponential shapes, which can only be separated by a partial-wave  
 1108 analysis. The different  $t'$  dependencies of the resonances also lead to a  $t'$ -dependent shape of the  
 1109  $m_{K\pi\pi}$  spectrum. For example, the relative strengths of the peaks in the low- $t'$  (figure 4.6c) and  
 1110 the high- $t'$  (figure 4.6d) region.

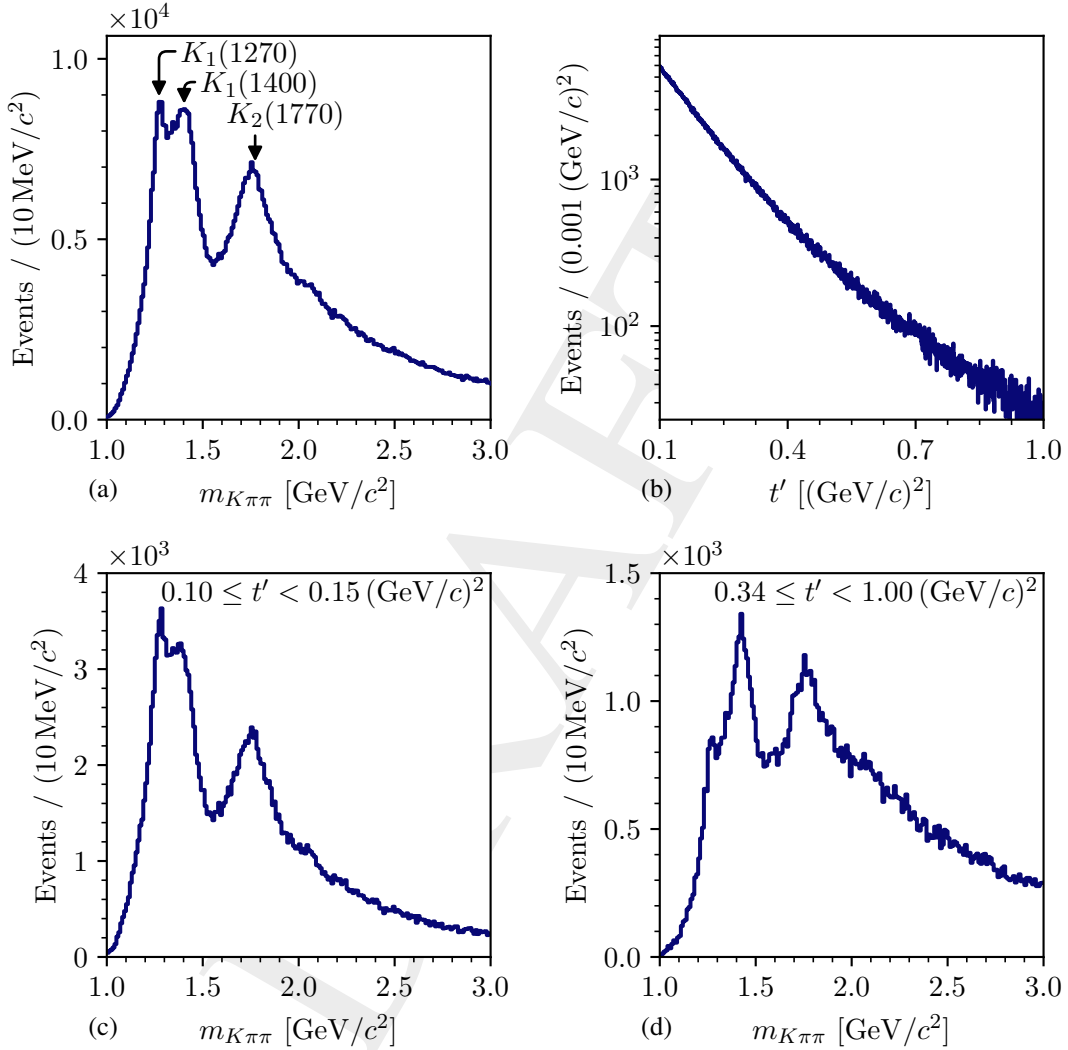


Figure 4.6: Invariant mass spectrum of the diffractively produced  $K^- \pi^- \pi^+$  system (a) for the full analyzed  $t'$  range and in (c) and (d) for the low- and high- $t'$  region, respectively. In (b) we show the corresponding  $t'$  spectrum. The arrows in (a) indicate well-known kaon resonances decaying into  $K^- \pi^- \pi^+$  according to the PDG [9].

1111 Also the invariant mass spectra of the  $K^-\pi^+$  and  $\pi^-\pi^+$  subsystems show clear peaks at the position  
 1112 of well-known resonances. The  $K^-\pi^+$ -mass spectrum shown in figure 4.7a is dominated by the  
 1113  $K^*(892)$  resonance. A second peak appears at about  $1.4 \text{ GeV}/c^2$  where two kaon resonances  
 1114 exist, the  $K_2^*(1430)$  and the  $K_0^*(1430)$ . Both resonances have a similar mass but a different spin.  
 1115 They can be separated only by a partial-wave analysis.

1116 The  $\pi^-\pi^+$  mass spectrum shown in figure 4.7b is dominated by the well-known  $\rho(770)$  resonances,  
 1117 sitting on a broad distribution. The shoulder in the high-mass tail of the  $\rho(770)$  at about  $1 \text{ GeV}/c^2$   
 1118 can be associated with the  $f_0(980)$  resonance. The higher-lying peak corresponds to the  $f_2(1270)$ .  
 1119 Similar structures are observed in the  $\pi^-\pi^+$  subsystem of the  $\pi^-\pi^-\pi^+$  final state [39]. The narrow  
 1120 peak at  $m_{\pi^-\pi^+} \approx 0.38 \text{ GeV}/c^2$  is due to a small contamination of the  $K^-\pi^-\pi^+$  sample from  
 1121 events of the reaction  $K^- + p \rightarrow K^-\phi(1020) + p$ , with  $\phi(1020) \rightarrow K^-K^+$ , where the RICH  
 1122 erroneously identified the second  $K^-$  and the  $K^+$ .<sup>[j]</sup> The wrong mass assumption for the final-state  
 1123 particles shifts the narrow  $\phi(1020)$  peak to about  $0.38 \text{ GeV}/c^2$ . From a coarse event selection  
 1124 of the  $K^-K^-K^+$  final state using COMPASS data, we estimated the  $K^-K^-K^+$  background to the  
 1125  $K^-\pi^-\pi^+$  sample to be below 4%.<sup>[k]</sup>

1126 The  $K^-\pi^-$  spectrum exhibits a broad continuous distribution with a maximum at about  $1 \text{ GeV}/c^2$ .  
 1127 No peaking or other resonant-like structures are observed, as expected as there are no known  
 1128 doubly-negatively charged light mesons.

1129 Finally, we compare our results to those from the ACCMOR collaboration [23] shown in  
 1130 figure 4.8. In their data, the peak in the  $K_2(1770)$  region of the  $m_{K\pi\pi}$  spectrum (see figure 4.8a) is  
 1131 less pronounced with respect to the double-peak in the  $K_1$  region (cf. figure 4.6a). This has two  
 1132 reasons. First, ACCMOR analyzed a lower  $t'$  region, which can have a different composition of  
 1133 resonances. Second, the experimental acceptance of our measurement drops with lower  $m_{K\pi\pi}$  (see  
 1134 figure D.35a). This suppresses the double-peak in the  $K_1$  region with respect to the peak in the  
 1135  $K_2(1770)$  region. The  $m_{K^-\pi^+}$  spectrum from ACCMOR shown in figure 4.8b exhibits clear peaks  
 1136 from the  $K^*(892)$  and the  $K_2^*(1430)$ , in agreement with our observations (cf. figure 4.7a). Also,  
 1137 their  $m_{\pi^-\pi^+}$  spectrum shown in figure 4.8c exhibits similar structures (cf. figure 4.7b). Changes  
 1138 in the relative strength of the observed structures might be caused by the different  $t'$  range and  
 1139 our experimental acceptance. Overall, at this level of the analysis the kinematic distributions  
 1140 from ACCMOR are consistent with our observations, while the smoothness of our distributions  
 1141 demonstrates the improved statistical precision due to our 3.6 times larger sample.

<sup>[j]</sup> Requiring the RICH to always identify the positive particle as a pion strongly suppresses the peak at about  $0.38 \text{ GeV}/c^2$  with respect to the rest of the spectrum. However, this requirement would also reduce the efficiency of the  $K^-\pi^-\pi^+$  selection by about 30%. Therefore, this cut was not applied in the  $K^-\pi^-\pi^+$  event selection.

<sup>[k]</sup> From the peak at about  $0.38 \text{ GeV}/c^2$  we estimated the  $\phi(1020)$  contamination of the  $K^-\pi^-\pi^+$  sample to be about 0.26%. From the  $m_{K^-K^+}$  spectrum of the COMPASS  $K^-K^-K^+$  sample, we estimated the fraction of  $\phi(1020)$  production in the  $K^-K^-K^+$  sample to be about 6.6%. We assumed, that the fraction of  $\phi(1020)$  in the  $K^-K^-K^+$  contamination of the  $K^-\pi^-\pi^+$  sample is the same as in the selected  $K^-K^-K^+$  sample.

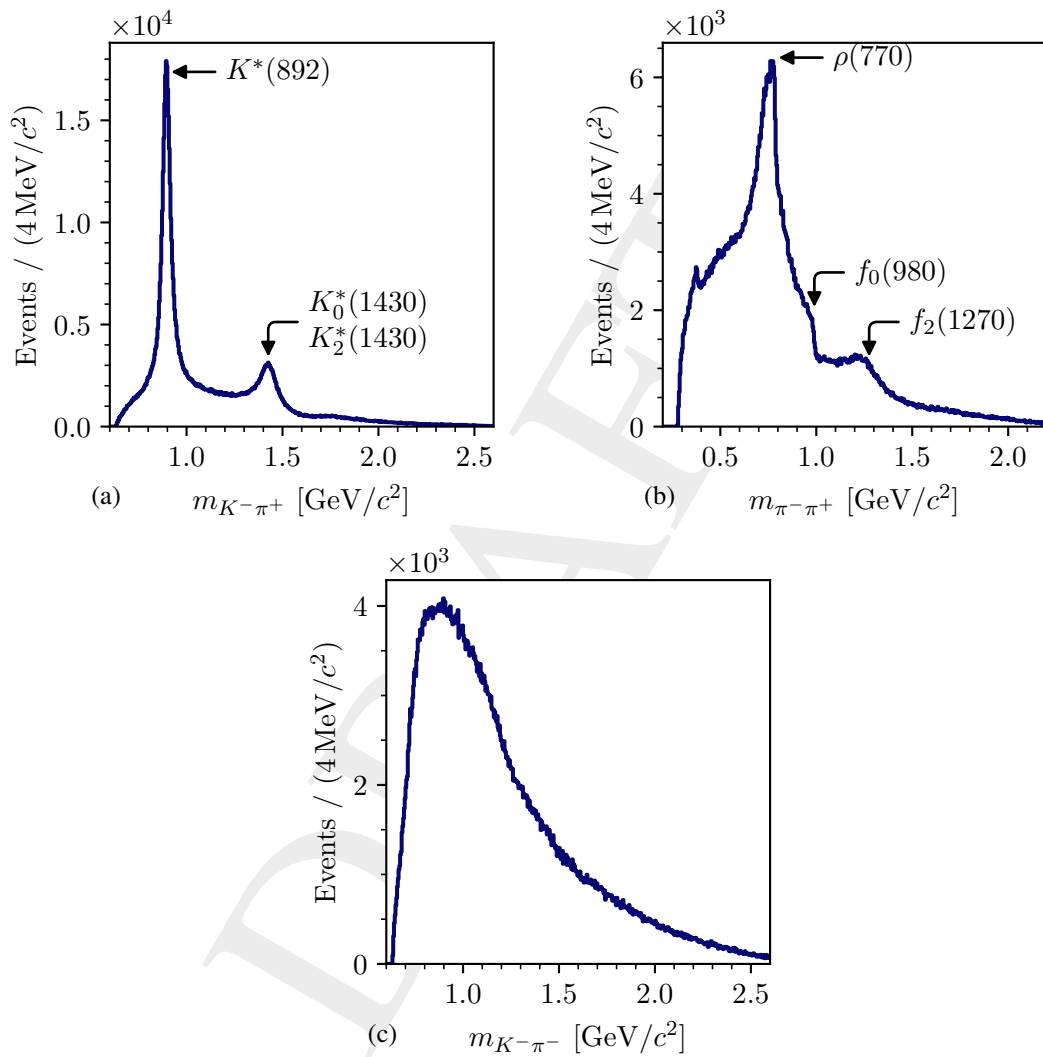


Figure 4.7: Invariant mass spectra of the two-body subsystems of the  $K^- \pi^- \pi^+$  final state: (a)  $K^- \pi^+$ , (b)  $\pi^- \pi^+$ , and (c)  $K^- \pi^-$ . The arrows indicate well-known resonances appearing in these two-body systems according to the PDG [9].

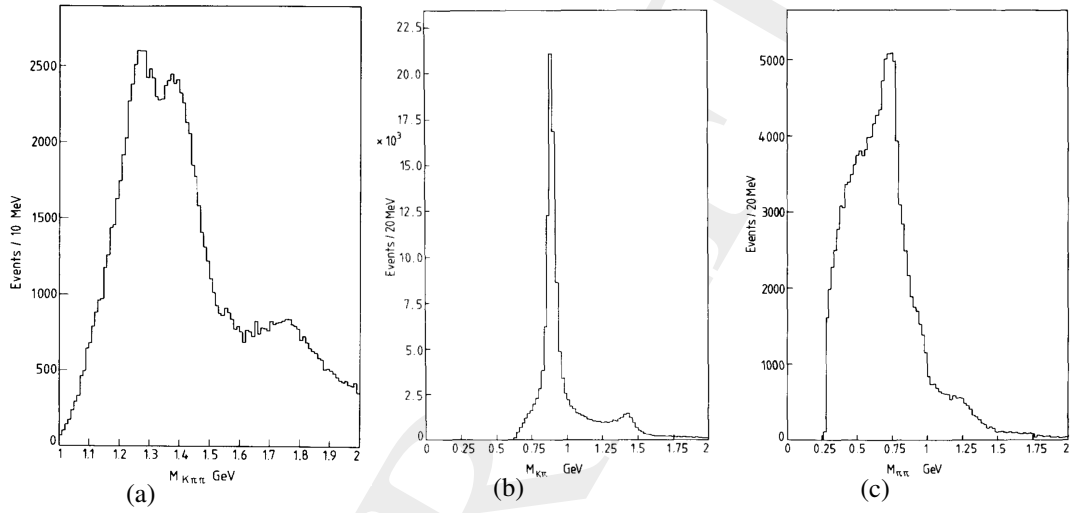


Figure 4.8: Kinematic distributions of the  $K^-\pi^-\pi^+$  final state in the range  $0 \leq t' \leq 0.7(\text{GeV}/c)^2$  as measured by the WA3 experiment and analyzed by ACCMOR [23]. (a) shows the  $m_{K\pi\pi}$  distribution. (b) and (c) show the invariant mass distribution of the  $K^-\pi^+$  and  $\pi^-\pi^+$  subsystem, respectively.





## 5 The Partial-Wave Decomposition

In order to separate the strange-meson resonances  $X^-$  appearing in the  $K^- \pi^- \pi^+$  system, which is produced in the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  (see figure 4.6a), and to identify their  $J^P$  quantum numbers, we performed a comprehensive partial-wave analysis (PWA) based on the  $K^- \pi^- \pi^+$  sample described in the previous chapter 4. We performed the partial-wave analysis in two stages. In the first stage called partial-wave decomposition (PWD), the data are decomposed into amplitudes coming from intermediate states  $X^-$  with various  $J^P$  quantum numbers and various decay paths. In the PWD, the  $m_{K\pi\pi}$  dependence of the reaction is not modeled explicitly, but our data are subdivided into narrow  $m_{K\pi\pi}$  bins, and the PWD is performed independently in these  $m_{K\pi\pi}$  bins. In this way, we determined the  $m_{K\pi\pi}$  dependence of the amplitudes from data. In the same spirit, we subdivided each  $m_{K\pi\pi}$  bin in four  $t'$  bins to also determine the  $t'$  dependence of the amplitudes. In the second analysis stage called resonance-model fit, the  $m_{K\pi\pi}$  dependence of the amplitudes is then modeled explicitly, which allows us to identify strange-meson resonances appearing in the  $K^- \pi^- \pi^+$  system and to measure their masses and widths.

An upper limit for the  $m_{K\pi\pi}$  bin widths are mainly given by the widths of the appearing strange-meson resonances, which are in the range of about  $100 \text{ MeV}/c^2$  or larger. Hence, we used for  $m_{K\pi\pi} < 2 \text{ GeV}/c^2$  a bin width of  $20 \text{ MeV}/c^2$ . For  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$  we used a bin width of  $40 \text{ MeV}/c^2$ , because the  $K^- \pi^- \pi^+$  sample size quickly shrinks towards high  $m_{K\pi\pi}$ , while at the same time strange-meson resonances typically become wider at higher masses. Given the approximately exponential shape of the  $t'$  spectrum, we subdivided our data into four  $t'$  bins, which we chose such that the number of events in the first bin, the second bin, and the last two bins combined is approximately the same.<sup>[a]</sup> The  $t'$ -bin borders are listed in table 5.1. In total, we split the analyzed kinematic range of  $1.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$  and  $0.1 \leq t' < 1.0 (\text{GeV}/c)^2$  into 300 ( $m_{K\pi\pi}, t'$ ) cells, in which the PWD was performed independently.

In this chapter, we first describe in section 5.1 the PWD formalism. In sections 5.2 to 5.4, we present extensions of this general approach that were developed for our analysis. In sections 5.5 and 5.6, we give a first glimpse on the results of the PWD. In sections 5.7 to 5.10, we present systematic and pseudodata studies of the PWD. The resonance-model fit, which used the results of the PWD as input, is presented in chapter 6. The physics results are discussed in chapter 7.

Table 5.1: Borders of the four  $t'$  bins as used for the partial-wave decomposition.

$[(\text{GeV}/c)^2]$	0.10	0.15	0.24	0.34	1.00
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<sup>[a]</sup> We rounded the  $t'$  bin borders to two significant digits in our analysis.

1171 **5.1 Method**1172 **5.1.1 Isobar Model and Coordinate System**

1173 The  $m_{K^-\pi^+}$  and  $m_{\pi^-\pi^+}$  distributions shown in figures 4.7a and 4.7b, respectively, are dominated  
 1174 by various two-body resonances. This indicates that the intermediate state  $X^-$  does not directly  
 1175 decay to  $K^-\pi^-\pi^+$ , but dominantly decays first into a two-body resonance  $\xi^0$  called isobar and the  
 1176 third remaining particle  $b^-$  called bachelor particle, and then the isobar decays into the two-body  
 1177 subsystem. This is schematically shown in figure 5.1. Figure 5.1a shows the graph if the isobar  
 1178 resonance is in the  $K^-\pi^+$  subsystem and hence the  $\pi^-$  is the bachelor particle. Figure 5.1b shows  
 1179 the graph if an isobar resonance is in the  $\pi^-\pi^+$  subsystem and hence the  $K^-$  is the bachelor  
 1180 particle. As the  $K^-\pi^-$  subsystem does not exhibit resonance signals (see figure 4.7c) and as there  
 1181 are no known resonances that decay to  $K^-\pi^-$ , we considered isobars only in the  $K^-\pi^+$  and  $\pi^-\pi^+$   
 1182 subsystems in the PWD. In summary, we employ the isobar model [70, 71], i.e. we split the  
 1183 reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  into the inelastic two-body scattering process  $K^- + p \rightarrow X^- + p$   
 1184 and a series of two successive two-body decays: (i)  $X^- \rightarrow \xi^0 b^-$ , (ii)  $\xi^0 \rightarrow K^-\pi^+$  or  $\xi^0 \rightarrow \pi^-\pi^+$

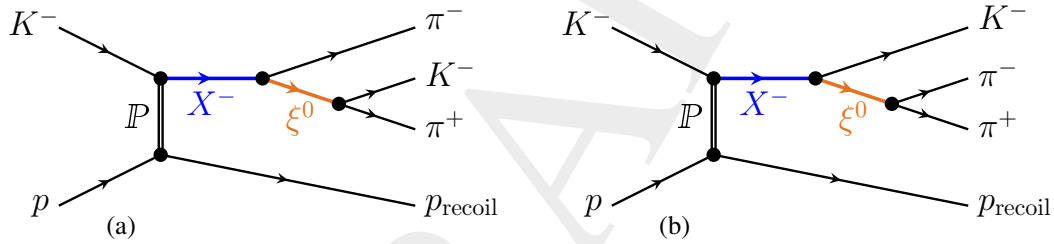


Figure 5.1: Schematic view of the reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  in the isobar model, where the intermediate state  $X^-$  successively decays to the  $K^-\pi^-\pi^+$  system via a two-body resonance  $\xi^0$  called isobar. (a) shows the reaction if the isobar resonance is in the  $K^-\pi^+$  subsystem. (b) show the reaction if the isobar resonance is in the  $\pi^-\pi^+$  subsystem. The third remaining particle  $b^-$  is called bachelor particle, which in (a) is the  $\pi^-$  and in (b) is the  $K^-$ .

1185 In order to disentangle the various contributions from the different intermediate states  $X^-$ , the  
 1186 PWD employs the full information from the measured kinematic distributions of the final-state  
 1187 particles. The choice of the kinematic variables that describe the reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$   
 1188 is not unique. A convenient definition is motivated by the isobar-model picture. The inelastic  
 1189 scattering reaction  $K^- + p \rightarrow X^- + p$  is described by the center-of-momentum energy  $s$ , which  
 1190 is constant due to the fixed beam momentum; the reduced squared four-momentum transfer  $t'$ ;  
 1191 and the invariant mass  $m_{K\pi\pi}$  of the  $K^-\pi^-\pi^+$  system. For fixed  $s$ ,  $m_{K\pi\pi}$  and  $t'$ , the  $X^-$  decay is  
 1192 described by five phase-space variables summarized by  $\tau$ . The decay  $X^- \rightarrow \xi^0 b^-$  is described  
 1193 in the  $X^-$  rest frame using the Gottfried-Jackson (GJ) frame shown in figure 5.2. This reference  
 1194 frame is a right-handed coordinate system, where the  $\vec{z}_{\text{GJ}}$  axis is given by the direction of the beam  
 1195  $K^-$  and the  $\vec{y}_{\text{GJ}}$  axis is given by the normal of the  $X^-$  production plane. The  $X^-$  production plane  
 1196 (orange plane in figure 5.2) is given by the momenta of the recoil proton and the beam  $K^-$ . Since  
 1197 in the  $X^-$  rest frame the momenta of the  $\xi^0$  and the bachelor particle are back to back, the  $X^-$

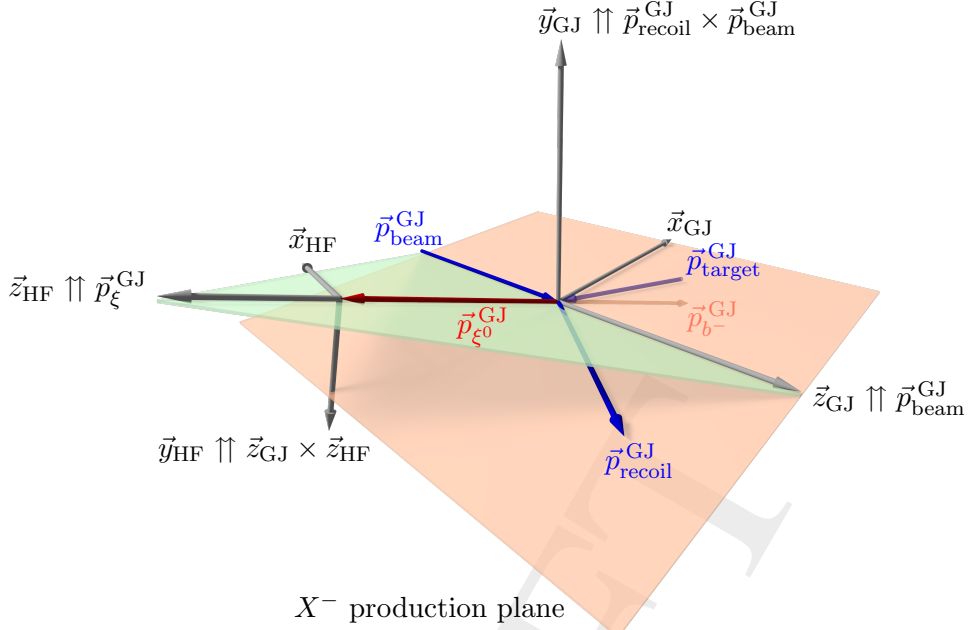


Figure 5.2: Definition of the Gottfried-Jackson (GJ) and helicity (HF) frames used to describe the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  with an intermediate state  $X^-$  in the  $K^- \pi^- \pi^+$  system decaying to a two-body isobar  $\xi^0$  and the bachelor particle  $b^-$ . The Gottfried-Jackson frame is defined in the  $X^-$  rest frame. The helicity frame is defined in the  $\xi^0$  rest frame. The momenta of the beam  $K^-$ , the target proton, and the recoiling proton in the Gottfried-Jackson frame are  $\vec{p}_{\text{beam}}^{\text{GJ}}$ ,  $\vec{p}_{\text{target}}^{\text{GJ}}$ , and  $\vec{p}_{\text{recoil}}^{\text{GJ}}$ , respectively. The unit vectors of the coordinate axes are labeled  $\vec{x}_i, \vec{y}_i, \vec{z}_i$ . In this work, we consider two cases, which yield different coordinate systems, one if the  $\xi^0$  is in the  $K^- \pi^- \pi^+$  subsystem and one if the  $\xi^0$  is in the  $\pi^- \pi^+$  subsystem. Taken from ref. [67] and adjusted.

1198 decay is described by two decay angles of one of the daughter particles. We chose the polar  
 1199 angle  $\theta_{\text{GJ}}$  and the azimuthal angle  $\phi_{\text{GJ}}$  of the isobar. The decay of the isobar  $\xi^0$  is described  
 1200 in its rest frame using the helicity frame (HF). The helicity frame is constructed by boosting  
 1201 from the  $X^-$  rest frame to the  $\xi^0$  rest frame. The  $\vec{z}_{\text{HF}}$  axis is given by the momentum of  $\xi^0$   
 1202 in the Gottfried-Jackson frame. The  $\vec{y}_{\text{HF}}$  axis is given by the normal of the plane (green plane in  
 1203 figure 5.2) that is defined by  $\vec{z}_{\text{GJ}}$  and the momentum of  $\xi^0$ . Since in the  $\xi^0$  rest frame the momenta  
 1204 of the two decay products are back to back, the  $\xi^0$  decay is described by two decay angles of  
 1205 one of the daughter particles. We chose the polar angle  $\theta_{\text{HF}}$  and the azimuthal angle  $\phi_{\text{HF}}$  of the  
 1206 negative decay product, which is either the  $K^-$  or the  $\pi^-$ . In addition to the four angles, the  
 1207 invariant mass of the two-body isobar subsystem completes the set of variables that span the  
 1208  $K^- \pi^- \pi^+$  phase space.

1209 Given that we consider isobars in the  $K^- \pi^+$  and  $\pi^- \pi^+$  subsystems, there are two different  
 1210 definitions of these phase-space variables that are used in the following: (i) if the isobar is in the  
 1211  $K^- \pi^+$  subsystem, the phase-space variables are  $m_{K\pi\pi}$ ,  $t'$ , and  $\tau^{K\pi} = (\theta_{\text{GJ}}^{K\pi}, \phi_{\text{GJ}}^{K\pi}, m_{K^- \pi^+}, \theta_{\text{HF}}^{K^-}, \phi_{\text{HF}}^{K^-})$ ;  
 1212 (ii) if the isobar is in the  $\pi^- \pi^+$  subsystem, the phase-space variables are  $m_{K\pi\pi}$ ,  $t'$ , and  $\tau^{\pi\pi} =$   
 1213  $(\theta_{\text{GJ}}^{\pi\pi}, \phi_{\text{GJ}}^{\pi\pi}, m_{\pi^- \pi^+}, \theta_{\text{HF}}^{\pi^-}, \phi_{\text{HF}}^{\pi^-})$ .

## 1214 5.1.2 Partial-Wave Decomposition Formalism

1215 In the following, we give a brief introduction into the PWD formalism. A detailed and general  
 1216 description of the PWD formalism used in our work can be found in ref. [72]. We mainly follow  
 1217 the derivations, notation, and conventions given in ref. [72]. All formulas, except explicitly  
 1218 stated otherwise are taken from ref. [72] or from references therein. The PWD formalism for the  
 1219 special case of the COMPASS  $\pi^- \pi^- \pi^+$  analysis, which is similar to our analysis, can be found in  
 1220 ref. [39].

### 1221 Cross Section

1222 The differential cross section for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  is given by

$$\frac{d\sigma}{d\Phi_4} = \frac{|\mathcal{M}|^2}{\mathfrak{F}}. \quad (5.1)$$

1223 Here, the flux factor,

$$\mathfrak{F} = 4 \sqrt{(p_{\text{beam}} p_{\text{target}})^2 - m_{\text{beam}}^2 m_{\text{target}}^2}, \quad (5.2)$$

1224 is approximately a constant given by the fixed beam momentum.  $\mathcal{M}$  is the Lorentz-invariant  
 1225 matrix element that encodes the whole dynamics of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ .<sup>[b]</sup> The  
 1226 differential phase-space element  $d\Phi_4$  of the  $K^- \pi^- \pi^+ p$  final state can be split into the two-body  
 1227 phase-space  $d\Phi_2$  of the  $X^- p$  system and the three-body phase-space  $d\Phi_3$  of the  $K^- \pi^- \pi^+$  final  
 1228 state, i.e.

$$d\Phi_4 = d\Phi_2 d\Phi_3 \frac{2m_{K\pi\pi}}{2\pi} dm_{K\pi\pi}. \quad (5.3)$$

1229 Expressing the two-body phase-space in terms of  $t'$  and the azimuthal angle  $\phi$  of the production  
 1230 plan around the beam-particle direction yields:

$$d\Phi_4 = \frac{1}{2(2\pi)^2} \frac{1}{\mathfrak{F}} d\phi dt' d\Phi_3 \frac{2m_{K\pi\pi}}{2\pi} dm_{K\pi\pi}, \quad (5.4)$$

1231 where the flux factor is appearing again (see ref. [72]). Since we consider unpolarized reactions,  
 1232 the matrix element does not depend on  $\phi$ . Hence, integration over  $\phi$  is trivial and yields for the  
 1233 differential cross section in equation (5.1):

$$\frac{d\sigma(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \frac{1}{\mathfrak{F}^2} \frac{1}{4\pi} \frac{2m_{K\pi\pi}}{2\pi} |\mathcal{M}(\tau, m_{K\pi\pi}, t')|^2. \quad (5.5)$$

1234 Finally, the number density; i.e. the distribution of the number  $N_{\text{ev}}$  of produced events, which is  
 1235 the number of events that were actually produced in the experiment, differential in  $m_{K\pi\pi}$ ,  $t'$ , and

<sup>[b]</sup> Amplitudes from various incoherent contributions may contribute to the reaction. At this point, we absorb these incoherent contributions in  $|\mathcal{M}|^2$  before we explicitly formulate them in equation (5.14).

1236 the 5-dimensional  $K^- \pi^- \pi^+$  phase-space  $d\Phi_3$ ; reads

$$\frac{dN_{\text{ev}}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \mathcal{L} \frac{d\sigma(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \frac{\mathcal{L}}{(2\pi\tilde{\delta})^2} m_{K\pi\pi} |\mathcal{M}(\tau, m_{K\pi\pi}, t')|^2, \quad (5.6)$$

1237 where  $\mathcal{L}$  is the integrated luminosity. We chose the distribution of the number of events to be  
 1238 differential in the Lorentz-invariant  $K^- \pi^- \pi^+$  phase-space element  $d\Phi_3(\tau; m_{K\pi\pi})$ , which contains  
 1239 the respective Jacobian that may appear from the explicit choice of the phase-space variables as  
 1240 discussed in section 5.1.3.

### 1241 Matrix Element for a Single Intermediate State

1242 We first formulate a model for  $|\mathcal{M}(\tau, m_{K\pi\pi}, t')|^2$  that considers only a single intermediate state  
 1243  $X^-$  and a single decay chain of  $X^-$ . The production, the propagation, and the decay of  $X^-$  are  
 1244 assumed to be independent of each other. Hence, the amplitude,

$$\mathcal{M}_{Kp \rightarrow Xp \rightarrow K\pi\pi}(\tau, m_{K\pi\pi}, t') = \mathcal{P}_{Kp \rightarrow Xp}(m_{K\pi\pi}, t') \mathcal{D}_X(m_{K\pi\pi}) \tilde{\Psi}_{X \rightarrow K\pi\pi}(\tau, m_{K\pi\pi}) \quad (5.7)$$

1245 factorizes into three parts: (i) an amplitude  $\mathcal{P}_{Kp \rightarrow Xp}(m_{K\pi\pi}, t')$  that models the production of  
 1246  $X^-$ , (ii) an amplitude  $\mathcal{D}_X(m_{K\pi\pi})$  that models the propagation of  $X^-$ , and (iii) an amplitude  
 1247  $\tilde{\Psi}_{X \rightarrow K\pi\pi}(\tau, m_{K\pi\pi})$  that models the decay of  $X^-$  via a particular decay chain.

### 1248 Decay Amplitudes

1249 The amplitude for the  $X^-$  decay shown in figure 5.3 can be calculated in the isobar model. It  
 1250 describes the decay of a certain intermediate state  $X^-$  with spin  $J$ , parity  $P$ , and spin projection  
 1251  $M^\varepsilon$ ,<sup>[c], [d]</sup> into the bachelor particle and a certain isobar with spin  $J_\xi$  and helicity  $\lambda_\xi$ . In addition,  
 1252 the bachelor particle and the isobar have a relative orbital angular momentum  $L$ . We call the  
 1253 combination,

$$a = J^P M^\varepsilon \xi b L, \quad (5.8)$$

1254 of these quantum number a partial wave label.<sup>[e]</sup>

1255 It is a well-established experimental fact that the strong interaction conserves parity. Parity con-  
 1256 servation can be implemented in the PWD formalism by using the so-called reflectivity basis [73]  
 1257 for the subprocess  $K^- + p \rightarrow X^- + p$ . The reflectivity operation is a space inversion followed by  
 1258 an 180° rotation about the production plane normal. This corresponds to a reflection through  
 1259 the production plane. As all momenta of the four particles of the subprocess  $K^- + p \rightarrow X^- + p$

[c] We define the reflectivity quantum number  $\varepsilon$  below.

[d] The  $\vec{z}_{\text{GJ}}$  axis in the Gottfried-Jackson frame is the quantization axis and defines the spin projection.

[e] For simplicity, the charge of the isobar and of the bachelor particle are dropped in the partial-wave labels. The spin  $J_\xi$  of the isobar does not explicitly appear in  $a$  as it is implicitly given by  $\xi$ , e.g.  $\xi = \rho(770)$  implies  $J_\xi = 1$ . The helicity  $\lambda_\xi$  of the isobar is also not given as it is an internal quantum number and summed over in equation (5.9).

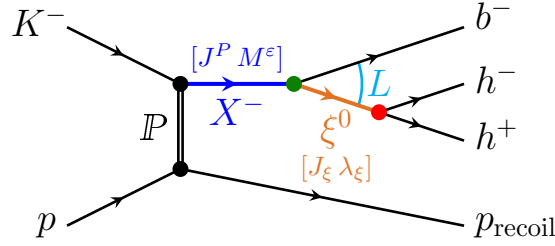


Figure 5.3: Schematic view of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  in the isobar model, where the intermediate state  $X^-$  with spin  $J$ , parity  $P$ , and spin projection  $M^\epsilon$  successively decays to the  $K^- \pi^- \pi^+$  final state via a two-body resonance  $\xi^0$  called isobar with spin  $J_\xi$  and helicity  $\lambda_\xi$ .  $L$  is the relative orbital angular momentum between the bachelor particle  $b^-$  and the isobar.  $h^\pm$  are the two final-state particles of the  $\xi^0$  decay. The colors correspond to the colors of the terms in equation (5.9).

1260 lie in the production plane by construction (see figure 5.2), the reflection operation leaves those  
 1261 momenta unchanged. In the following, we construct decay amplitudes that are eigenfunctions of  
 1262 the reflectivity operator with eigenvalues  $\varepsilon$  called reflectivity. For mesons, the reflectivity can be  
 1263  $\varepsilon = \pm 1$ .<sup>[f]</sup> Partial waves with different  $\varepsilon$  do not interfere due to parity conservation [73].

1264 In the reflectivity basis,  $M$  is defined to be  $M \geq 0$ . For each  $M$  in the range  $0 < M \leq J$ , there  
 1265 is one state with  $\varepsilon = +1$  and one with  $\varepsilon = -1$ . In addition, there is one state with  $M = 0$  and  
 1266  $\varepsilon = P(-1)^J$ .<sup>[g]</sup> Hence, also in the reflectivity basis there are in total  $2J + 1$  states, as expected for  
 1267 the total multiplicity of a state with spin  $J$ .

1268 The main advantage of using the reflectivity basis is that in the limit of a high center-of-momentum  
 1269 energy, the reflectivity is approximately identical to the naturality of the exchange particle in the  
 1270 scattering process [74–76]. Since at COMPASS energies the scattering process is dominated  
 1271 by Pomeron exchange, which has positive naturality, dominantly positive reflectivity states are  
 1272 produced.<sup>[h]</sup> Hence, we may neglect negative-reflectivity states, which drastically reduces the  
 1273 amount of states, i.e. partial waves, that need to be considered in the PWD by about a factor  
 1274 two.<sup>[i]</sup>

<sup>[f]</sup> In general, the reflectivity of bosons is  $\varepsilon = \pm 1$ .

<sup>[g]</sup> A detailed explanation can be found in section 5.2.3 of ref. [72].

<sup>[h]</sup> It was shown in ref. [48] that even at the high center-of-momentum energy at COMPASS,  $f_2$  exchange also has some contribution to the scattering process. As the  $f_2$  exchange has also positive naturality, we still expect the reaction to be dominated by positive-reflectivity states. Ref. [48] did not find significant contributions from exchanges with negative naturality.

<sup>[i]</sup> For the wave-set selection discussed in section 5.2, we performed a study where we also considered partial waves with negative reflectivity. However, none of the negative-reflectivity waves picked up significant intensity.

1275 Following the derivation in ref. [72], the total decay amplitude for a partial wave  $a$  reads

$$\begin{aligned}
 \tilde{\Psi}_a(\tau, m_{K\pi\pi}) &= \sum_{\lambda_\xi} \alpha_{X \rightarrow \xi b L} \sqrt{\frac{2L+1}{4\pi}} \left[ {}^\varepsilon D_{M\lambda_\xi}^J(\phi_{\text{GJ}}, \theta_{\text{GJ}}, 0) \right]^* F_L(m_{K\pi\pi})(L, 0; J_\xi, \lambda_\xi | J, \lambda_\xi) \\
 &\quad \times \mathcal{D}_\xi(m_{h^- h^+}) \\
 &\quad \times \alpha_\xi \sqrt{\frac{2J_\xi+1}{4\pi}} \left[ D_{\lambda_\xi 0}^{J_\xi}(\phi_{\text{HF}}, \theta_{\text{HF}}, 0) \right]^* F_{J_\xi}(m_{h^- h^+}),
 \end{aligned} \tag{5.9}$$

1276 i.e. factorizes into three parts represented by the three lines in equation (5.9). The colors match  
 1277 the respective parts in figure 5.3.

1278 The first line shown in green represents the amplitude of the two-body decay  $X^- \rightarrow \xi^0 b^-$ . Here,  
 1279 the complex-valued coupling  $\alpha_{X \rightarrow \xi b L}$  encodes the strength and relative phase of the  $X^-$  decay  
 1280 into  $\xi^0 b^-$  with a given  $L$ . The Wigner  $D$ -function in the reflectivity basis,  ${}^\varepsilon D_{M\lambda_\xi}^J(\phi_{\text{GJ}}, \theta_{\text{GJ}}, 0)$ ,  
 1281 describes the dependence of the decay amplitude on the angles in the  $X^-$  decay (see equation  
 1282 (177) in ref. [72]). The centrifugal-barrier factor  $F_L(m_{K\pi\pi})$  accounts for the additional energy  
 1283 needed to produce an orbital angular momentum of  $L$ . It is a model-dependent term, which  
 1284 modifies the coupling at the  $X^-$  decay vertex. We used the parameterization from von Hippel and  
 1285 Quigg [77].<sup>[j]</sup> Finally, the Clebsch-Gordan coefficient  $(L, 0; J_\xi, \lambda_\xi | J, \lambda_\xi)$  describes the coupling  
 1286 of the orbital-angular momentum  $L$  and the isobar spin  $J_\xi$  to the  $X^-$  spin  $J$  in the  $L$ - $S$  coupling  
 1287 scheme used here.<sup>[k]</sup>

1288 The second line shown in orange represents the propagation amplitude of the isobar. It is  
 1289 given by the dynamic amplitude  $\mathcal{D}_\xi(m_{h^- h^+})$  of the isobar resonance as a function of the invariant  
 1290 mass  $m_{h^- h^+}$  of the two-body subsystem, i.e. as a function of  $m_{K^- \pi^+}$  or  $m_{\pi^- \pi^+}$ . For most of  
 1291 the considered isobar resonances, we used a relativistic Breit-Wigner amplitude. The various  
 1292 dynamic amplitudes are separately discussed in section 5.1.4.

1293 The third line shown in red represents the amplitude of the two-body decay of the isobar. Here,  
 1294 the complex-valued coupling  $\alpha_\xi$  encodes the strength and relative phase of the decay to  $K^- \pi^+$  or  
 1295  $\pi^- \pi^+$ . The Wigner  $D$ -function  $D_{\lambda_\xi 0}^{J_\xi}(\phi_{\text{HF}}, \theta_{\text{HF}}, 0)$  [78, 79] describes the dependence of the total  
 1296 decay amplitude on the angles in the  $\xi^0$  decay.  $F_{J_\xi}(m_{h^- h^+})$  is the centrifugal-barrier factor in the  
 1297  $\xi^0$  decay. As the two final-state particles are spin-less, the orbital angular momentum between  
 1298 them equals to  $J_\xi$ . The same parameterization is used as for  $F_L(m_{K\pi\pi})$ .

1299 The helicity  $\lambda_\xi$  of the intermediate isobar is an intermediate quantum number. The corresponding  
 1300 decay amplitudes are constraint by the other quantum numbers and the Clebsch-Gordan coefficient.  
 1301 Hence, equation (5.9) contains a coherent sum over all allowed helicities, such that decay  
 1302 amplitudes with different helicities interfere.

<sup>[j]</sup> See appendix D in ref. [72] for the definition of the centrifugal-barrier factors using  $z = [q(m_{K\pi\pi}, m_{h^- h^+}, m_{b^-})/q_R]^2$ ,  
 where  $q$  is the two-body break-up momentum of the  $X^- \rightarrow \xi^0 b^-$  decay [see equation (5.41)] and  $q_R = 197.3 \text{ MeV}/c$ .

<sup>[k]</sup> Other Clebsch-Gordan coefficients that appear according to the general formula in equation (152) of ref. [72] are  
 one in our case of three spin-less final-state particles.

1303 One should note that the isobar model is only an approximation for the actual physical process.  
 1304 For example, it neglects all kinds of rescattering effects among all three final-state particles, and it  
 1305 neglects a direct three-body decay of  $X^-$ . However, such effects are expected to be small, except  
 1306 for very special cases, e.g. if triangle singularities appear in the rescattering amplitudes [80].

1307 The total decay amplitude as given by equation (5.9) can be calculated up to the in general  
 1308 unknown couplings  $\alpha_{X \rightarrow \xi b L}$  and  $\alpha_\xi$ . To remove these unknowns, we define the normalized decay  
 1309 amplitudes  $\Psi'_a$ , also simply called decay amplitudes, in the following way:

$$\Psi'_a(\tau, m_{K\pi\pi}) \equiv \frac{\tilde{\Psi}'_a(\tau, m_{K\pi\pi})}{\alpha_{X \rightarrow \xi b L} \alpha_\xi \sqrt{\mathfrak{R}_a(m_{K\pi\pi})}}. \quad (5.10)$$

1310 Here, we additionally divide by the square root of the wave-normalization integral,<sup>[1]</sup> which is  
 1311 given by the integral of the absolute-squared of the total decay amplitude without couplings over  
 1312 the  $(m_{K\pi\pi}, t')$  kinematic cell and over the  $K^- \pi^- \pi^+$  phase space, i.e.<sup>[m]</sup>

$$\mathfrak{R}_a(m_{K\pi\pi}) = \int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' \int d\Phi_3(\tau) \left| \frac{\tilde{\Psi}'_b(\tau, \tilde{m}_{K\pi\pi})}{\alpha_{X \rightarrow \xi b L} \alpha_\xi} \right|^2. \quad (5.11)$$

1313  $\mathfrak{R}_a$  incorporates the  $K^- \pi^- \pi^+$  phase-space volume accessible at  $m_{K\pi\pi}$  and can be interpreted as  
 1314 the phase-space volume filled by partial wave  $a$ .

### 1315 Multiple Intermediate States and Incoherent Contributions

1316 The amplitude in equation (5.7) describes the production and propagation of a single intermediate  
 1317 state  $X^-$  and its decay via a single decay path. However, a state can decay into the  $K^- \pi^- \pi^+$   
 1318 final state via various decay chains, i.e. via various isobars and various values for the orbital angular  
 1319 momentum  $L$ . Also, as already seen in the  $m_{K\pi\pi}$  distribution in figure 4.6a, various states  $X^-$   
 1320 appear in our data. As these are all intermediate states, they interfere and thus have to be added  
 1321 up coherently to obtain the total amplitude. Hence, equation (5.7) needs to be extended:

$$\mathcal{M}(\tau, m_{K\pi\pi}, t') = \sum_{a \in \mathbb{W}} \left\{ \sum_{k \in \mathbb{S}_a} \mathcal{P}_{k,a}(m_{K\pi\pi}, t') \mathcal{D}_k(m_{K\pi\pi}) \alpha_{k \rightarrow \xi b L} \right\} \alpha_\xi \sqrt{\mathfrak{R}_a(m_{K\pi\pi})} \Psi'_a(\tau, m_{K\pi\pi}). \quad (5.12)$$

1322 Here, we use the normalized decay amplitudes given in equation (5.10). The outer sum runs  
 1323 over the set  $\mathbb{W}$  of all considered partial waves, i.e. over all considered  $J^P M^E$  quantum number  
 1324 combinations of  $X^-$  and over all considered decay paths. We discuss in section 5.2 how we chose  
 1325  $\mathbb{W}$ . The inner sum runs over all intermediate states  $X^-$  labeled by  $k$  that may appear in partial

<sup>[1]</sup> Dividing by the wave-normalization integral yields the convenient property that the diagonal elements of the integral matrix defined in equation (5.22) are one.

<sup>[m]</sup> The wave-normalization integral is proportional to the  $t'$ -bin width. As we used different  $t'$ -bin widths in our analysis (see table 5.1),  $\mathfrak{R}_a(m_{K\pi\pi})$  in principle also depends on  $t'$ . We omit this  $t'$  dependence in the formulas for simplicity.



1326 wave  $a$ , e.g. it runs over ground and excited states with the same  $J^P$  quantum numbers. Since the  
 1327 production amplitude not only depends on which state  $k$  is produced, but also depends on the  
 1328 spin-projection  $M^\varepsilon$  with which this state is produced,  $\mathcal{P}_{k,a}(m_{K\pi\pi}, t')$  has an additional wave label  
 1329  $a$ , which includes  $M^\varepsilon$ .

1330 The PWD model for the distribution of the number  $N_{\text{ev}}$  of produced events differential in  $m_{K\pi\pi}$ ,  
 1331  $t'$ , and the 5-dimensional  $K^-\pi^-\pi^+$  phase-space  $d\Phi_3$  is obtained by inserting equation (5.12) in  
 1332 equation (5.6):

$$\frac{d\widehat{N}_{\text{ev}}^{\text{coh}}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \left| \sum_{a \in \mathbb{W}} \sqrt{\frac{\mathcal{L}}{(2\pi\delta)^2}} \sqrt{m_{K\pi\pi}} \left\{ \sum_{k \in \mathbb{S}_a} \mathcal{P}_{k,a}(m_{K\pi\pi}, t') \mathcal{D}_k(m_{K\pi\pi}) \alpha_{k \rightarrow \xi b L} \right\} \alpha_\xi \sqrt{\mathfrak{N}_a(m_{K\pi\pi})} \Psi_a(\tau, m_{K\pi\pi}) \right|^2. \quad (5.13)$$

1333 We use a hat to indicate that  $\widehat{N}_{\text{ev}}$  is the PWD model prediction for the actual quantity  $N_{\text{ev}}$ .

1334 Up to now, we considered perfect coherence of the partial-wave amplitudes. However, there are  
 1335 also reactions where the corresponding amplitudes do not interfere and hence have to be summed  
 1336 incoherently in the total cross section. For example, scattering reactions with spin flip and spin  
 1337 non-flip of the target proton have to be summed at the cross-section level as the proton spin was  
 1338 not measured. Another example are background processes, which are discussed in section 5.3.  
 1339 Generally, incoherent contributions are implemented in our formalism by an incoherent sum over  
 1340 various coherent sectors labeled by  $z$  that may contribute to our data sample. Hence, the PWD  
 1341 model for the distribution of the number of produced events reads

$$\mathcal{I}(\tau, m_{K\pi\pi}, t') \equiv \frac{d\widehat{N}_{\text{ev}}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \sum_z \left| \sum_{a \in \mathbb{W}_z} \sqrt{\frac{\mathcal{L}}{(2\pi\delta)^2}} \sqrt{m_{K\pi\pi}} \left\{ \sum_{k \in \mathbb{S}_a} \mathcal{P}_{k,a}^z(m_{K\pi\pi}, t') \mathcal{D}_k(m_{K\pi\pi}) \alpha_{k \rightarrow \xi b L} \right\} \alpha_\xi \sqrt{\mathfrak{N}_a(m_{K\pi\pi})} \Psi_a(\tau, m_{K\pi\pi}) \right|^2. \quad (5.14)$$

1342 The quantity  $\mathcal{I}$  is also called the model intensity. In general, the sets  $\mathbb{W}_z$  of partial waves  
 1343 may be different in the coherent sectors. Also, the production amplitudes may be different for  
 1344 different production processes. Hence,  $\mathcal{P}_{k,a}^z(m_{K\pi\pi}, t')$  has an additional  $z$  label. The propagation  
 1345 depends only on the intermediate state  $k$  and the decay amplitude is completely determined by  
 1346 the partial-wave label  $a$ . Hence, both amplitudes do not have a  $z$  label.

1347 In addition to the partial waves defined in equation (5.8), we included a single so-called flat wave  
 1348 in our model, which has a flat decay amplitude, i.e.  $\Psi_{\text{flat}}(\tau, m_{K\pi\pi}) = \text{const}$ . It is added incoherently  
 1349 to the other partial waves, i.e. there is an own coherent sector containing only the flat wave. This  
 1350 flat wave effectively models incoherent background in our data that has an isotropic phase-space  
 1351 distribution.

1352 **Transition Amplitudes**

1353 Within the isobar model, the decay amplitudes are known and can be calculated without free  
 1354 parameters. We combine all other terms in equation (5.14), which are partly unknown, to the  
 1355 so-called transition amplitudes

$$\mathcal{T}_a^z(m_{K\pi\pi}, t') \equiv \sqrt{\frac{\mathcal{L}}{(2\pi\mathfrak{F})^2}} \sqrt{m_{K\pi\pi}} \left\{ \sum_{k \in \mathbb{S}_a} \mathcal{P}_{k,a}^z(m_{K\pi\pi}, t') \mathcal{D}_k(m_{K\pi\pi}) \alpha_{k \rightarrow \xi b L} \right\} \alpha_\xi \sqrt{\mathfrak{N}_a(m_{K\pi\pi})}. \quad (5.15)$$

1356 The transition amplitudes of a partial wave  $a$  incorporate the production and propagation of all  
 1357 intermediate states that may appear in wave  $a$ . As the transition amplitudes contain the couplings  
 1358  $\alpha_{k \rightarrow \xi b L}$  and  $\alpha_\xi$ , they incorporate also the strengths and phases of the decays of the intermediate  
 1359 and isobar states. Using the transition amplitudes simplifies equation (5.14) to

$$\mathcal{I}(\tau, m_{K\pi\pi}, t') = \sum_z \left| \sum_{a \in \mathbb{W}_z(m_{K\pi\pi}, t')} \mathcal{T}_a^z(m_{K\pi\pi}, t') \Psi_a(\tau, m_{K\pi\pi}) \right|^2. \quad (5.16)$$

1360 It is important to note, that the transition amplitudes depend only on  $m_{K\pi\pi}$  and  $t'$ . The known  
 1361 decay amplitudes are the only terms that depend on the  $K^- \pi^- \pi^+$  phase-space variables  $\tau$ . As  
 1362 mentioned at the beginning of this section, we performed the PWD independently in narrow  
 1363  $(m_{K\pi\pi}, t')$  cells. We chose these cells to be sufficiently narrow so that we can assume the transition  
 1364 amplitudes to be approximately constant within each cell. Hence, the  $m_{K\pi\pi}$  and  $t'$  dependencies  
 1365 of the transition amplitudes are not explicitly modeled in the PWD, but complex-valued piecewise  
 1366 constant functions are used instead to approximate these dependencies in a model-independent  
 1367 way. For a given  $(m_{K\pi\pi}, t')$  cell, the constant transition amplitudes are the free parameters that  
 1368 are determined in the PWD fits described in section 5.1.3. Using this binned approach, the  
 1369  $m_{K\pi\pi}$  and  $t'$  dependence of the transition amplitudes are measured in the PWD. As indicated in  
 1370 equation (5.16), also the set  $\mathbb{W}_z(m_{K\pi\pi}, t')$  of partial waves may depend on  $m_{K\pi\pi}$  and  $t'$ , which is  
 1371 discussed in section 5.2.

 1372 **Spin-Density Matrix**

1373 Expanding the absolute-value-squared term in equation (5.16) yields

$$\mathcal{I}(\tau, m_{K\pi\pi}, t') = \sum_z \sum_{a, b \in \mathbb{W}_z(m_{K\pi\pi}, t')} \mathcal{T}_a^z(m_{K\pi\pi}, t') \left[ \mathcal{T}_b^z(m_{K\pi\pi}, t') \right]^* \Psi_a(\tau, m_{K\pi\pi}) \left[ \Psi_b(\tau, m_{K\pi\pi}) \right]^*, \quad (5.17)$$

1374 where the transition amplitudes appear in pairs. Exchanging the two sums in equation (5.17), the  
 1375 model intensity can be expressed in terms of the so-called spin-density matrix

$$\rho_{ab}(m_{K\pi\pi}, t') = \sum_z \mathcal{T}_a^z(m_{K\pi\pi}, t') \left[ \mathcal{T}_b^z(m_{K\pi\pi}, t') \right]^*. \quad (5.18)$$

1376 If a wave  $a$  does not appear in coherent sector  $z$ , the corresponding transition amplitude is  
 1377 zero. This means, if waves  $a$  and  $b$  appear only in different coherent sectors, the corresponding  
 1378 spin-density matrix element is zero.<sup>[n]</sup> Using the spin-density matrix, the model intensity in  
 1379 equation (5.17) reads<sup>[o]</sup>

$$\mathcal{I}(\tau, m_{K\pi\pi}, t') = \sum_{a,b \in \mathbb{W}(m_{K\pi\pi}, t')} \Psi_a(\tau, m_{K\pi\pi}) \rho_{ab}(m_{K\pi\pi}, t') \left[ \Psi_b(\tau, m_{K\pi\pi}) \right]^*. \quad (5.19)$$

1380 It is important to note that the transition amplitudes cannot be uniquely determined, because any  
 1381 unitary transformation  $\mathcal{U}_{z'z}$  of the transition amplitudes,

$$\mathcal{T}'_{a^{z'}}(m_{K\pi\pi}, t') = \sum_z \mathcal{U}_{z'z} \mathcal{T}_a^z(m_{K\pi\pi}, t'), \quad (5.20)$$

1382 results in the same model intensity [81]. The reason is, that the transition amplitudes always  
 1383 appear in pairs in equation (5.17). Also, the spin-density matrix is invariant under such a unitary  
 1384 transformation. Hence, the measured transition amplitudes  $\mathcal{T}_a^z(m_{K\pi\pi}, t')$  are in general different  
 1385 from the transition amplitudes  $\mathcal{T}_a^p(m_{K\pi\pi}, t')$  of individual physics processes  $p$ , e.g. spin flip and  
 1386 spin non-flip, because  $p = z' \neq z$ .

1387 The measured transition amplitudes  $\mathcal{T}_a^z(m_{K\pi\pi}, t')$  that appear in equation (5.16) are only an  
 1388 effective parameterization of the spin-density matrix. Different parameterizations of the spin-  
 1389 density matrix are possible in order to fix the arbitrary unitary transformation. We used the  
 1390 so-called Chung-Trueman parameterization [73], which is explained in Appendix E of ref. [72].

1391 A model parameter that needs to be chosen is the rank of the spin-density matrix, which corre-  
 1392 sponds to the number of incoherent sectors in the sum over  $z$  in equation (5.16).<sup>[p]</sup> Our choice  
 1393 for the rank of the spin-density matrix is discussed in section 5.3.

## 1394 Observables

1395 The most important observable is the model intensity given in equation (5.19) as it is related to  
 1396 the distribution of the measured  $K^-\pi^-\pi^+$  sample.

<sup>[n]</sup> For example, if  $z$  labels the two coherent sectors with positive and negative reflectivity, which do not interfere, the wave set of the coherent sector with positive reflectivity and the wave set of the coherent sector with negative reflectivity are disjoint. Hence, the corresponding spin-density matrix has block-diagonal form, where one block corresponds to positive-reflectivity waves and the other block corresponds to negative-reflectivity waves.

<sup>[o]</sup> In equation (5.19), the sum goes over the full set  $\mathbb{W}(m_{K\pi\pi}, t')$  of all partial waves from all coherent sectors, i.e.  $\mathbb{W}(m_{K\pi\pi}, t') = \bigcup_z \mathbb{W}_z(m_{K\pi\pi}, t')$ .

<sup>[p]</sup> As discussed above, we included an incoherent flat wave in our model. However, we do not count the flat wave for what we call the rank of the PWD model or the rank of the spin-density matrix, because the main analysis yields practically zero intensity for the flat wave as discussed in section 5.3. This means, e.g., that a spin-density matrix of a rank=3 PWD model, i.e. a PWD model with a rank=3 spin-density matrix, technically has a rank of 4.

1397 The estimate for the total number of produced events in a  $(m_{K\pi\pi}, t')$  cell can be calculated by  
 1398 integrating equation (5.19) over the ranges of the kinematic  $(m_{K\pi\pi}, t')$  cell and over all five  
 1399  $K^-\pi^-\pi^+$  phase-space variables  $\tau$ , i.e. <sup>[q]</sup>

$$\begin{aligned}\widehat{N}_{\text{ev}}(m_{K\pi\pi}, t') &= \int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' \int d\Phi_3(\tau) \mathcal{I}(\tau, \tilde{m}_{K\pi\pi}, \tilde{t}') \\ &= \sum_{a,b \in \mathbb{W}(m_{K\pi\pi}, t')} \rho_{ab}(m_{K\pi\pi}, t') \int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' \int d\Phi_3(\tau) \Psi_a(\tau, \tilde{m}_{K\pi\pi}) [\Psi_b(\tau, \tilde{m}_{K\pi\pi})]^* \\ &= \sum_{a,b \in \mathbb{W}(m_{K\pi\pi}, t')} \rho_{ab}(m_{K\pi\pi}, t') I_{ab}(m_{K\pi\pi}, t').\end{aligned}\quad (5.21)$$

1400 In the last line, we introduce the so-called phase-space integral matrix

$$I_{ab}(m_{K\pi\pi}, t') \equiv \int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' \int d\Phi_3(\tau) \Psi_a(\tau, \tilde{m}_{K\pi\pi}) [\Psi_b(\tau, \tilde{m}_{K\pi\pi})]^*. \quad (5.22)$$

1401 Limiting the sum in equation (5.17) to only a single partial wave  $a$  yields the expected number of  
 1402 produced events for this wave, i.e.

$$\widehat{N}_a(m_{K\pi\pi}, t') \equiv \rho_{aa}(m_{K\pi\pi}, t') I_{aa}(m_{K\pi\pi}, t') = \rho_{aa}(m_{K\pi\pi}, t'). \quad (5.23)$$

1403 Here, we use that  $I_{aa}(m_{K\pi\pi}, t') = 1$ , due to the normalization of the decay amplitudes in equa-  
 1404 tion (5.10).  $\widehat{N}_a(m_{K\pi\pi}, t')$  is also called the intensity of a partial wave and equals to the corre-  
 1405 sponding diagonal element of the spin-density matrix. Accordingly, we call  $\widehat{N}_{\text{ev}}(m_{K\pi\pi}, t')$  defined  
 1406 in equation (5.21) also the total model intensity.

1407 As explained in section 2.2, we split our total data set into three subsets ( $i$ ) with slightly different  
 1408 experimental acceptances  $\eta^{(i)}(\tau, m_{K\pi\pi}, t')$ . The PWD model for the distribution of the number  
 1409  $N_{\text{ev}}^{(i)}$  of produced events in data set ( $i$ ) reads

$$\frac{d\widehat{N}_{\text{ev}}^{(i)}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \hat{r}^{(i)}(m_{K\pi\pi}, t') \frac{d\widehat{N}_{\text{ev}}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \hat{r}^{(i)}(m_{K\pi\pi}, t') \mathcal{I}(\tau, m_{K\pi\pi}, t'). \quad (5.24)$$

1410 The so-called data-set fraction, i.e. the fraction of produced events in data set ( $i$ ), are given by

$$\hat{r}^{(i)}(m_{K\pi\pi}, t') = \frac{d\widehat{N}_{\text{ev}}^{(i)}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} \bigg/ \frac{d\widehat{N}_{\text{ev}}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') \bigg/ \widehat{N}_{\text{ev}}(m_{K\pi\pi}, t'). \quad (5.25)$$

<sup>[q]</sup> In the second line, the fact that our piecewise parameterization for the transition amplitudes and hence the spin-density matrix is constant within a  $(m_{K\pi\pi}, t')$  cell is used.

1411 The data-set fractions fulfill the condition

$$\sum_{(i)} \hat{r}^{(i)}(m_{K\pi\pi}, t') = 1. \quad (5.26)$$

1412 As the data-set fractions correspond to the number of produced events and not to the number  
 1413 of measured events, they cannot be directly calculated from the fractions of measured events in  
 1414 the  $K^- \pi^- \pi^+$  sample. Therefore, the  $\hat{r}^{(i)}(m_{K\pi\pi}, t')$  are free real-valued parameters in the PWD fits  
 1415 and their values are determined from data. The actual data-set fractions are global constants, i.e.  
 1416 independent of  $(m_{K\pi\pi}, t')$ . However, as the PWD fits are performed independently in  $(m_{K\pi\pi}, t')$   
 1417 cells, independent parameters for the data-set fraction are used in each  $(m_{K\pi\pi}, t')$  cell. The  
 1418 consistency of the extracted the data-set fractions is discussed in section 5.5.

1419 In order to compare the model intensity to the measured distributions, the experimental acceptance  
 1420 has to be taken into account. The acceptance distorts the measured distribution of events with  
 1421 respect to the model intensity, i.e. with respect to the distribution of produced events. The PWD  
 1422 model for the distribution of the number  $\bar{N}_{\text{ev}}^{(i)}$  of measured events in data set  $(i)$  differential in  
 1423  $m_{K\pi\pi}$ , in  $t'$ , and in the 5-dimensional  $K^- \pi^- \pi^+$  phase-space  $d\Phi_3$  reads<sup>[r]</sup>

$$\frac{d\bar{N}_{\text{ev}}^{(i)}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \eta^{(i)}(\tau, m_{K\pi\pi}, t') \hat{r}^{(i)}(m_{K\pi\pi}, t') \mathcal{I}(\tau, m_{K\pi\pi}, t'). \quad (5.27)$$

1424 The acceptance models  $\eta^{(i)}(\tau, m_{K\pi\pi}, t')$ ; i.e. the models for the probability to measure an event  
 1425 that was produced with  $m_{K\pi\pi}, t'$ , and  $\tau$ ; are obtained by Monte Carlo simulations of the detector  
 1426 as described in appendix C.2.

1427 Analogously to equation (5.21), the expected total number of measured events in data set  $(i)$  in a  
 1428  $(m_{K\pi\pi}, t')$  cell is calculated as

$$\begin{aligned} \bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') &= \int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' \int d\Phi_3(\tau) \eta^{(i)}(\tau, \tilde{m}_{K\pi\pi}, \tilde{t}') \hat{r}^{(i)}(\tilde{m}_{K\pi\pi}, \tilde{t}') \mathcal{I}(\tau, \tilde{m}_{K\pi\pi}, \tilde{t}') \\ &= \sum_{a,b \in \mathbb{W}(m_{K\pi\pi}, t')} \rho_{ab}(m_{K\pi\pi}, t') \hat{r}^{(i)}(m_{K\pi\pi}, t') \bar{I}_{ab}^{(i)}(m_{K\pi\pi}, t'). \end{aligned} \quad (5.28)$$

1429 Here, the so-called acceptance-integral matrix,

$$\bar{I}_{ab}^{(i)}(m_{K\pi\pi}, t') \equiv \int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' \int d\Phi_3(\tau) \eta^{(i)}(\tau, \tilde{m}_{K\pi\pi}, \tilde{t}') \Psi_a(\tau, \tilde{m}_{K\pi\pi}) \left[ \Psi_b(\tau, \tilde{m}_{K\pi\pi}) \right]^*, \quad (5.29)$$

1430 appears, which takes into account the experimental acceptance of data set  $(i)$ .

<sup>[r]</sup> In equation (5.27), we neglect detector resolution effects that may lead to a smearing of the variables  $(\tau, m_{K\pi\pi}, t')$ , because of the good detector resolution of COMPASS (see appendix C.4). Incorporating these effects would require a convolution of equation (5.27) with the detector resolution function. The calculation of such high-dimensional convolution integrals is computationally prohibitively expensive.

1431 Finally, the PWD model for the distribution of the number  $\bar{N}_{\text{ev}}$  of measured events in all data sets  
 1432 reads

$$\frac{d\widehat{N}_{\text{ev}}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \sum_{(i)} \frac{d\widehat{N}_{\text{ev}}^{(i)}(\tau, m_{K\pi\pi}, t')}{d\Phi_3 dm_{K\pi\pi} dt'} = \left\{ \sum_{(i)} \eta^{(i)}(\tau, m_{K\pi\pi}, t') \hat{r}^{(i)}(m_{K\pi\pi}, t') \right\} \mathcal{I}(\tau, m_{K\pi\pi}, t'), \quad (5.30)$$

1433 and the estimated total number of measured events in all data sets in a  $(m_{K\pi\pi}, t')$  cell is

$$\widehat{N}_{\text{ev}}(m_{K\pi\pi}, t') = \sum_{(i)} \widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') = \sum_{a,b \in \mathbb{W}(m_{K\pi\pi}, t')} \rho_{ab}(m_{K\pi\pi}, t') \left\{ \sum_{(i)} \hat{r}^{(i)}(m_{K\pi\pi}, t') \bar{I}_{ab}^{(i)}(m_{K\pi\pi}, t') \right\}. \quad (5.31)$$

### 1434 5.1.3 Maximum-Likelihood Fit

1435 In order to measure the  $m_{K\pi\pi}$  and  $t'$  dependence of the spin-density matrix elements, we subdivided  
 1436 our data into narrow bins in  $m_{K\pi\pi}$  and in  $t'$ . The number of events per  $(m_{K\pi\pi}, t')$  cell is  
 1437 between 10 and 7000 events with about 2400 events on average. We fitted the PWD model in  
 1438 equation (5.16) independently in each of the 300  $(m_{K\pi\pi}, t')$  cells to data. The free parameters in  
 1439 these fits are the transition amplitudes  $\{\mathcal{T}_a^z\}$ , which are complex-valued constants within each  
 1440  $(m_{K\pi\pi}, t')$  cell,<sup>[S]</sup> and the data-set fractions  $\{\hat{r}^{(i)}\}$ , which are real-valued constants within one  
 1441  $(m_{K\pi\pi}, t')$  cell. We performed an unbinned extended maximum-likelihood fit in each  $(m_{K\pi\pi}, t')$   
 1442 cell, where we maximized the likelihood function  $\mathcal{L}_{\text{PWD}}$  with respect to the free fit parameters.

### 1443 Likelihood Function

1444 First, we formulate the likelihood function  $\mathcal{L}_{\text{PWD}}^{(i)}$  for a single data set. This likelihood function  
 1445 is the joint probability density function of the measured events in the given  $(m_{K\pi\pi}, t')$  cell, which  
 1446 is the product of the probability density functions of the single events. The probability density  
 1447 function of a single event is proportional to the density of the measured number of events in the  
 1448 kinematic variables  $\tau, m_{K\pi\pi}, t'$  as given in equation (5.27) and reads

$$\begin{aligned} p^{(i)}(\tau; m_{K\pi\pi}, t') &= \frac{\Phi_3(\tau; m_{K\pi\pi}) \eta^{(i)}(\tau, m_{K\pi\pi}, t') \hat{r}^{(i)}(m_{K\pi\pi}, t') \mathcal{I}(\tau, m_{K\pi\pi}, t')}{\int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' d\tau \Phi_3(\tau; m_{K\pi\pi}) \eta^{(i)}(\tau, m_{K\pi\pi}, t') \hat{r}^{(i)}(m_{K\pi\pi}, t') \mathcal{I}(\tau, m_{K\pi\pi}, t')} \\ &= \frac{\Phi_3(\tau; m_{K\pi\pi}) \eta^{(i)}(\tau, m_{K\pi\pi}, t') \hat{r}^{(i)}(m_{K\pi\pi}, t') \mathcal{I}(\tau, m_{K\pi\pi}, t')}{\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')}. \end{aligned} \quad (5.32)$$

<sup>[S]</sup> In the Chung-Trueman parameterization of the spin-density matrix, some transition amplitudes are zero and some are real-valued by construction.

1449 Here, we express the probability density for an explicit choice for the phase-space variables  
 1450  $\tau$  using  $d\Phi_3 = d\tau\Phi_3(\tau; m_{K\pi\pi})$ , where  $\Phi_3(\tau; m_{K\pi\pi})$  is the density of states in the phase-space,  
 1451 which includes the Jacobian term that arises from the choice of variables. Interestingly, the  
 1452 normalization integral, which appears in the denominator in equation (5.32), equals to the  
 1453 predicted number of measured events for the given  $(m_{K\pi\pi}, t')$  cell in equation (5.28).

1454 The intensity model enters linear in the numerator and the denominator of equation (5.32) and  
 1455 the transition amplitudes appear quadratic in the intensity model in equation (5.16). Hence,  
 1456  $p^{(i)}(\tau; m_{K\pi\pi}, t')$  is invariant under a multiplication of all transition amplitudes by a common con-  
 1457 stant, i.e.  $\mathcal{T}_a^z(m_{K\pi\pi}, t') \rightarrow c\mathcal{T}_a^z(m_{K\pi\pi}, t')$ . The same holds for the data-set fraction  $\hat{r}^{(i)}(m_{K\pi\pi}, t')$ .

1458 To fix the scale of the transition amplitudes and the data-set fraction,<sup>[1]</sup> the extended maximum-  
 1459 likelihood formalism is used. The corresponding extended likelihood function reads

$$\mathcal{L}_{\text{PWD}}^{(i)}(m_{K\pi\pi}, t') = \frac{\left[\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')\right]^{\bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')} e^{-\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')}}{\bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')!} \prod_{k=1}^{\bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')} p^{(i)}(\tau^k; m_{K\pi\pi}^k, t'^k). \quad (5.33)$$

1460 The fraction in equation (5.33) is the Poisson probability to actually measure  $\bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')$  events  
 1461 given that we expect  $\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')$  events according to equation (5.28).

1462 Inserting equation (5.32) in equation (5.33) yields

$$\begin{aligned} \mathcal{L}_{\text{PWD}}^{(i)}(m_{K\pi\pi}, t') &= \frac{e^{-\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')}}{\bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')!} \left[\hat{r}^{(i)}(m_{K\pi\pi}, t')\right]^{\bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')} \\ &\times \prod_{k=1}^{\bar{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')} \Phi_3(\tau^k; m_{K\pi\pi}^k) \eta^{(i)}(\tau^k, m_{K\pi\pi}^k, t'^k) \mathcal{I}(\tau^k, m_{K\pi\pi}^k, t'^k). \end{aligned} \quad (5.34)$$

1463 Here, the facts are used that the denominator of the probability density in equation (5.32) cancels  
 1464 with the  $\left[\widehat{N}_{\text{ev}}^{(i)}\right]^{\bar{N}_{\text{ev}}^{(i)}}$  term of the Poisson probability and that the data-set fraction is the same for all  
 1465 events within one  $(m_{K\pi\pi}, t')$  cell.

1466 As the data sets are independent, the total likelihood is the product of the likelihoods of the  
 1467 individual data sets, i.e.

$$\mathcal{L}_{\text{PWD}}(m_{K\pi\pi}, t') = \prod_{(i)} \mathcal{L}_{\text{PWD}}^{(i)}(m_{K\pi\pi}, t'). \quad (5.35)$$

<sup>[1]</sup> The transition amplitudes and the data-set fraction have two independent scales to be fixed, while the extended maximum-likelihood formalism gives only one constraint. The other constraint is given by the normalization condition of the data-set fraction parameters according to equation (5.26). This is discussed below in detail for multiple data sets.

1468 Instead of maximizing  $\mathcal{L}_{\text{PWD}}$ , it is numerically more stable to minimize the negative log-  
 1469 likelihood

$$-\ln \mathcal{L}_{\text{PWD}}(m_{K\pi\pi}, t') = -\sum_{(i)} \ln \mathcal{L}_{\text{PWD}}^{(i)}(m_{K\pi\pi}, t'). \quad (5.36)$$

1470 Inserting equation (5.34) into equation (5.36) yields

$$-\ln \mathcal{L}_{\text{PWD}}(m_{K\pi\pi}, t') = -\sum_{(i)} \left\{ -\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') - \ln [\overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')!] \right. \\
 + \overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') \ln [\hat{r}^{(i)}(m_{K\pi\pi}, t')] \\
 \left. + \sum_{k=1}^{\overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')} \ln [\Phi_3(\tau^k; m_{K\pi\pi}^k) \eta^{(i)}(\tau^k, m_{K\pi\pi}^k, t'^k) \mathcal{I}(\tau^k, m_{K\pi\pi}^k, t'^k)] \right\}. \quad (5.37)$$

1471 We can split this into multiple sub-terms

$$-\ln \mathcal{L}_{\text{PWD}}(m_{K\pi\pi}, t') = -\sum_{(i)} \left\{ \overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') \ln [\hat{r}^{(i)}(m_{K\pi\pi}, t')] - \widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') \right\} \\
 - \sum_{(i)} \sum_{k=1}^{\overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')} \ln [\mathcal{I}(\tau^k, m_{K\pi\pi}^k, t'^k)] \\
 + \sum_{(i)} \ln [\overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')!] \\
 - \sum_{(i)} \sum_{k=1}^{\overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')} \ln [\Phi_3(\tau^k; m_{K\pi\pi}^k) \eta^{(i)}(\tau^k, m_{K\pi\pi}^k, t'^k)]. \quad (5.38)$$

1472 The first line (blue) in equation (5.38) represents the  $N_{\text{dataset}}$  conditions arising from the Poisson  
 1473 terms of the extended maximum-likelihood ansatz. Together with the normalization condition for  
 1474 the data-set fraction in equation (5.26),<sup>[u]</sup> they constrain the  $N_{\text{dataset}}$  data-set fraction parameters  
 1475 and the absolute common scale of the transition amplitudes.

1476 The second line (orange) in equation (5.38) takes into account the distribution of the data in the  
 1477  $K^-\pi^-\pi^+$  phase space. It constrains the transition amplitudes.

1478 The last two lines (green) do not contain any free fit parameters. Hence, they are constant in the  
 1479 likelihood maximization and can be dropped. Especially noteworthy, the experimental acceptance  
 1480 for each of the measured events  $\eta^{(i)}(\tau^k, m_{K\pi\pi}^k)$ , which is computationally very expensive to  
 1481 calculate, can be dropped. The experimental acceptance enters only via the calculation of

<sup>[u]</sup> We implemented the normalization condition for the data-set fraction parameters by allowing for only  $(N_{\text{dataset}} - 1)$  free data-set fraction parameters, while one data-set fraction parameter is calculated for each iteration from the  $(N_{\text{dataset}} - 1)$  free data-set fraction parameters using equation (5.26).



1482  $\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')$  via the acceptance-integral matrices in equation (5.29). Thus, the acceptance does  
 1483 not need to be calculated for each measured event in the PWD fit, but only the acceptance-  
 1484 integral matrix has to be calculated using Monte Carlo integration techniques. Furthermore, the  
 1485 acceptance-integral matrix does not contain any free fit parameters and can thus be calculated  
 1486 before the PWD fit. This drastically reduces the computational costs of evaluating the negative  
 1487 log-likelihood. Still, the computational costs for all PWD fits performed in this analysis are of  
 1488 the order of a million CPUh. Also, the  $K^-\pi^-\pi^+$  phase-space  $\Phi_3(\tau; m_{K\pi\pi})$ , which incorporates  
 1489 the Jacobian from the explicit choice of the set of phase-space variables, can be dropped.

## 1490 PWD Fit Procedure

1491 In order to obtain the maximum-likelihood estimates for the transition amplitudes and data-set  
 1492 fractions, the negative log-likelihood function in equation (5.38) is minimized dropping the  
 1493 constant terms shown in green.<sup>[v]</sup>

1494 The start-parameter values for the transition amplitudes and data-set fraction are generated in two  
 1495 steps. In the first step, values for the real and imaginary parts of the transition amplitudes are ran-  
 1496 domly drawn from a uniform distribution in the range from  $-\sqrt{\widehat{N}_{\text{ev}}(m_{K\pi\pi}, t')}$  to  $\sqrt{\widehat{N}_{\text{ev}}(m_{K\pi\pi}, t')}$ .  
 1497 In the second step, the data-set fractions and the absolute scale of the transition amplitudes are  
 1498 calculated such that  $\widehat{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t') = \overline{N}_{\text{ev}}^{(i)}(m_{K\pi\pi}, t')$  based on the transition amplitudes that were  
 1499 obtained in the first step. This second step turned out to be mandatory in the case of fitting  
 1500 multiple data sets in order to achieve a stable fit that reliably finds the parameter values that  
 1501 correspond to the smallest negative log-likelihood value. Fits without this second step get easily  
 1502 trapped in local minima of the likelihood function far away from the physical solution.

### 1503 5.1.4 Dynamic Amplitudes of the Isobars

1504 So far, we introduced in sections 5.1.1 to 5.1.3 the well-established PWD formalism. Before  
 1505 being able to perform a PWD fit to our  $K^-\pi^-\pi^+$  sample, an explicit PWD model has to be  
 1506 constructed. We discuss the construction of the wave set and extensions of the PWD formalism  
 1507 that are special to this analysis in sections 5.2 to 5.4. Important choices when formulating an  
 1508 explicit PWD model are the employed parameterizations for the dynamic amplitudes of the  
 1509 isobar resonances. For most of the isobar resonances considered in this analysis, we used a  
 1510 relativistic Breit-Wigner amplitude [see equation (5.39) below]. However, the  $K\pi$  and  $\pi\pi$   $S$ -wave  
 1511 amplitudes are not approximated well by Breit-Wigner amplitudes.

1512 For the  $\pi\pi$   $S$ -wave amplitude, we used the same approach as in the COMPASS  $\pi^-\pi^-\pi^+$  analy-  
 1513 sis [39]. The  $\pi\pi$   $S$ -wave amplitude contains dominantly three poles: the  $f_0(500)$ , the  $f_0(980)$ ,

<sup>[v]</sup> As minimizer, we used the low-memory BFGS (LBFGS) [82–84] implementation of the NLOpt package [85]. This algorithm approximates the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm [86–89] and is a quasi-Newton method that was designed to have a low memory requirement.

1514 and the  $f_0(1500)$ . The couplings of each of these three poles to the total amplitude are different  
 1515 for different intermediate states  $X^-$  that decay to the  $\pi\pi$   $S$ -wave system. Therefore, we separated  
 1516 the total  $\pi\pi$   $S$ -wave amplitude into three independent partial waves, each with its own transition  
 1517 amplitude: (i) The  $f_0(1500)$  is parameterized by a relativistic Breit-Wigner amplitude [see equa-  
 1518 tion (5.39) below], (ii) the  $f_0(980)$  is parameterized by the so-called Flatté parameterization [see  
 1519 equation (5.43) below], (iii) the “remaining” broad  $\pi\pi$   $S$ -wave component [see equation (5.44)  
 1520 below], which contains the  $f_0(500)$ .

1521 Analogously to the  $\pi\pi$   $S$ -wave amplitude, the  $K\pi$   $S$ -wave amplitude contains dominantly three  
 1522 poles: the  $K_0^*(700)$ , the  $K_0^*(1430)$ , and the  $K_0^*(1950)$ . However, in contrast to the  $\pi\pi$   $S$ -wave  
 1523 amplitude, where the small width of the  $f_0(980)$  allows us to separate it from the broad  $\pi\pi$   
 1524  $S$ -wave component, the larger width of the  $K_0^*(1430)$  prohibits such an approach for the  $K\pi$   
 1525  $S$ -wave amplitude. Therefore, we present below an alternative approach to simultaneously take  
 1526 into account all three poles [see equations (5.50) and (5.51) below].

### 1527 Relativistic Breit-Wigner Amplitude

1528 In this analysis, we used a relativistic Breit-Wigner amplitude [46, 90] of the form

$$\mathcal{D}_{\text{BW}}(m; m_0, \Gamma_0) = \frac{m_0 \Gamma_0}{m^2 - m_0^2 - i m_0 \Gamma(m)}, \quad (5.39)$$

1529 where  $m_0$  and  $\Gamma_0$  are the nominal mass and width of the resonance, respectively. The mass-  
 1530 dependent width is modeled by the sum over the decay channels  $i$

$$\Gamma(m) = \sum_i \Gamma_i(m) = \sum_i \Gamma_i \frac{q_i(m)}{m} \frac{m_0}{q_i(m_0)} \frac{F_{L_0}^2(m)}{F_{L_0}^2(m_0)}, \quad (5.40)$$

1531 which takes into account the opening of the phase-space for the decay channel  $i$  in the two-body  
 1532 approximation. The two-body break-up momentum,

$$q_i(m) = q(m, m_1, m_2) = \frac{\sqrt{[m^2 - (m_1 + m_2)^2][m^2 - (m_1 - m_2)^2]}}{2m}, \quad (5.41)$$

1533 is given by the masses  $m_1$  and  $m_2$  of the daughter particles.  $F_{L_0}(m)$  is the centrifugal barrier factor  
 1534 as used in the decay amplitudes, where  $L_0$  is the orbital angular momentum between the daughter  
 1535 particles. The partial decay widths  $\Gamma_i$  sum up to the total decay width, i.e.  $\Gamma_0 = \sum_i \Gamma_i$ .

1536 For the parameterizations of the dynamic amplitudes of isobars, we included in the sum in  
 1537 equation (5.40) only the  $K^- \pi^+$  or the  $\pi^- \pi^+$  decay channel, depending on the isobar, such that

$$\Gamma(m) = \Gamma_0 \frac{q(m)}{m} \frac{m_0}{q(m_0)} \frac{F_{J_\xi}^2(m)}{F_{J_\xi}^2(m_0)}. \quad (5.42)$$

1538 As the final-state particles are spin less, the orbital angular momentum between them equals to  
 1539 the isobar spin, i.e.  $L_0 = J_\xi$ . The mass  $m_0$  and width  $\Gamma_0$  of the isobar resonances are taken from  
 1540 the PDG [91].<sup>[w]</sup>

#### 1541 Flatté Parameterization for the $f_0(980)$

1542 The  $f_0(980)$  is very close in mass to the  $K\bar{K}$  threshold, which leads to strong deviations  
 1543 of the amplitude from a Breit-Wigner shape. To take this into account, we employed the  
 1544 Flatté parameterization [93] for the  $f_0(980)$  isobar using the formula and the parameters deter-  
 1545 mined by BESIII [94]

$$\mathcal{D}_{\text{Flatté}}(m) = \frac{1}{m_0^2 - m^2 - i(g_{\pi\pi} \varphi_2^{\pi\pi}(m) + g_{K\bar{K}} \varphi_2^{K\bar{K}}(m))}. \quad (5.43)$$

1546 Here, the  $\varphi_2^i(m)$  are the two-body phase spaces terms for the two decay channels  $i = \pi\pi$  and  
 1547  $i = K\bar{K}$  that are analytically continued below the threshold where they become complex-valued,  
 1548 and the  $g_i$  are the couplings.

#### 1549 AMPK Parameterization for the Broad $\pi\pi$ $S$ -Wave Component

1550 The broad  $\pi\pi$   $S$ -wave component, which contains the  $f_0(500)$  is parameterized following the  
 1551 ansatz suggested by the VES collaboration [95]. The so-called  $M$  solution obtained from  
 1552 analyzing  $\pi\pi \rightarrow \pi\pi$  scattering and defined by equations (3.15) and (3.20) in ref. [96] provides a  
 1553 parameterization of the  $\pi\pi$   $S$ -wave amplitude, which also includes the  $f_0(980)$  pole. In order to  
 1554 remove the  $f_0(980)$  from this amplitude, the parameters  $f_1^1, f_2^1, f_1^3, c_{11}^4$ , and  $c_{22}^4$  and all diagonal  
 1555 elements of the  $M$  matrix were set to zero. Finally, we used the  $\pi\pi \rightarrow \pi\pi$  element of the  $T$ -matrix  
 1556 ( $T_{11}$ ) defined in equation (3.15) in ref. [96] as the amplitude for the broad  $\pi\pi$   $S$ -wave component  
 1557 called  $[\pi\pi]_S^{\text{AMPK}}$ :

$$\mathcal{D}_{\text{AMPK}}(m) = T_{11}(m). \quad (5.44)$$

1558 Figure 5.4 illustrates the intensity and the real and imaginary parts of this amplitude.

#### 1559 Palano-Pennington Parameterization for the $K\pi$ $S$ -Wave

1560 A variety of elaborate models for the  $K\pi$   $S$ -wave amplitude are on the market [97–101]. However,  
 1561 many of them suffer from covering only a limited mass range, typically up to at most  $1.5 \text{ GeV}/c^2$ .  
 1562 However, analyzing an  $m_{K\pi\pi}$  range up to  $3 \text{ GeV}/c^2$  demands a  $K\pi$   $S$ -wave amplitude that is  
 1563 valid up to  $m_{K\pi\pi} \approx 2.9 \text{ GeV}/c^2$ . We tried different parameterizations such as the classic LASS

<sup>[w]</sup> For some resonances, the PDG lists more than one average value. The masses and widths that were used in these cases are listed in ref. [92].

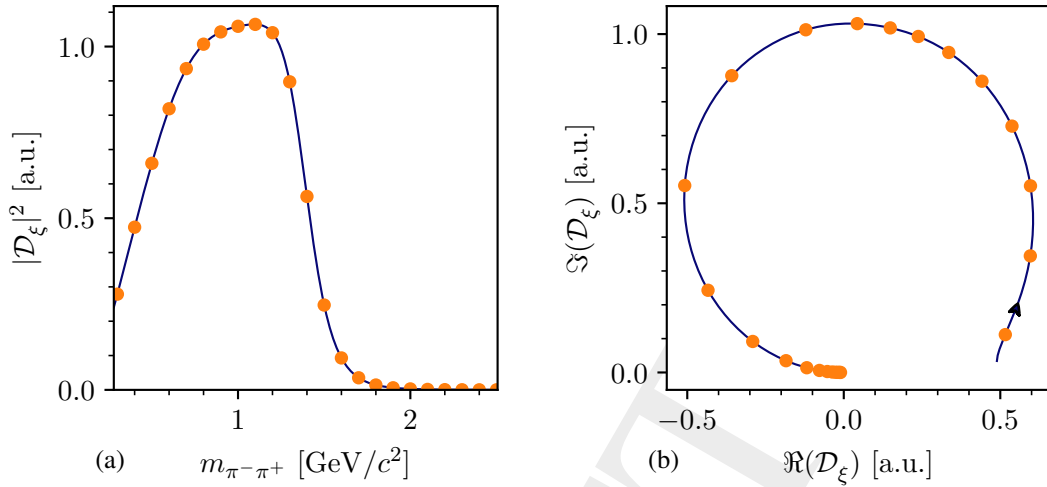


Figure 5.4: Dynamic amplitude of the  $[\pi\pi]_S^{\text{AMPK}}$  isobar. (a) shows the intensity as a function of  $m_{\pi^-\pi^+}$ , (b) shows the Argand diagram, i.e. real vs. imaginary part of the dynamic amplitude of the  $[\pi\pi]_S^{\text{AMPK}}$  isobar. The orange dots in the Argand diagram are drawn at the same  $m_{\pi^-\pi^+}$  values as the corresponding orange dots in the intensity spectrum. The black arrow indicates the direction of increasing  $m_{\pi^-\pi^+}$ . Figure 10 in ref. [39], which also shows the dynamic amplitude of the  $[\pi\pi]_S^{\text{AMPK}}$  isobar, is wrong due to a mistake. Here, we show the correct amplitude.

1564 parameterization [97] with parameters taken from ref. [102] and the generalized LASS (GLASS)  
 1565 parameterization [99] with parameters taken from ref. [103]. At the end we obtained the best  
 1566 results in terms of likelihood and in terms of fit stability using an approach that simultaneously  
 1567 takes into account all three  $K_0^*$  poles as explained in detail in the following.

1568 The scattering amplitude for the process  $i \rightarrow f$ , e.g.  $K\pi \rightarrow K\pi$  or  $K\eta \rightarrow K\pi$ , can be described in  
 1569 terms of the  $T$  matrix. If the final state  $f$  is not produced in a scattering process, but in the decay  
 1570 of a heavier state, as in our case, the decay amplitude  $F_f$  can be written in terms of the  $Q$  vector  
 1571 equation

$$F_f(m) = \sum_i T_{if}(m) Q_i(m), \quad (5.45)$$

1572 where  $m$  is the invariant mass of the initial and final state.  $Q_i$  represents the production of the  
 1573 intermediate state  $i$  in the decay, which then rescatters to the final state  $f$ . The rescattering is  
 1574 expressed by the  $T$ -matrix element  $T_{if}$ . The  $T$  matrix is independent of the process. Thus, it can  
 1575 be determined from other experiments, e.g. from  $K\pi \rightarrow K\pi$  scattering experiments, and used  
 1576 as input here. Typically, the elements  $Q_i(m)$  are parameterized by polynomials in  $m^2$ , with the  
 1577 leading term being constant. Using equation (5.45) as isobar parameterizations in equation (5.9)  
 1578 and taking into account only the leading term  $Q_i(m) \approx \text{const}$ , allows us to merge the sum  $\sum_i$  in  
 1579 equation (5.45) and the sum  $\sum_a$  over different waves in equation (5.16). Hence, the different  
 1580 states  $i$  can be interpreted as independent partial waves. The constants  $Q_i$  can be absorbed  
 1581 into the transition amplitudes of the waves with the dynamic isobar amplitudes given by the  
 1582 corresponding  $T$ -matrix element  $T_{if}$ .

1583 We took the  $T$ -matrix elements from a two-channel  $K$ -matrix parameterization in ref. [100], with  
 1584 the two channels  $1 = K\pi$  and  $2 = K\eta$ . One should note that despite  $K\eta$  is in principle the first  
 1585 inelastic channel, it is well known from measurements that the inelasticity actually starts at the  
 1586 higher-lying threshold of the  $K\eta'$  channel. Therefore, the second channel should be interpreted  
 1587 as an effective inelastic channel, in addition to  $K\pi$ .

1588 We shortly recapitulate the most important formulas here.<sup>[x]</sup> The  $T$ -matrix elements relevant for  
 1589 the  $K\pi$  final state read in terms of the  $K$ -matrix elements  $K_{ij}$ :

$$T_{11} = \frac{K_{11} - i\varphi_2^2 \det K}{\delta}, \quad \text{and} \quad T_{21} = T_{12} = \frac{K_{12}}{\delta}. \quad (5.46)$$

1590 Here,  $\det K = K_{11}K_{22} - K_{12}^2$ ,  $\varphi_2^i$  is the two-body phase space for the channel  $i$ , analytically  
 1591 continued for energies below the corresponding threshold, and<sup>[y]</sup>

$$\delta = 1 - i\varphi_2^1 K_{11} - i\varphi_2^2 K_{22} - \varphi_2^1 \varphi_2^2 \det K. \quad (5.47)$$

1592 The  $K$ -matrix elements are parameterized by a sum of two poles at  $s_a$  and  $s_b$  and a third-order  
 1593 polynomial:

$$K_{ij} = \frac{(s - s_A)}{s_{K\pi}} \left[ \sum_{\alpha=a,b} \frac{g_i^\alpha g_j^\alpha}{s_\alpha - s} + \sum_{n=0}^3 C_{ij,n} X^n \right], \quad (5.48)$$

1594 where

$$X = \frac{2s - (s_{\text{top}} + s_{\text{bot}})}{s_{\text{top}} - s_{\text{bot}}} \quad (5.49)$$

1595 depends on  $s = m^2$ . The parameters  $s_{K\pi} = m_K^2 + m_\pi^2$ ,  $s_A = 0.87753 s_{K\pi}$ ,  $s_{\text{top}} = 5.832 \text{ GeV}^2$ , and  
 1596  $s_{\text{bot}} = 0.36 \text{ GeV}^2$  are fixed. The remaining parameters were determined in ref. [100] by a fit to  
 1597 scattering data from LASS [97] and Estabrooks et. al. [104] and to BaBar data on the decay  
 1598  $\eta_c \rightarrow \bar{K}K\pi$  [105] (see TABLE I in ref. [100]).

1599 Finally, the two dynamic functions included in the PWD are

$$\mathcal{D}_{[K\pi]_S^{K\pi}}(m) = T_{11}(s = m^2) \quad (5.50)$$

$$\mathcal{D}_{[K\pi]_S^{K\eta}}(m) = T_{12}(s = m^2). \quad (5.51)$$

1600 Figures 5.5 and 5.6 show the isobar dynamic amplitudes in the  $m_{K-\pi^+}$  range relevant for this  
 1601 analysis.

1602 The  $T_{11}$  element as determined in ref. [100] exhibits an unphysical behavior in the mass region  
 1603 above  $2.5 \text{ GeV}/c^2$  as there are no experimental data to constrain the amplitude in this region.  
 1604 Thus, we set both amplitudes  $\mathcal{D}_{[K\pi]_S^{K\pi}}(m) = 0$  and  $\mathcal{D}_{[K\pi]_S^{K\eta}}(m) = 0$  above  $m = 2.4 \text{ GeV}/c^2$ .

<sup>[x]</sup> There are some known typos in the formulas of ref. [100], which are corrected here.

<sup>[y]</sup> In ref. [100],  $\Delta$  was used instead of  $\delta$ .

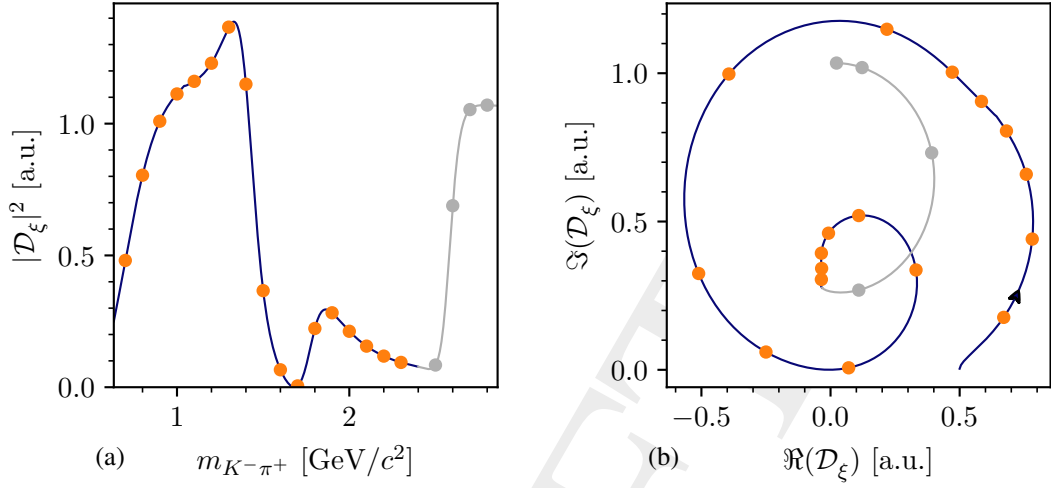


Figure 5.5: Same as figure 5.4, but showing the dynamic amplitude of the  $[K\pi]_S^{K\pi}$  isobar. The gray lines and points are the extrapolation beyond the region where we set the amplitude to zero.

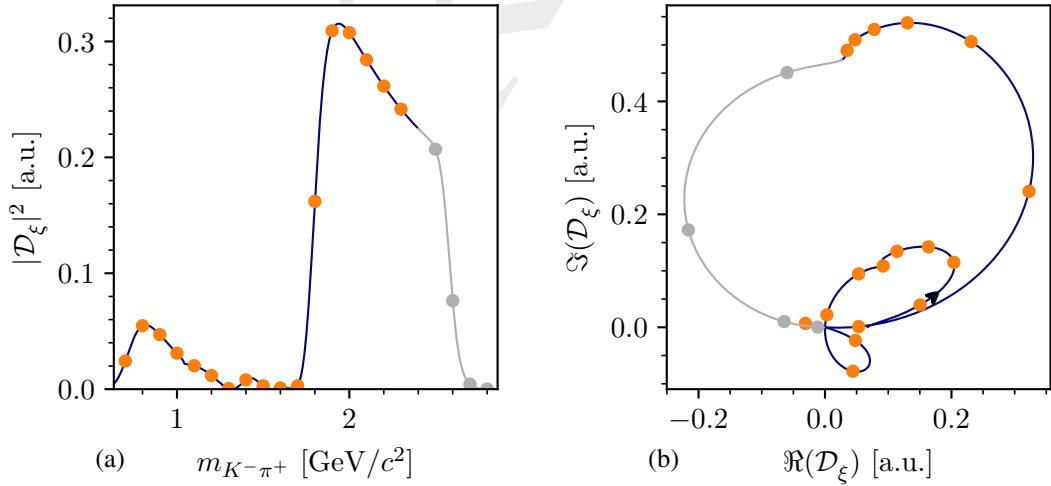


Figure 5.6: Same as figure 5.4, but showing the dynamic amplitude of the  $[K\pi]_S^{K\eta}$  isobar. The gray lines and points are the extrapolation beyond the region where we set the amplitude to zero.

## 5.2 Wave-Set Selection

In principle there is an infinite number of possible partial waves that may contribute to the data, e.g. as the spins and orbital angular momenta can take any integer number. Not all of these partial waves might be realized in reality and not all of the realized partial waves might contribute significantly to the  $K^- \pi^- \pi^+$  sample such that they can be resolved with the given precision of the measured data.<sup>[z]</sup> As we measured only a finite amount of data and only a finite amount of computing resources is available, we have to truncate the sum over partial waves in the intensity model in equation (5.16) by selecting a certain set of partial waves, the so-called wave set, that we include in the model. On the one hand, a too large wave set causes overfitting in the PWD fit, because the number of fit parameters is approximately proportional to the number of partial waves included in the wave set. Overfitting can lead to findings in the PWD that arise from noise in the data [106]. This is an issue especially in amplitude analysis like the PWD, because the coherent sum squared over complex-valued amplitudes like in equation (5.16) introduces non-linear effects in the model. For example, two or more amplitudes may destructively interfere with each other. Such a destructive interference may lead to large artificial enhancements of the interfering amplitudes, while it leads to only a small change in the total model intensity and thus to only a small change in description of the data, which may be misused to describe noise in the data. In addition, an overfitted model is less robust against systematic effects, e.g. from background processes like  $K^- + p \rightarrow K^- K^- K^+ + p$  that also entered the  $K^- \pi^- \pi^+$  sample (see section 4.2). On the other hand, a too small wave set, i.e. a wave set that is missing waves that significantly contribute to the data, may lead to artifacts in the results of the PWD, because it leaves structures in the data that arise from the missed waves undescribed. These structures might be partly accounted for in the PWD fit by the waves that are included in the wave set. This might lead to artificial structures in these waves. Additionally, the missed waves may contain interesting physics signals that we would miss. As we present in this work the so-far world's largest sample of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , we are especially interested in such weak signal that were not seen before. Therefore, the goal of the wave-set selection is to find a minimal wave set that is sufficient to describe all significant structures in the  $K^- \pi^- \pi^+$  sample.

Traditionally, these wave sets had been constructed by hand in the following iterative process. Starting from a wave set constructed based on previous knowledge, partial waves are manually added or removed. Then, the result of a PWD of these modified wave sets is studied. Based on pre-defined criteria the modified wave set is accepted or rejected. Such a criterion can be whether a newly added wave shows “significant intensity”. Also, likelihood-ratio tests are used to decide whether removing a wave leads to a similar good description of the data such that the wave set without the corresponding wave can be accepted. This procedure of adding and removing waves is repeated until a “good enough” wave set is found. Following this approach potentially introduces observer bias. The selection of waves that are added or removed is a personal choice,

<sup>[z]</sup> In addition to the diffractive scattering reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , for which the partial waves were constructed in section 5.1.2, there are other processes, e.g. Deck-like reactions (see section 2.1.1) or incoherent background from reactions like  $K^- + p \rightarrow K^- K^- K^+ + p$ , that also contribute to the  $K^- \pi^- \pi^+$  sample. As the partial waves were not constructed to describe these processes, their contribution in the  $K^- \pi^- \pi^+$  sample projects in principle to all partial waves, but not all of these projections contribute significantly to the data.

1642 because not all possible combinations of adding and removing waves can be tested. This holds  
 1643 especially for partial-wave analyses, where the contribution of a partial wave to the data is caused  
 1644 not only by its own intensity, but also by its interference with other partial waves [107]. A partial  
 1645 wave may become significant only when it is added together with other waves. Also, often the  
 1646 decisions when to accept or reject a wave and when to stop the procedure is taken based on  
 1647 subjective criteria, which are hard to quantify and thus hard to reproduce.

1648 In this work, we minimized this potential observer bias by inferring the wave set from data.  
 1649 Various techniques exist for construction optimal models that consist of sets of individual  
 1650 components, e.g. in our case partial-waves. These model-selection techniques have applications  
 1651 also in other fields, e.g. in machine learning. They all have in common that they select an  
 1652 optimal subset of model components that is sufficient to describe the data from a large pool of  
 1653 potentially possible components. Such a method was first applied to partial-wave analyses in  
 1654 ref. [107]. At COMPASS, such methods were applied in the analysis of the reaction  $\pi^- + p \rightarrow$   
 1655  $\pi^- \pi^- \pi^- \pi^+ \pi^+ + p$  [67] and  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  [43, 108]. They all share the same idea. First, a  
 1656 large set of waves, the so-called wave pool, is systematically constructed by including all waves  
 1657 that are expected to potentially contribute to the data (see section 5.2.1). In the second step, the  
 1658 so-called wave-set selection fit, the data are fitted using the whole wave pool. However, using  
 1659 the likelihood in equation (5.38) would lead to massive overfitting, as the wave pool is typically  
 1660 much larger than the wave set needed to describe the data. In order to circumvent overfitting,  
 1661 regularization techniques are applied to the wave-set selection fit, with the goal to suppress  
 1662 insignificant waves (see section 5.2.2). In the third step, the waves that acquire significant  
 1663 intensity in the wave-set selection fit are selected for the wave set (see section 5.2.5). In the  
 1664 final step, the set of selected waves is fitted to the data, without regularization. This fit yields  
 1665 the final results for the PWD (see section 5.5). Applying this approach to each  $(m_{K\pi\pi}, t')$  cell  
 1666 yields an individual wave set for each cell. Due to the finite amount of measured data, there  
 1667 are fluctuations of the wave set between neighboring  $(m_{K\pi\pi}, t')$  cells. Such fluctuations can be  
 1668 suppressed by impose a continuity criterion in the wave-set selection (see section 5.2.3).

### 1669 5.2.1 Construction of the Wave Pool

1670 As a starting point for the wave-set selection, we had to construct a pool of partial waves that  
 1671 on the one hand contains all waves that potentially contribute significantly to our data, but that  
 1672 on the other hand is still manageable in size. In order to avoid bias from the construction of  
 1673 the wave pool, we considered large ranges of the partial-wave quantum numbers. We included  
 1674 partial-waves with spin  $J \leq 7$  and orbital angular-momentum  $L \leq 7$ . We considered only waves  
 1675 with positive reflectivity<sup>[aa]</sup> and with spin projections  $M = 0, 1, 2$ . Finally, we considered twelve  
 1676 isobars that are known to decay to the  $\pi^- \pi^+$  and  $K^- \pi^+$  final state [91], six in the  $\pi^- \pi^+$  subsystem  
 1677 and six in the  $K^- \pi^+$  subsystem. They are listed in table 5.2.

---

<sup>[aa]</sup> Due to the high beam momentum, we assumed that production via Pomeron exchange dominates our data, which produces only positive-reflectivity waves (see section 5.1). Also, in a wave-set selection study including negative-reflectivity waves, none of the negative-reflectivity waves picked up significant intensity.



Table 5.2: Two-body isobars included in the systematic construction of the wave pool. The first row shows the quantum numbers. The second row gives the name of the isobar resonance. The third row gives the parametrization used in the PWD model.

$J_{\xi}^{PC}$	0 <sup>++</sup>		1 <sup>--</sup>	2 <sup>++</sup>	3 <sup>--</sup>	
$\pi^{-}\pi^{+}$ isobars	$[\pi\pi]_S^{\text{AMPK}}$	$f_0(980)$	$f_0(1500)$	$\rho(770)$	$f_2(1270)$	$\rho_3(1690)$
Amplitude	section 5.1.4	(5.43)	(5.39)	(5.39)	(5.39)	(5.39)
$J_{\xi}^P$	0 <sup>+</sup>		1 <sup>-</sup>		2 <sup>+</sup>	3 <sup>-</sup>
$K^{-}\pi^{+}$ isobars	$[K\pi]_S^{K\pi}$	$[K\pi]_S^{K\eta}$	$K^*(892)$	$K^*(1680)$	$K_2^*(1430)$	$K_3^*(1780)$
Amplitude	(5.50)	(5.51)	(5.39)	(5.39)	(5.39)	(5.39)

1678 Within these weak limitations, we included all combinations of quantum numbers and isobars  
1679 that are allowed by the conservation laws of strong interaction. This resulted in a large wave pool  
1680 of 596 partial waves plus the incoherent flat wave to be fitted to the data. The pool of considered  
1681 partial waves is much larger than the wave set constructed by hand in the ACCMOR analysis [23],  
1682 which consisted of only 21 waves with  $J \leq 2$  and  $L \leq 2$ . Compared to other analyses that applied  
1683 wave-set selection techniques, the challenge in the analysis presented here is to determine the  
1684 wave set from a large wave pool with only a limited amount of data. The wave pool in ref. [107]  
1685 consisted of only 40 waves. In the COMPASS  $\pi^{-}\pi^{-}\pi^{+}$  analysis we used a wave-pool of similar  
1686 size, but the  $\pi^{-}\pi^{-}\pi^{+}$  sample is about 100 times larger than the  $K^{-}\pi^{-}\pi^{+}$  sample analyzed in this  
1687 work.<sup>[ab]</sup>

1688 Assuming that the  $K^{-}\pi^{-}\pi^{+}$  sample is dominated by high-energy diffractive scattering, which is  
1689 a coherent process,<sup>[ac]</sup> we used a rank=1 model for the wave-selection fit, i.e. we use a PWD  
1690 model with a rank=1 spin-density matrix as discussed in section 5.1.2. The number of 1194 free  
1691 parameters<sup>[ad]</sup> of the PWD model is small enough to be determined by the limited amount of  
1692 data and also technically manageable.<sup>[ae]</sup>

<sup>[ab]</sup> In addition to the minimization of bias from the wave pool, another argument for constructing a larger wave pool is that we require the PWD model to be flexible enough to describe also background contributions to the  $K^{-}\pi^{-}\pi^{+}$  sample as discussed in section 5.3. This is a challenge especially in this work, where the expected background from other processes of about 10 % is large compared to, e.g., the COMPASS  $\pi^{-}\pi^{-}\pi^{+}$  analysis.

<sup>[ac]</sup> As discussed in section 5.1, spin flip of the target proton is suppressed at COMPASS energies.

<sup>[ad]</sup> The real and imaginary parts of the transition amplitudes of the 596 waves, with one of them being real-valued to account for the unknown global phase, plus a real-valued amplitude for the flat wave, plus two data-set fraction parameters, i.e.  $2 \cdot 596 - 1 + 1 + 2 = 1194$

<sup>[ae]</sup> A rank=3 model would have nearly three times the number of parameters as the rank=1 model.

1693 **5.2.2 Regularization of the Likelihood Function**

1694 Using the wave pool in a fit of equation (5.38) to the data would lead to massive overfitting, as  
 1695 the number of free parameters is larger than the number of events in some  $(m_{K\pi\pi}, t')$  cells. In  
 1696 order to avoid this, we used regularization methods. There are different approaches to implement  
 1697 regularization. Here, we added for each coherent sector<sup>[af]</sup>  $z$  and each partial wave  $a$  in the  
 1698 wave pool a so-called regularization term  $\ln \mathcal{L}_{\text{Reg}}$  to the log-likelihood that imposes a penalty on  
 1699  $|\mathcal{T}_a^z| \neq 0$ , i.e.<sup>[ag]</sup>

$$\ln \mathcal{L}'_{\text{WSS}} = \ln \mathcal{L}_{\text{PWD}} + \sum_{z,a} \ln \mathcal{L}_{\text{Reg}} [|\mathcal{T}_a^z|; \{p_{\text{Reg}}\}]. \quad (5.52)$$

1700 Here,  $\ln \mathcal{L}_{\text{PWD}}$  is the log-likelihood function of the PWD as defined in equation (5.38), which  
 1701 contains the information from the data sample and  $\{p_{\text{Reg}}\}$  represents the set of additional pa-  
 1702 rameters of the regularization term, which must be tuned. A wave that does not significantly  
 1703 contribute to the data has no support from  $\mathcal{L}_{\text{PWD}}$  and is therefore driven by the regularization  
 1704 term, which is designed to suppress this wave such that  $|\mathcal{T}_a^z| \rightarrow 0$ .

1705 Different forms for the regularization term are possible. We used the Cauchy regularization:

$$\ln \mathcal{L}_{\text{Reg}} [|\mathcal{T}_a^z|; \Gamma_a^z] = -\ln \left[ 1 + \frac{|\mathcal{T}_a^z|^2}{(\Gamma_a^z)^2} \right], \quad (5.53)$$

1706 which had been already applied successfully in the COMPASS analysis of the reaction  $\pi^- + p \rightarrow$   
 1707  $\pi^- \pi^- \pi^- \pi^+ \pi^+ + p$  [67]. Its free parameter  $\Gamma_a^z$  sets the scale for the magnitude of the transition  
 1708 amplitude and thereby the strength of the regularization. Figure 5.7a shows the shape of the  
 1709 Cauchy regularization term in the complex plane of a transition amplitude. The term has a  
 1710 maximum at  $|\mathcal{T}_a^z| = 0$ , as required to suppress insignificant waves.

1711 We also performed tests using a LASSO regularization<sup>[ah]</sup>, a ridge regression,<sup>[ai]</sup> or a combination  
 1712 of both. None gave satisfactory results. Either the intensities even of large and significant waves  
 1713 were heavily suppressed or the intensities of insignificant waves were not suppressed enough  
 1714 to perform a selection. We obtained similar results in the wave-set selection performed in the  
 1715 COMPASS  $\pi^- \pi^- \pi^+$  analysis [43]. We concluded, that LASSO regularization or ridge regression  
 1716 cannot handle well the large dynamic range of the partial-wave intensities of up to five orders  
 1717 of magnitude. However, in the Cauchy regularization the logarithm brings the intensities to a  
 1718 common scale on, which the regularization was performed. Furthermore, to study the systematic  
 1719 effects of the wave set on the results of the PWD we constructed another wave set using principles  
 1720 of information field theory as discussed in section 5.7.2.

<sup>[af]</sup> We used a rank=1 model with only one coherent sector for the 596 partial waves of the wave pool plus one sector containing the incoherent flat wave.

<sup>[ag]</sup> Here, we drop the  $m_{K\pi\pi}$  and  $t'$  dependence for simplicity.

<sup>[ah]</sup> LASSO regularization uses the following regularization term [109]:  $\ln \mathcal{L}_{\text{Reg}} [|\mathcal{T}_a^z|; \lambda] = -\lambda |\mathcal{T}_a^z|$ .

<sup>[ai]</sup> Ridge regression uses the following regularization term [110]:  $\ln \mathcal{L}_{\text{Reg}} [|\mathcal{T}_a^z|; \lambda] = -\lambda |\mathcal{T}_a^z|^2$ .

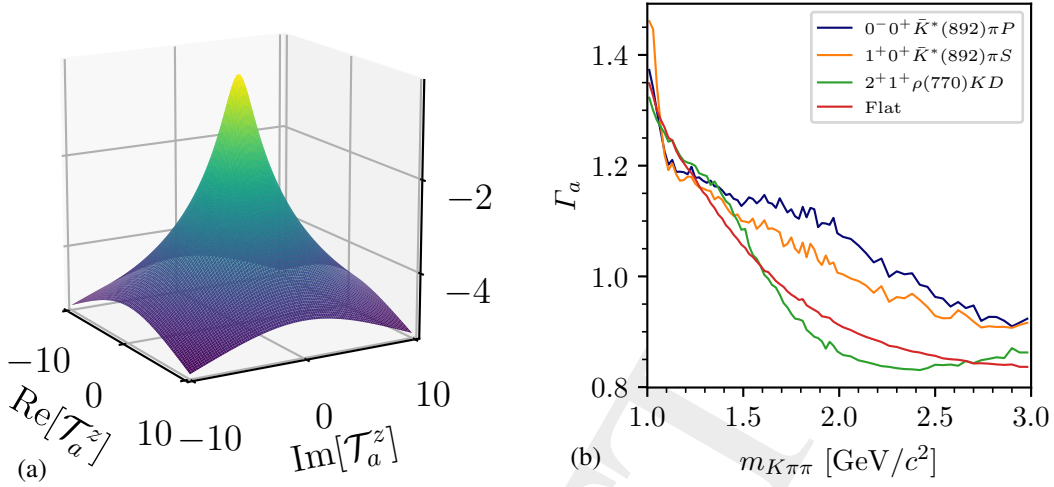


Figure 5.7: Properties of the Cauchy regularization term. (a) shows  $\ln \mathcal{L}_{\text{Reg}}$  in the complex plane of a transition amplitude  $\mathcal{T}_a^z$ . (b) shows the dependence of  $\Gamma_a$  on  $m_{K\pi\pi}$  defined in equation (5.56) for four selected partial waves in the lowest  $t'$  bin.

1721 Whether a wave is significant and hence should be included in the wave set depends on whether  
 1722 its intensity is large enough to be resolved with the given precision of our data. However, the  
 1723 partial-wave intensities corresponds to the produced number of events if the data would contain  
 1724 only the given wave, while the precision of the data depends on the total number of measured  
 1725 events. Therefore, the partial-wave intensity cannot be compared directly to the precision of  
 1726 the data, but acceptance effects have to be taken into account. As the acceptance is different for  
 1727 different partial waves,<sup>[aj]</sup> this requires a different scale parameter  $\Gamma_a^z$  in the Cauchy regularization  
 1728 term for each of the waves in the wave pool, which needs to be tuned. The same scale parameter  
 1729 can be used if the same wave appears in different coherent sectors  $z$ , i.e.  $\Gamma_a^z = \Gamma_a$ . In order to  
 1730 reduce this task to one common scale parameter for all waves, we applied the regularization  
 1731 penalty to the number,<sup>[ak]</sup>

$$\widehat{N}_a^z = |\mathcal{T}_a^z|^2 \bar{I}_{aa}, \quad (5.54)$$

1732 of measured events predicted for wave  $a$  by the model, i.e. the expected number of measured  
 1733 events if the data would contain only wave  $a$ . As  $\widehat{N}_a^z$  incorporates the acceptance effects it allowed  
 1734 us to use a common scale parameter  $\Gamma$  in the regularization, i.e.

$$\ln \mathcal{L}_{\text{Reg}} [|\mathcal{T}_a^z|; \Gamma] = -\ln \left[ 1 + \frac{\widehat{N}_a^z}{\Gamma^2} \right]. \quad (5.55)$$

<sup>[aj]</sup> As the acceptance is strongly modulated in the phase-space variables (see section 5.6), the average acceptance of a partial wave depends on the phase-space distribution of the given wave.

<sup>[ak]</sup> Here, the diagonal element of the acceptance-integral matrix  $\bar{I}_{aa}^{2008}(m_{K\pi\pi}, t')$  enters, which is the average acceptance of wave  $a$  [see equation (5.29)]. As the experimental acceptance of the three different data sets considered in this analysis are very similar, we used for simplicity only the acceptance-integral matrix of the 2008 data set in the regularization term.

1735 We implemented this in equation (5.53) by using a different parameter  $\Gamma_a$  for each wave in each  
 1736  $(m_{K\pi\pi}, t')$  cell<sup>[a1]</sup> given by

$$\Gamma_a(m_{K\pi\pi}, t') \equiv \frac{\Gamma}{\sqrt{\bar{I}_{aa}(m_{K\pi\pi}, t')}}. \quad (5.56)$$

1737 This is shown for four exemplary selected waves in figure 5.7b. The overall drop of  $\Gamma_a$  for all  
 1738 partial waves is caused by the rise of the acceptance towards higher masses (see figure C.4b).  
 1739 Also, the different acceptances of the waves due to their different kinematic distributions of the  
 1740 final-state particles is taken into account here. This means that a wave with larger intensity can  
 1741 be less significant than a wave with smaller intensity if the former has a lower acceptance and  
 1742 thereby effectively contributes less to the measured data.

1743 In this analysis, we chose  $\Gamma = 0.36$ . This value was tuned such that the effect from the Cauchy  
 1744 regularization is as weak as possible in order to not strongly bias the results of significant waves  
 1745 with large intensities, while still being strong enough to suppress insignificant waves, which is  
 1746 necessary to perform the wave-set selection. Using equation (5.56), the choice of  $\Gamma$  becomes  
 1747 independent of the acceptance of the analyzed channel. A similar value for  $\Gamma$  was found in the  
 1748 COMPASS  $\pi^-\pi^-\pi^+$  analysis, where a different final state with a completely different acceptance  
 1749 was studied [43].

### 1750 5.2.3 Imposing Continuity of the Wave Set in $m_{K\pi\pi}$

1751 As the wave sets for each  $(m_{K\pi\pi}, t')$  cell were inferred from data, they exhibit statistical fluctua-  
 1752 tions. For example, almost every of the considered 596 waves appeared in at least one  $(m_{K\pi\pi}, t')$   
 1753 cell when we fitted equation (5.52) to the data. To suppress these fluctuations, we imposed  
 1754 continuity of the wave sets in  $m_{K\pi\pi}$ . This was done by fitting multiple neighboring  $m_{K\pi\pi}$  bins  
 1755 simultaneously in one fit and by adding another penalty term for each wave that favors the  
 1756 corresponding transition amplitudes to be continuous in  $m_{K\pi\pi}$ . We do not impose a continuity  
 1757 condition in  $t'$ .

1758 As a measure of discontinuity, we used the sum of the squared deviations of the transition  
 1759 amplitudes of one  $m_{K\pi\pi}$  bin to the neighboring bin at  $m_{K\pi\pi} + \Delta m_{K\pi\pi}$  in a limited  $m_{K\pi\pi}$  range  
 1760  $(m_{K\pi\pi}^{\text{Start}}, m_{K\pi\pi}^{\text{End}})$ .<sup>[am]</sup>

$$\ln \mathcal{L}_{\text{Cont}} \left[ \mathcal{T}_a^z(m_{K\pi\pi}^{\text{Start}}, t'), \dots, \mathcal{T}_a^z(m_{K\pi\pi}^{\text{End}}, t'); \lambda \right] = - \sum_{m_{K\pi\pi}=m_{K\pi\pi}^{\text{Start}}}^{m_{K\pi\pi}^{\text{End}}-\Delta m_{K\pi\pi}} \lambda \left| \mathcal{T}_a^z(m_{K\pi\pi}, t') - \mathcal{T}_a^z(m_{K\pi\pi} + \Delta m_{K\pi\pi}, t') \right|^2. \quad (5.57)$$

<sup>[a1]</sup> The acceptance and thereby  $\bar{I}_{aa}(m_{K\pi\pi}, t')$  depends on  $m_{K\pi\pi}$  and  $t'$ .

<sup>[am]</sup> We used  $\lambda = 0.8$ , which was tuned in a similar way as the  $\Gamma$  parameter of the Cauchy regularization (see section 5.2.2).

1761 The total log-likelihood function of the wave-set selection fit across multiple  $m_{K\pi\pi}$  bins reads

$$\ln \mathcal{L}_{\text{WSS}} = \sum_{m_{K\pi\pi}=m_{K\pi\pi}^{\text{Start}}}^{m_{K\pi\pi}^{\text{End}}} \ln \mathcal{L}'_{\text{WSS}}(m_{K\pi\pi}; t') + \sum_{z,a} \ln \mathcal{L}_{\text{Cont}} [\mathcal{T}_a^z(m_{K\pi\pi}^{\text{Start}}, t'), \dots, \mathcal{T}_a^z(m_{K\pi\pi}^{\text{End}}, t'); \lambda]. \quad (5.58)$$

1762 Maximizing  $\ln \mathcal{L}_{\text{WSS}}$ , large fluctuations among neighboring bins are suppressed.

1763 Since different  $m_{K\pi\pi}$  regions are dominated by different resonances, the wave set is necessarily a  
 1764 function of  $m_{K\pi\pi}$ . Therefore, we included only a limited range of 15 consecutive  $m_{K\pi\pi}$  bins that  
 1765 are fitted simultaneously in the wave-set selection fit. Still, the wave-set selection was carried  
 1766 out for each  $(m_{K\pi\pi}, t')$  cell individually using seven  $m_{K\pi\pi}$  bins above and seven  $m_{K\pi\pi}$  bins below  
 1767 the  $(m_{K\pi\pi}, t')$  cell for which the wave-set selection was performed. <sup>[an], [ao]</sup>

## 1768 5.2.4 Sub-Threshold Decays of Isobar Resonances

1769 The invariant mass of a two-body subsystem at a given three-body mass  $m_{K\pi\pi}$  is kinematically  
 1770 limited to be below  $m_{K\pi\pi} - m_b$ , where  $m_b$  is the mass of the bachelor particle. If this limit  
 1771 is smaller than the nominal mass  $m_{\xi,0}$  of an isobar resonance in the corresponding two-body  
 1772 subsystem we can only observe the low-mass tail of the resonance. Waves in  $m_{K\pi\pi}$  regions,  
 1773 where  $m_{K\pi\pi} - m_b$  is much smaller than  $m_{\xi,0}$ , the so-called sub-threshold waves, are not expected  
 1774 to contribute significantly to the data, because the low-mass tail of the isobar resonances results  
 1775 in a small decay amplitude of the corresponding wave. In addition, the low-mass tail of the isobar  
 1776 amplitude of a sub-threshold wave has no clear signature, which would allow to unambiguously  
 1777 distinguish this wave from other waves with the same quantum numbers but with a different  
 1778 isobar resonance. For example, the phase of the isobar amplitude is approximately constant. This  
 1779 lack of a clear signature of sub-threshold waves leads to ambiguities that are known, e.g. from  
 1780 the COMPASS  $\pi^- \pi^- \pi^+$  analysis [43], to cause artifacts in the PWD.

1781 Therefore, we fixed the amplitude of partial waves with heavy isobars <sup>[ap]</sup> to be zero below a  
 1782 certain threshold  $m_{K\pi\pi}^{\xi, \text{thr}}$  in the wave-set selection fits. We chose this threshold such that above  
 1783  $m_{K\pi\pi}^{\xi, \text{thr}}$ , we are able to observe a significant part of the phase motion of the amplitude of the  
 1784 isobar. Therefore, the threshold is defined by the two-body mass, where the phase motion of the  
 1785 amplitude of the isobar is 1/8 of the total phase motion.

<sup>[an]</sup> At the borders of the  $m_{K\pi\pi}$  spectrum, we still included 15  $m_{K\pi\pi}$  bins, but the  $m_{K\pi\pi}$  cell for which the wave-set selection fit was performed was no longer in the center of this range.

<sup>[ao]</sup> To avoid effects due to the change in the chosen  $m_{K\pi\pi}$  binning, we used for all 15 bins the same bin width in  $m_{K\pi\pi}$  as in the  $(m_{K\pi\pi}, t')$  cell, for which the wave-selection fit was performed. For example, for  $(m_{K\pi\pi}, t')$  cells around  $m_{K\pi\pi} = 2 \text{ GeV}/c^2$ , where the bin width changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$ , we used in the wave-set selection fits for wave sets at  $m_{K\pi\pi} < 2 \text{ GeV}/c^2$  bins of  $20 \text{ MeV}/c^2$  width, also for those of the 15 bins with  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$ ; and vice versa for wave sets at  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$ .

<sup>[ap]</sup> We applied these thresholds to waves with  $K^*(1680)$ ,  $K_3^*(1780)$ ,  $f_0(980)$ ,  $f_0(1500)$ , and  $f_2(1270)$  isobars.

1786 This translates into an  $m_{K\pi\pi}$  threshold of<sup>[aq]</sup>

$$m_{K\pi\pi}^{\xi,\text{thr}} = m_b + m_{\xi,0} - 1.5 \Gamma_{\xi,0}, \quad (5.59)$$

1787 below which the respective partial wave amplitude was fixed to be zero in the wave-set selection  
1788 fit. Here,  $\Gamma_{\xi,0}$  is the nominal width of the isobar.

1789 This approach has two effects. First, for  $(m_{K\pi\pi}, t')$  cells below  $m_{K\pi\pi}^{\xi,\text{thr}}$  a wave with isobar resonance  
1790  $\xi$  was not included in the selected wave sets. Second, as we fitted 15 consecutive cells in  $m_{K\pi\pi}$  to  
1791 impose continuity (see section 5.2.3), the wave-set selection fits for  $(m_{K\pi\pi}, t')$  cells just above  
1792  $m_{K\pi\pi}^{\xi,\text{thr}}$  also included  $(m_{K\pi\pi}, t')$  cells below  $m_{K\pi\pi}^{\xi,\text{thr}}$ . For those cells below  $m_{K\pi\pi}^{\xi,\text{thr}}$ , we also fixed the  
1793 amplitude of the sub-threshold waves to zero. Due to the zero amplitude of sub-threshold waves  
1794 in  $(m_{K\pi\pi}, t')$  cells below  $m_{K\pi\pi}^{\xi,\text{thr}}$ , the continuity criterion in equation (5.57) leads to an additional  
1795 regularization of the corresponding waves in  $(m_{K\pi\pi}, t')$  cells above  $m_{K\pi\pi}^{\xi,\text{thr}}$ . Consequently,  $m_{K\pi\pi}^{\xi,\text{thr}}$  is  
1796 not a hard threshold, but a constraint that smoothly becomes weaker for higher  $m_{K\pi\pi}$ , similar to  
1797 how we expect such a wave to contribute to the data.

## 1798 5.2.5 Results of the Wave-Set Selection Fit

1799 Following the procedure described in sections 5.2.1 to 5.2.4, we fitted the likelihood in equa-  
1800 tion (5.58) to the data to obtain a wave set for each  $(m_{K\pi\pi}, t')$  cell. We performed 700 attempts  
1801 with random start parameter values for each cell in order to account for possible multimodality  
1802 of  $\ln \mathcal{L}_{\text{WSS}}$ . From these 700 fit attempts, the best fit result, i.e. the result with the largest log-  
1803 likelihood value, is used to determine the wave set. As shown in figure 5.8a, for many  $(m_{K\pi\pi}, t')$   
1804 cells, the best result was found multiple times, but there are some cells where the best result was  
1805 found only once. These bins suffer from multimodality of  $\ln \mathcal{L}_{\text{WSS}}$ , which seems to be more  
1806 pronounced in the high- $m_{K\pi\pi}$  region. As an example, figure 5.8b show the likelihood distribution  
1807 of a  $(m_{K\pi\pi}, t')$  cell where the best solution was found only once. This distribution exhibits a 500  
1808 units wide continuous peak<sup>[ar]</sup> from which we conclude, that  $\ln \mathcal{L}_{\text{WSS}}$  has a very large number  
1809 of local minima, which, however, yield similar description of the data. Similar results were  
1810 observed in other applications of the Cauchy regularization [43, 67]. A possible explanation  
1811 for this multimodality is the non-convex shape of the Cauchy regularization in equation (5.53),  
1812 which is known to induce multimodality [43, 111, 112].

1813 In order to decide which waves enter the wave set, we ordered the waves by intensity in each  
1814  $(m_{K\pi\pi}, t')$  cell as shown in figure 5.9. Figure 5.9b shows the typical behavior in an  $(m_{K\pi\pi}, t')$   
1815 cell in the high-mass region. The intensities obtained from the best result (orange points) fall

<sup>[aq]</sup> Here, we used a relativistic Breit-Wigner amplitude and the nominal isobar mass and width from ref. [91] to determine this threshold.

<sup>[ar]</sup> The first bin of the histogram shown in figure 5.8b has more than 300 entries and not 1 entry as it would be expected for the likelihood distribution of a  $(m_{K\pi\pi}, t')$  cell where the best solution was found only once. The reason is that in order to show the spread in  $\ln \mathcal{L}$ , the bin width of this histogram was chosen much wider than the 0.1 units in  $\ln \mathcal{L}_{\text{WSS}}$  different, which define two solutions to be the same. Therefore, the first bin contains multiple different solutions.

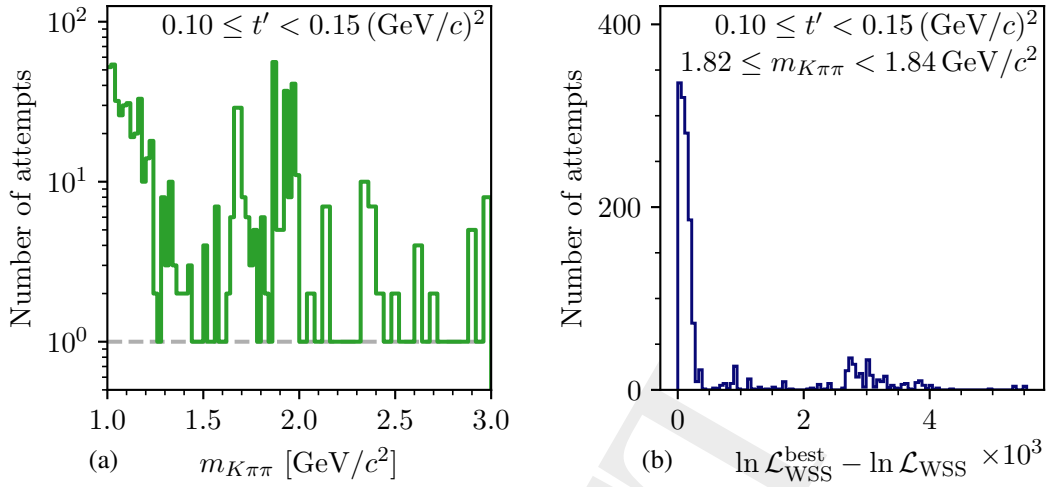


Figure 5.8: Stability of the wave-set selection fits. (a) shows the number of fit results that yielded the best solution, i.e. an  $\ln \mathcal{L}_{\text{WSS}}$  value at most 0.1 units smaller than the overall largest  $\ln \mathcal{L}_{\text{WSS}}$  value found in all 700 fit attempts, as a function of  $m_{K\pi\pi}$  in the lowest  $t'$  bin. (b) shows the distribution of the  $\ln \mathcal{L}_{\text{WSS}}$  values obtained by minimizing equation (5.58) relative to the overall largest  $\ln \mathcal{L}_{\text{WSS}}$  value of the best fit result from the wave-set selection fit in one  $(m_{K\pi\pi}, t')$  cell.

1816 continuously until they reach a value of  $|\mathcal{T}_a^z|^2 \approx 5$ , where the intensity distribution has a jump  
 1817 discontinuity. The jump is followed by a long tail of about 550 waves nearly all of them with  
 1818  $|\mathcal{T}_a^z|^2 \ll 1$ . The waves in this tail do not significantly contribute to the data. Therefore, we  
 1819 selected all waves with an intensity above a threshold given by the jump (black horizontal line in  
 1820 figure 5.9). The sub-optimal solutions with lower  $\ln \mathcal{L}_{\text{WSS}}$  are shown by the other colored points.  
 1821 They exhibit a significant spread around the best solution, especially for the deselected waves.  
 1822 The reason for this is, that insignificant waves are not pulled to exactly zero intensity by the  
 1823 Cauchy regularization.<sup>[as]</sup> This leaves some freedom to the fit to distribute intensity among the  
 1824 waves in the deselected tail without having a large influence on  $\ln \mathcal{L}_{\text{WSS}}$ . As these fluctuations  
 1825 mainly affects the deselected waves that have an intensity well below the threshold, it does not  
 1826 strongly influence the selection of the wave set.

1827 Figure 5.9a shows the typical behavior in the low-mass region. Also here, we observe a clear jump  
 1828 at a similar intensity of  $|\mathcal{T}_a^z|^2 \approx 5$ . In addition, we observe small jumps at higher intensities, i.e. in  
 1829 the region of the selected waves. They seem to be driven by correlations among neighboring  $m_{K\pi\pi}$   
 1830 bins, because if we did not use equation (5.57), those small jumps were much less pronounced.

1831 Overall, the jumps always appear at a similar intensity of the order of 1, which means that a wave  
 1832 has to contribute with a common minimum intensity to the data in order to be resolved. Still,  
 1833 we determined the thresholds individually for each  $(m_{K\pi\pi}, t')$  cell using the method discussed in  
 1834 appendix D.1.1. All waves that in the wave-set selection fit have an intensity above the respective

<sup>[as]</sup> This is because the gradient of  $\ln \mathcal{L}_{\text{Reg}}$  is zero at  $|\mathcal{T}_a^z| = 0$ . Other regularization approaches, e.g. LASSO, do not have this drawback, but require special minimization techniques.

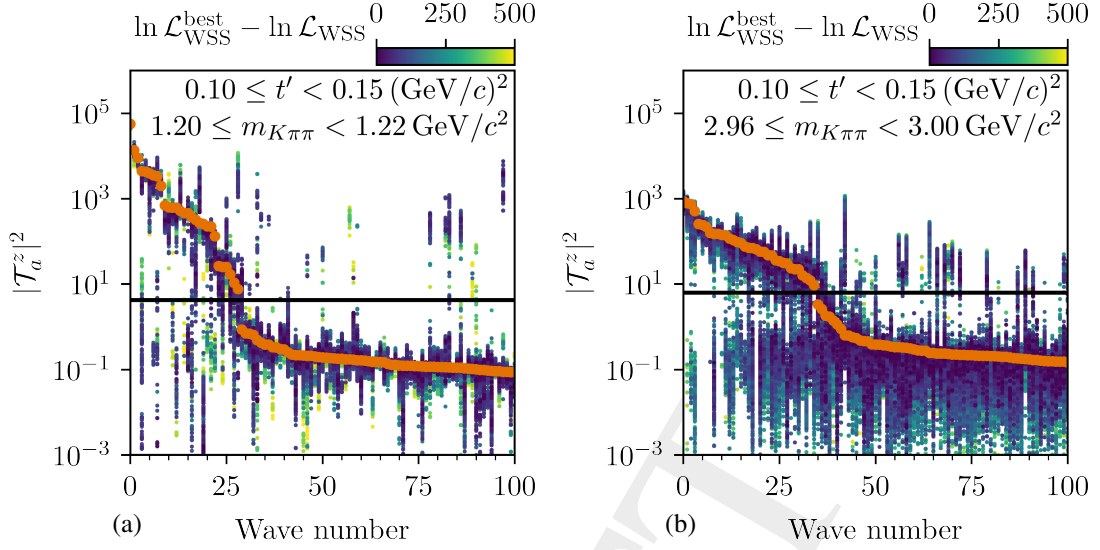


Figure 5.9: Partial waves ordered by their intensity in two neighboring  $m_{K\pi\pi}$  bins in the lowest  $t'$  bin. The waves are ordered by intensity as obtained from the best result in each cell and numbered accordingly. The orange points show the best result out of 700 fit attempts. The other colored points show the results from the other fit attempts. Their color represents  $\ln \mathcal{L}_{\text{WSS}}^{\text{best}} - \ln \mathcal{L}_{\text{WSS}}$ . Only results where this difference is smaller than 500 units are plotted. Only the 100 waves with the largest intensity are shown. The black horizontal line marks the threshold, above which waves were selected for the wave set.

1835 threshold entered the wave set of the given  $(m_{K\pi\pi}, t')$  cell. The incoherent flat wave was always  
 1836 included in the selected wave set, independent of the result of the wave-set selection.

## 1837 5.2.6 The Selected Wave-Set

1838 As discussed above, we determined the wave set individually for each  $(m_{K\pi\pi}, t')$  cell. Hence, a  
 1839 wave might be deselected in individual cells, while it is selected in the neighboring cells. This  
 1840 is observed, e.g., in the tails of  $K^-\pi^-\pi^+$  resonances where the intensity becomes small and  
 1841 fluctuates around the threshold above which the wave is selected. However, this leads to a bias  
 1842 towards larger intensities when studying such waves in the resonance-model fit discussed in  
 1843 chapter 6. This is because statistical fluctuations towards smaller intensities favor the wave to be  
 1844 deselected and thus are not considered in the  $\chi^2$  statistics used in the RMF, while fluctuations  
 1845 towards larger intensities favor the wave to be selected and thus are considered in the RMF. To  
 1846 circumvent this effect, we manually included waves that show interesting signals into the wave  
 1847 sets of all  $(m_{K\pi\pi}, t')$  cells considered by the resonance-model fit, independent of the result of  
 1848 the wave-set selection fit. The list of those waves is given in table D.1 in the appendix. As this  
 1849 procedure adds only a few waves in a few  $(m_{K\pi\pi}, t')$  cells, it only weakly affects other waves in  
 1850 the PWD. We verified this by comparing the results of two PWD fits. One using the wave set  
 1851 directly obtained from the wave-set selection fits and one using the modified wave set.



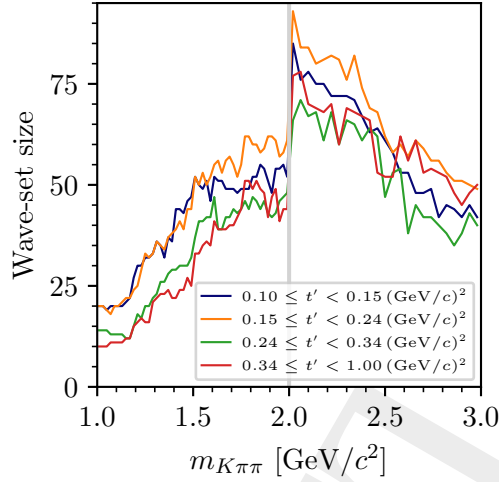


Figure 5.10: Number of waves in the selected wave sets of the individual  $(m_{K\pi\pi}, t')$  cells as a function of  $m_{K\pi\pi}$ . The different line colors represent the four  $t'$  bins. The gray line indicates the  $m_{K\pi\pi}$  value where we changed from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins in  $m_{K\pi\pi}$ .

1852 The size of the selected wave sets exhibits a pronounced  $m_{K\pi\pi}$  dependence as shown in figure 5.10.  
 1853 The wave-set size ranges from about 15 waves in the lowest  $m_{K\pi\pi}$  bins that contain only a few  
 1854 events up to about 80 waves in the  $2 \text{ GeV}/c^2$  region. The wave-set size rises with increasing  
 1855  $m_{K\pi\pi}$  up to about  $2 \text{ GeV}/c^2$  because at higher masses more decay channels and higher spins  
 1856 contribute. As expected, doubling the  $m_{K\pi\pi}$  bin width at  $2 \text{ GeV}/c^2$  leads to a jump of the wave-set  
 1857 size, because more waves can be resolved due to the larger number of events. No significant  
 1858 discontinuity at  $2 \text{ GeV}/c^2$  is observed in the results for the transition amplitudes (see section 5.5).  
 1859 Above about  $2 \text{ GeV}/c^2$ , the wave-set size decreases again, because the number of events becomes  
 1860 smaller. Similarly, the selected wave set is smaller in the two highest  $t'$  bins (green and red lines  
 1861 in figure 5.10), which have about half the number of events compared to the two lowest  $t'$  bins  
 1862 (blue and orange lines in figure 5.10).

1863 Overall, 238 partial waves<sup>[at]</sup> were selected in at least one  $(m_{K\pi\pi}, t')$  cell. Most of them were  
 1864 selected over wide continuous  $m_{K\pi\pi}$  ranges such as the  $0^- 0^+ [K\pi]_S^{K\pi} \pi S$  wave shown in fig-  
 1865 ure 5.11. This proves that the continuity condition in equation (5.57) works. About 90 of 238  
 1866 waves appear only in a few individual  $(m_{K\pi\pi}, t')$  cells such as the  $0^- 0^+ \rho_3(1690) K F$  wave shown  
 1867 in figure 5.11. This represents the statistical uncertainty of the wave set.<sup>[au]</sup> The complete list  
 1868 of selected partial waves can be found in appendix D.1.3 in figures D.3 to D.34. As expected  
 1869 from the observed structures in the  $m_{K^- \pi^+}$  and  $m_{\pi^- \pi^+}$  distribution shown in figures 4.7a and 4.7b,  
 1870 respectively, a large fraction of the selected partial waves represent decays to ground-state isobar  
 1871 resonances like the  $K^*(892)$ ,  $K_2^*(1430)$ ,  $\rho(770)$ , or the  $f_2(1270)$ . Furthermore, the selected partial

<sup>[at]</sup> This does not include the incoherent flat wave.

<sup>[au]</sup> We studied the influence of these about 90 noisy waves on the other waves, by performing a PWD using a wave set without these noisy waves. The results are consistent with those from the PWD using the complete 238-wave set.

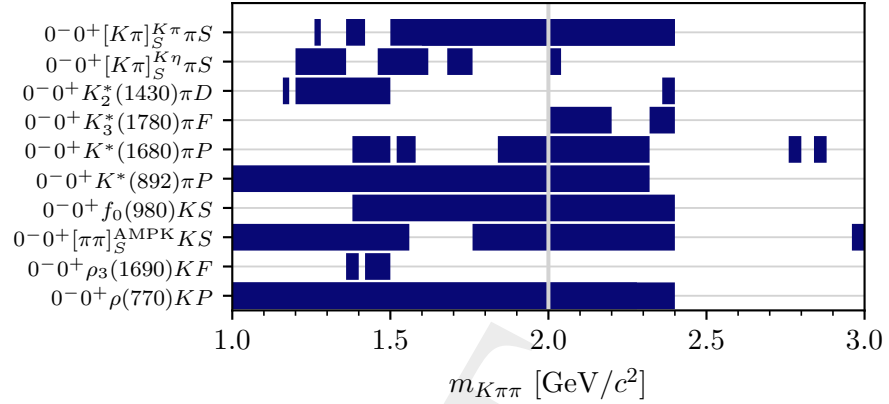


Figure 5.11: Mass ranges of selected waves with  $J^P = 0^-$  in the lowest  $t'$  bin. The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

1872 waves are dominated by waves with  $J \lesssim 5$ , which is consistent with previous observations as  
 1873 there is no known or expected strange-meson resonance with  $J > 5$  (see figure 1.1). Therefore,  
 1874 we conclude that the wave-set selection yielded reasonable results. We substantiate this statement  
 1875 when studying the agreement between the PWD model and data in section 5.6.

1876 Finally, the so-called 238-wave set that we inferred from data using the wave-set selection  
 1877 approach as discussed in this section was used in equation (5.16) as the model for the PWD of  
 1878 the measured  $K^- \pi^- \pi^+$  data. In addition, it was also used for many pseudodata studies discussed  
 1879 in sections 5.8, 5.10, and 6.4.

### 1880 5.3 Modeling Incoherent Background Processes

1881 As discussed in section 5.1, the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  is dominantly a coherent process.  
 1882 In the PWD, it can be modeled therefore by a rank=1 spin-density matrix in equation (5.18).  
 1883 However, also events from other processes passed the event selection discussed in section 4.1 and  
 1884 thereby entered the  $K^- \pi^- \pi^+$  sample. For example, there is contamination of beam pions in the  
 1885  $K^- \pi^- \pi^+$  sample (see section 3.1.6). These beam pions may also undergo diffractive scattering  
 1886 reactions leading to a final state with three charged particles, i.e. the reaction  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$ .  
 1887 We expect this  $\pi^- \pi^- \pi^+$  background to be the largest background component in the  $K^- \pi^- \pi^+$   
 1888 sample as discussed in detail in section 5.10. Another source of background are reactions with  
 1889 three kaons in the final state, i.e.  $K^- + p \rightarrow K^- K^- K^+ + p$ . Such events entered the  $K^- \pi^- \pi^+$  sample  
 1890 due to limitations of the final-state particle identification. We estimated the  $K^- K^- K^+$  background  
 1891 to be about 4% as discussed in section 4.2. All these background processes include different, i.e.  
 1892 distinguishable final-state particles. Therefore, these processes cannot be modeled as a sum of  
 1893 coherent amplitudes, but the corresponding amplitudes have to be summed incoherently.

1894 In order to treat these incoherent background processes using the formalism developed in sec-  
 1895 tion 5.1, we formulated a spin-density matrix of the 238-wave set with rank  $> 1$ . This allows  
 1896 for incoherence in the PWD model and thereby takes into account the incoherent background  
 1897 components in an effective way. In section 5.3.1, we give a detailed motivation for this approx-  
 1898 imation. We know of at least three processes contributing to the  $K^- \pi^- \pi^+$  sample: the signal  
 1899 reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , and the background reactions  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  and  
 1900  $K^- + p \rightarrow K^- K^- K^+ + p$ . Consequently, we formulated the PWD model in equation (5.19)  
 1901 using a rank=3 spin-density matrix. In order to study whether a PWD model using a rank=3  
 1902 spin-density matrix is sufficient to take into account all incoherent background processes, we  
 1903 performed a study in which we used a much larger rank. i.e. a rank=6 spin-density matrix. This  
 1904 study yielded results consistent with those from the rank=3 PWD fits, which suggests that the  
 1905 additional freedom in the rank=6 PWD fits from the almost two times larger number of free  
 1906 parameters is not needed to describe the data. Thus, we conclude that the PWD model using  
 1907 a rank=3 spin-density matrix, which is called rank=3 model in the following, is sufficient to  
 1908 effectively take into account the incoherent background processes.

1909 As discussed in section 5.2, the 238-wave set was constructed based on a rank = 1 model.  
 1910 Historically, we initially had used a rank=1 model not only for the wave-set selection fits, but also  
 1911 for the final PWD, analogously to the COMPASS  $\pi^- \pi^- \pi^+$  analysis [39]. Unfortunately, it turned  
 1912 out that a later state of the analysis the incoherent background processes play a significant role,  
 1913 i.e. when describing the results of the PWD in terms of a resonance model as done in the RMF  
 1914 described in chapter 6. Hence, we had to take into account the incoherent background processes  
 1915 in the RMF by incoherently adding background components to the coherent resonance model for  
 1916 the process  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . However, describing the results of the PWD that were based  
 1917 on the coherent rank=1 model by an incoherent resonance model would have been inconsistent.  
 1918 Thus, we had to treat the incoherent background processes also at the level of the PWD by using  
 1919 a rank=3 model. Performing the wave-set selection again would have been very time-consuming  
 1920 and computationally very expensive. Hence, we used the 238-wave set, which is based on a  
 1921 rank=1 model, for the PWD using the rank=3 model, because by switching to a rank=3 model  
 1922 we only added more freedom to the fit as the rank=1 model is a subset of the rank=3 model.  
 1923 Furthermore, we observe overall the same structures in the partial waves when comparing the  
 1924 results using the rank=3 and the rank=1 models. When introducing the higher rank, we observe  
 1925 the largest change in the incoherent flat wave. While the flat wave contributed about 2 % to the  
 1926 total intensity when using the rank=1 model, it became practically zero when using the rank=3  
 1927 model. As the flat wave models background from events where the three final state particles are  
 1928 uncorrelated, the zero intensity of the flat wave indicates that there is a negligible fraction of such  
 1929 events in the  $K^- \pi^- \pi^+$  sample. This underlines the selectivity of the event selection presented in  
 1930 section 4.1. The non-vanishing flat wave when using the rank=1 model accounted for part of the  
 1931 incoherent background processes, as it was the only incoherent model component in the rank=1  
 1932 model. However, as final-state particles from incoherent background processes are correlated,  
 1933 the flat wave is only a rough approximation for these contributions only for data samples where  
 1934 these incoherent backgrounds are small, e.g. in the COMPASS  $\pi^- \pi^- \pi^+$  analysis [39].

1935 **5.3.1 Effective Background Description using a Higher Rank**

1936 In order to include the incoherent background processes in the PWD model, one would need to  
 1937 write the total probability  $P(\tau^{K\pi\pi})$  to measure an event as a sum of probabilities of the  $K^-\pi^-\pi^+$   
 1938 and the background processes, bkg, i.e. <sup>[av]</sup>

$$P(\tau^{K\pi\pi}) = P^{K\pi\pi}(\tau^{K\pi\pi}) + \sum_{\text{bkg}} P^{\text{bkg}}(\tau^{\text{bkg}}) \cdot J(\text{bkg} \rightarrow K\pi\pi). \quad (5.60)$$

1939 Here, the phase-space variables  $\tau^{K\pi\pi}$  (see section 5.1.1) are used to formulate the total probability.  
 1940 Depending on which process  $p$  we are assuming for the event, its probability to be measured  
 1941 is described by a different set of phase-space variables  $\tau^p$ . This introduces additional Jacobian  
 1942 terms  $J$  that arise due to the transformation from the set  $\tau^p$  of variables to  $\tau^{K\pi\pi}$ . Modeling the  
 1943 individual probabilities analogously to equation (5.32), yields: <sup>[aw]</sup>

$$P(\tau^{K\pi\pi}) \propto \eta^{K\pi\pi}(\tau^{K\pi\pi}) \cdot \mathcal{I}_{K\pi\pi}^{K\pi\pi}(\tau^{K\pi\pi}) + \sum_{\text{bkg}} \eta^{\text{bkg}}(\tau^{\text{bkg}}) \cdot \mathcal{I}_{\text{bkg}}^{\text{bkg}}(\tau^{\text{bkg}}) \cdot J(\text{bkg} \rightarrow K\pi\pi). \quad (5.61)$$

1944 Here,  $\eta^p$  is the experimental acceptance of the event assuming that it is of process  $p$ , and  $\mathcal{I}_q^p$  is  
 1945 the model intensity formulated according to equation (5.16) for events produced by process  $q$  but  
 1946 modeled in terms of partial waves assuming the process  $p$ . For example,  $\mathcal{I}_{K\pi\pi}^{K\pi\pi}$  is the intensity  
 1947 model for the  $K^-\pi^-\pi^+$  component in the data formulated in terms of partial waves of the reaction  
 1948  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  as given in equation (5.10).

1949 Including the incoherent background processes according to equation (5.61) is impossible mainly  
 1950 due to two reasons. First, this would require a model for  $\mathcal{I}_{\text{bkg}}^{\text{bkg}}$  as input. However, for most  
 1951 background processes such as  $K^- + p \rightarrow K^- K^- K^+ + p$ , such a model is unknown. <sup>[ax]</sup> Second, the  
 1952 calculation of the difference acceptances  $\eta^p(\tau^p)$  of the various processes is not feasible here. As  
 1953 shown in section 5.1.3, for a single process, the acceptance of each event can be combined from  
 1954 all events to one summand,  $\sum_k \eta^{K\pi\pi}(\tau_k^{K\pi\pi})$ , in the  $\ln \mathcal{L}_{\text{PWD}}$  in equation (5.38). This summand is  
 1955 independent of the fit parameters. Thus, this term can be dropped from the likelihood function, i.e.  
 1956 it can be ignored in the maximum-likelihood fits. <sup>[ay]</sup> However, for multiple processes we would  
 1957 have to use equation (5.61), where the acceptance is not a global coefficient, but the various  
 1958 processes contribute with different acceptances. Therefore, for multiple processes the acceptance  
 1959 of each event cannot be combined to one summand in  $\ln \mathcal{L}_{\text{PWD}}$  and thus cannot be dropped.  
 1960 Hence, we would need to determine the acceptance individually for each measured event and  
 1961 for each considered process. In practice, it is not feasible to determine these acceptances in a  
 1962 reasonable amount of time. <sup>[az]</sup> This prevents us from using equation (5.61).

<sup>[av]</sup> For simplicity, we drop the dependencies on  $m_{K\pi\pi}$  and  $t'$  here.

<sup>[aw]</sup> For simplicity, we omit the constant normalization factor.

<sup>[ax]</sup> The only exception is for the  $\pi^-\pi^-\pi^+$  background, for which we determined such a model in the COMPASS  $\pi^-\pi^-\pi^+$  analysis [39].

<sup>[ay]</sup> The acceptance is still correctly considered in the maximum-likelihood fits. It enters via the acceptance-integral matrix given in equation (5.29).

<sup>[az]</sup> As described in section 5.1, we implemented acceptance effects in the PWD in the acceptance-integral matrix

1963 We circumvented these limitations and took into account the incoherent background processes by  
 1964 effectively modeling the background contributions and their acceptances in terms of an intensity  
 1965 model consisting of partial waves of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , i.e. we used

$$\mathcal{I}_{\text{bkg}}^{K\pi\pi}(\tau^{K\pi\pi}) \equiv \frac{\eta^{\text{bkg}}(\tau^{\text{bkg}})}{\eta^{K\pi\pi}(\tau^{K\pi\pi})} \mathcal{I}_{\text{bkg}}^{\text{bkg}}(\tau^{\text{bkg}}) \cdot J(\text{bkg} \rightarrow K\pi\pi). \quad (5.62)$$

1966 With this, the total probability in equation (5.61) reads

$$P(\tau^{K\pi\pi}) \propto \eta^{K\pi\pi}(\tau^{K\pi\pi}) \cdot \mathcal{I}_{K\pi\pi}^{K\pi\pi}(\tau^{K\pi\pi}) + \sum_{\text{bkg}} \eta^{K\pi\pi}(\tau^{K\pi\pi}) \cdot \mathcal{I}_{\text{bkg}}^{K\pi\pi}(\tau^{K\pi\pi}). \quad (5.63)$$

1967 Now, each model intensity is multiplied by the same acceptance  $\eta^{K\pi\pi}$ . Therefore, the acceptance  
 1968 can be factored out and dropped in the likelihood function, which resolves the issue of determining  
 1969  $\eta^{K\pi\pi}$  on an event-by-event basis.

1970 Still, a model  $\mathcal{I}_{\text{bkg}}^{K\pi\pi}$  for the background processes is needed. However, as all terms in equa-  
 1971 tion (5.63) are functions of the same set  $\tau^{K\pi\pi}$  of phase-space variables,  $\mathcal{I}_{\text{bkg}}^{K\pi\pi}$  can be modeled in  
 1972 terms of partial waves of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , analogously to equation (5.16).  
 1973 This yields for the probability of an event:<sup>[ba]</sup>

$$P \propto \eta^{K\pi\pi} \left[ \sum_{z_{K\pi\pi}} \left| \sum_{a \in \mathbb{W}} \mathcal{T}_a^{z_{K\pi\pi}} \Psi_a^{z_{K\pi\pi}} \right|^2 + \sum_{\text{bkg}} \sum_{z_{\text{bkg}}} \left| \sum_{a \in \mathbb{W}_{z_{\text{bkg}}}} \mathcal{T}_a^{z_{\text{bkg}}} \Psi_a^{z_{\text{bkg}}} \right|^2 \right]. \quad (5.64)$$

1974 Grouping all incoherent sums over the coherent sectors  $z$  into a single sum and using the same  
 1975 wave set  $\mathbb{W}$  with the same set  $\{\Psi_a\}$  of decay amplitudes for all coherent sectors allows us to  
 1976 describe the  $K^- \pi^- \pi^+$  signal and the background processes by a single condensed expression:

$$P \propto \eta^{K\pi\pi} \left[ \underbrace{\sum_{\mathfrak{p}=\{z_{K\pi\pi}, z_{\pi\pi\pi}, z_{KKK}, \dots\}} \left| \sum_{a \in \mathbb{W}} \mathcal{T}_a^{\mathfrak{p}} \Psi_a \right|^2}_{\equiv \mathcal{I}_{\text{tot}}^{K\pi\pi}} \right], \quad (5.65)$$

1977 i.e. by a single total model intensity  $\mathcal{I}_{\text{tot}}^{K\pi\pi}$ . Finally,  $\mathcal{I}_{\text{tot}}^{K\pi\pi}$  can be written in terms of a single  
 1978 spin-density matrix [see equation (5.18)]

$$\rho_{ab} = \sum_{\mathfrak{p}=\{z_{K\pi\pi}, z_{\pi\pi\pi}, z_{KKK}, \dots\}} \mathcal{T}_a^{\mathfrak{p}} [\mathcal{T}_b^{\mathfrak{p}}]^*. \quad (5.66)$$

---

defined in equation (5.29). We calculated the elements of this matrix by a Monte Carlo integration based on one reconstructed pseudodata sample. Here, we would need to determine the acceptance individually for each measured event and for each considered process. This would require generating more and orders of magnitude larger pseudodata samples and is thus computationally extremely expensive.

<sup>[ba]</sup> For simplicity, we drop the dependence on  $\tau^{K\pi\pi}$  here as it is the same for all functions.

1979 The rank of this matrix and thereby the rank of the PWD model is given by the incoherent  
 1980 processes, i.e. by the sum over  $p$ . Equation (5.65) has the same form as equation (5.32) with  
 1981 coherent sectors now representing the  $K^-\pi^-\pi^+$  signal and the various background processes.  
 1982 Therefore, when taking into account the incoherent background by using a rank  $> 1$  PWD model,  
 1983 we can use the same PWD formalism described in section 5.1, e.g. the same decay amplitudes  
 1984 and the same likelihood function. Just the number of free parameters increases when using a  
 1985 model with a higher rank.

1986 As explained in section 5.1, in the PWD fits the measurable quantities are the spin-density matrix  
 1987 elements. The transition amplitudes  $\mathcal{T}_a^z$  in equation (5.18) are an effective parameterization of  
 1988 the spin-density matrix. In general, they are different from the transition amplitudes  $\mathcal{T}_a^p$  of the  
 1989 various physics processes  $p$  in equation (5.66) by an unknown unitary transformation. Thus, we  
 1990 cannot determine the transition amplitudes of the individual processes uniquely. Therefore, we  
 1991 cannot separate the  $K^-\pi^-\pi^+$  signal from the background processes at the stage of the PWD. This  
 1992 is only possible at the level of the RMF as discussed in chapter 6.

1993 In summary, using a PWD model with rank = 3 allows us to take into account incoherent  
 1994 background processes in an effective way, while still employing the formalism presented in  
 1995 section 5.1. This, however, requires the  $K^-\pi^-\pi^+$  PWD model to be flexible enough to approximate  
 1996 the phase-space distribution of the background processes according to equation (5.62). We studied  
 1997 this approximation for the dominant  $\pi^-\pi^-\pi^+$  background as discussed in section 5.10.2. Overall,  
 1998 the PWD model using the 238-wave set is able to approximate the  $\pi^-\pi^-\pi^+$  background in the  
 1999  $K^-\pi^-\pi^+$  sample. Also in the resonance-model fit, we find consistent results for the background  
 2000 contributions in the  $K^-\pi^-\pi^+$  sample as presented in section 6.2, which was the initial motivation  
 2001 to formulate a rank=3 PWD model.

## 2002 5.4 Improving Estimates of Partial-Wave Decomposition Results

2003 The physics quantities that we determine in the PWD fits are the real and imaginary parts of the  
 2004 spin-density matrix elements defined in equation (5.18). Our estimates for the values of these  
 2005 quantities, together with the corresponding statistical uncertainties and correlations, enter the  
 2006 RMFs as discussed in section 6.1.5. Hence, in addition to a precise and accurate estimation of  
 2007 the values of the spin-density matrix elements, we aim for an accurate estimate of their statistical  
 2008 uncertainties and correlations.<sup>[bb]</sup> The latter are represented by the entries of the covariance  
 2009 matrix of the spin-density matrix elements.

2010 Performing a maximum-likelihood fit of equation (5.38) to the measured  $K^-\pi^-\pi^+$  sample yields  
 2011 the optimal parameter values for the fit parameters, i.e. the real and imaginary parts of the  
 2012 transition amplitudes  $^{\text{MLE}}\mathcal{T}_a^z$  and the data-set fraction parameters. These optimal values are  
 2013 called maximum-likelihood estimates. The covariance matrix of the fit parameters is estimated

---

<sup>[bb]</sup> Systematic uncertainties are discussed in section 5.7.

2014 by evaluating the inverse of the Hessian matrix of the log-likelihood function at its maxi-  
 2015 mum (see equation (40.12) in ref. [9]). The observables we are actually interested in are the  
 2016 spin-density matrix elements that are calculated from the transition amplitudes according to  
 2017 equation (5.18). The maximum-likelihood estimates of the spin-density matrix elements are  
 2018 calculated by inserting  $^{\text{MLE}}\mathcal{T}_a^z$  into equation (5.18). The corresponding covariance matrix is  
 2019 calculated using linear uncertainty propagation, i.e. by a linear approximation of equation (5.18),  
 2020 (see equation (40.42) in ref. [9]).

2021 This maximum-likelihood approach was used in previous partial-wave analyses [39, 113, 114]  
 2022 to obtain the estimates of the values and covariance matrix of the spin-density matrix elements.  
 2023 However, this approach has limitations. First, the uncertainty estimation of the fit parameters  
 2024 assumes that the log-likelihood function is approximated well a multivariate Gaussian function  
 2025 in the fit parameters, which is true only for large data samples. For finite sample sizes as in this  
 2026 analysis, this approximation may lead to biased uncertainties as discussed in ref. [108]. Second,  
 2027 the linear uncertainty propagation is only an approximation when calculating the uncertainties  
 2028 of observables that depend in a non-linear way on the fit parameters. For example, the real and  
 2029 imaginary parts of the spin-density matrix elements depend on the products of real and imaginary  
 2030 parts of the transition amplitudes:

$$\Re(\rho_{ab}) = \sum_z \left[ \Re(\mathcal{T}_a^z) \Re(\mathcal{T}_b^z) + \Im(\mathcal{T}_a^z) \Im(\mathcal{T}_b^z) \right] \quad (5.67)$$

$$\Im(\rho_{ab}) = \sum_z \left[ \Im(\mathcal{T}_a^z) \Re(\mathcal{T}_b^z) - \Re(\mathcal{T}_a^z) \Im(\mathcal{T}_b^z) \right]. \quad (5.68)$$

2031 The linear uncertainty propagation is a sufficient approximation only if the relative uncertainties  
 2032 on the transition amplitudes are small. To overcome these approximations, we applied the method  
 2033 of Bootstrapping [115] in order to obtain better estimates for the values and the covariance matrix  
 2034 of the observables, e.g. of spin-density matrix elements. This is discussed in the following  
 2035 section 5.4.1.

### 2036 5.4.1 The Bootstrapping Method

2037 In this section, we explain the Bootstrapping method on the example of spin-density matrix  
 2038 elements. The same method can be applied for any other observable, e.g. for the data-set ratio  
 2039 parameters. For the purpose of notation, we collect all real and imaginary parts of the spin-density  
 2040 matrix elements in one real-valued vector  $\vec{\lambda}$ .  $\lambda_i$  is the  $i^{\text{th}}$  entry of  $\vec{\lambda}$  as defined in equation (6.20),  
 2041 i.e. the real or imaginary part of one spin-density matrix element. The maximum-likelihood  
 2042 estimates  $\lambda_i^{\text{MLE}}$  of the spin-density matrix elements depend on the data sample from which  
 2043 they were determined. The data sample is subject to statistical fluctuations. These fluctuations  
 2044 propagate to  $\lambda_i^{\text{MLE}}$ , which means that they are also statistically distributed quantities. The  
 2045 uncertainties of  $\lambda_i^{\text{MLE}}$  and the correlations between them are given by the covariance matrix  
 2046  $\text{Cov}[\lambda_i^{\text{MLE}}, \lambda_j^{\text{MLE}}]$  of this distribution.

2047 We approximated the underlying distribution of  $\lambda_i^{\text{MLE}}$  by a finite set  $\{\lambda_i^{(h)}\}$  that is distributed  
 2048 accordingly. Obtaining such a set requires a set of data samples indexed by  $h$ , where each  
 2049 of these samples is distributed in the same way as the measured  $K^-\pi^-\pi^+$  sample. Since we  
 2050 cannot remeasure the  $K^-\pi^-\pi^+$  sample multiple times, we employed an approximation method  
 2051 that belongs to the class of so-called resampling methods [115, 116], to construct random data  
 2052 samples from the measured  $K^-\pi^-\pi^+$  sample. The size of these data samples must be the identical  
 2053 to the size of the measured  $K^-\pi^-\pi^+$  sample, because the precision of the data determines the  
 2054 number of waves that can be resolved in the partial-wave decomposition (see section 5.2).  
 2055 Applying the 238-wave set, which was optimized for the measured  $K^-\pi^-\pi^+$  sample, to a smaller  
 2056 data sample may lead to overfitting and thereby bias the distribution of  $\lambda_i^{\text{MLE}}$ . This constrains the  
 2057 choice of applicable resampling methods.

2058 Due to the limitations discussed above, we used the Bootstrapping method [115]. Based on  
 2059 this method we generated  $N_{\text{BS}}$  Bootstrapping samples indexed by  $h$  by randomly drawing  $\bar{N}_{\text{ev}}$   
 2060 events from the  $\bar{N}_{\text{ev}}$  measured events of the  $K^-\pi^-\pi^+$  sample. This means that in a Bootstrapping  
 2061 sample  $h$  some of the measured events are used more than once.<sup>[bc]</sup> The distribution of the  
 2062 Bootstrapping samples approximates the underlying distribution of the  $K^-\pi^-\pi^+$  sample.<sup>[bd]</sup>  
 2063 Thus, they allow us to approximate the distribution of any observable obtained from the  $K^-\pi^-\pi^+$   
 2064 sample. For example, to study the distribution of the spin-density matrix elements, we determined  
 2065 their maximum-likelihood estimates  $\lambda_i^{(h)}$  for each Bootstrapping sample  $h$ . To this end, we first  
 2066 performed a maximum-likelihood fit of equation (5.38) to each Bootstrapping sample, which  
 2067 yielded the maximum-likelihood estimates of the transition amplitudes. Then, we calculated for  
 2068 each Bootstrapping sample the spin-density matrix elements  $\lambda_i^{(h)}$  from the maximum-likelihood  
 2069 estimates of the transition amplitudes.

2070 This procedure yielded for each spin-density matrix element  $i$  a set  $\{\lambda_i^{(h)}\}$  of  $N_{\text{BS}}$  estimates, one  
 2071 from each Bootstrapping sample  $h$ . These sets approximate the underlying physical distribution  
 2072 of the spin-density matrix elements. Thus, they allow us to estimate the covariance matrix of the  
 2073 spin-density matrix elements

$$\text{Cov}[\lambda_i^{\text{MLE}}, \lambda_j^{\text{MLE}}] = \frac{1}{N_{\text{BS}} - 1} \sum_{h=1}^{N_{\text{BS}}} (\lambda_i^{(h)} - \langle \lambda_i \rangle) (\lambda_j^{(h)} - \langle \lambda_j \rangle). \quad (5.69)$$

2074 The mean value of the spin-density matrix elements, called Bootstrapping mean value, reads

$$\langle \lambda_i \rangle = \frac{1}{N_{\text{BS}}} \sum_{h=1}^{N_{\text{BS}}} \lambda_i^{(h)}. \quad (5.70)$$

<sup>[bc]</sup> When adding an event to the Bootstrapping sample, we randomly selected it from the full sample of measured events.

<sup>[bd]</sup> Formally, we approximated the underlying distribution of the  $K^-\pi^-\pi^+$  sample by the empirical distribution that is based on the measured  $K^-\pi^-\pi^+$  sample [see equation (1.6) in ref. [117]]. Then we drew a set of samples from this empirical distribution, which are the Bootstrapping samples.



2075 It is also used to approximate the bias on  $\lambda_i^{\text{MLE}}$  [117]:

$$\text{bias}[\lambda_i^{\text{MLE}}] \approx \langle \lambda_i \rangle - \lambda_i^{\text{MLE}}. \quad (5.71)$$

2076 For each  $(m_{K\pi\pi}, t')$  cell we generated  $N_{\text{BS}} = 2000$  Bootstrapping samples. For each Bootstrapping  
 2077 sample indexed by  $h$  in each  $(m_{K\pi\pi}, t')$  cell we performed 50 maximum-likelihood fit attempts of  
 2078 equation (5.38) with randomly chosen start-parameter values. The fit with the largest likelihood  
 2079 value determined the maximum-likelihood estimate  $\lambda_i^{(h)}$  for Bootstrapping sample  $h$ . In total,  
 2080 we performed  $30 \times 10^6$  single PWD fits to obtain the Bootstrapping results discussed in the  
 2081 following section 5.4.2.

## 2082 5.4.2 Comparison of Bootstrapping and Maximum-Likelihood Estimates

2083 First, we compare the Bootstrapping and maximum-likelihood estimates of the intensities, i.e.  
 2084 the diagonal spin-density matrix elements. From each of the  $N_{\text{BS}} = 2000$  Bootstrapping samples  
 2085 for each  $(m_{K\pi\pi}, t')$  cell we obtained an estimate for the partial-wave intensities. As an example,  
 2086 the distributions of the Bootstrapping estimates of the intensity of the  $1^+ 0^+ \rho(770) K S$  wave  
 2087 are shown by the histograms in figures 5.12a and 5.12b for two neighboring  $m_{K\pi\pi}$  bins. Both  
 2088 distributions are approximated well by a Gaussian (orange curve) with expectation value and  
 2089 width given by the mean and standard deviation of the Bootstrapping distribution according to  
 2090 equations (5.69) and (5.70), respectively:

$$\mu_i = \langle \lambda_i \rangle \quad \text{and} \quad \sigma_i = \sqrt{\text{Cov}[\lambda_i^{\text{MLE}}, \lambda_i^{\text{MLE}}]}. \quad (5.72)$$

2091 In general, using the mean and the standard deviation of the distribution as the expectation value  
 2092 and width of a Gaussian yield the best possible Gaussian approximation of this distribution  
 2093 independent of the actual shape of the distribution.<sup>[be]</sup> We find similar agreement with a Gaussian  
 2094 for most partial-waves that have an intensity value that is large compared to the uncertainty.

2095 The red curves in figure 5.12 represent Gaussian distributions with expectation value and width  
 2096 given by the maximum-likelihood estimates of the intensity value and its uncertainty from the  
 2097  $K^- \pi^- \pi^+$  sample. In figure 5.12a, the maximum-likelihood estimate yielded a slightly smaller  
 2098 intensity and a slightly larger uncertainty compared to the estimates from Bootstrapping. Also in  
 2099 figure 5.12b, the maximum-likelihood estimate of the intensity is only slightly smaller, but the  
 2100 uncertainty estimate is unreasonably larger. We observe similarly large uncertainties from the  
 2101 maximum-likelihood estimate in a few other  $(m_{K\pi\pi}, t')$  cells. We suspect these unreasonably large  
 2102 uncertainties to arise from numerical instabilities due to the large number of free parameters  
 2103 in the rank = 3 PWD model, which lead to an approximately singular Hessian matrix of the  
 2104 likelihood function. We did not observe such unreasonably large uncertainties when using a

<sup>[be]</sup> Using the mean and standard deviation of the distribution as expectation value and width of the Gaussian approximation minimizes the Kullback-Leibler divergence [118], which is a measure how different the Gaussian approximation is with respect to the true distribution.

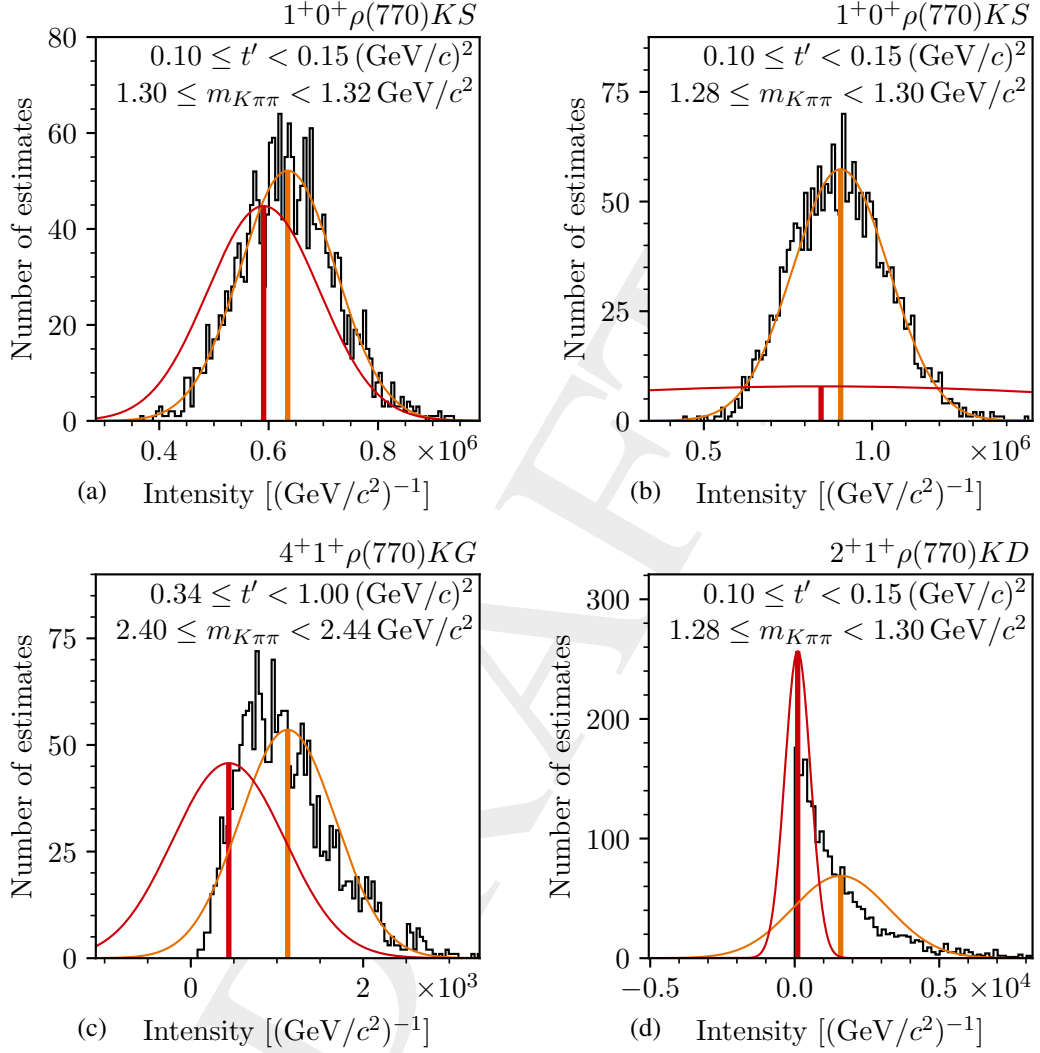


Figure 5.12: Distribution of the intensity estimates for selected partial-waves in the given  $(m_{K\pi\pi}, t')$  cells as obtained from the Bootstrapping samples (histograms). The orange curves are Gaussian distributions with expectation values and widths given by the mean values (vertical orange lines) and standard deviations of the distributions. The red curves are Gaussian distributions with expectation values and widths given by the maximum-likelihood estimates of the intensity value (vertical red lines) and its uncertainty, respectively. (a) and (b) show the intensity of the  $1^+ 0^+ \rho(770) K S$  wave in two neighboring  $m_{K\pi\pi}$  bins. (c) shows the intensity of the  $4^+ 1^+ \rho(770) K G$  wave. (d) shows the intensity of the  $2^+ 1^+ \rho(770) K D$  wave from a PWD using a rank=1 PWD model. (a) to (c) were obtained using a rank=3 PWD model.

2105 rank=1 PWD model. As we did not use the maximum-likelihood estimates of the uncertainties  
 2106 in this analysis, we did not study this effect further.

2107 For partial-waves in  $(m_{K\pi\pi}, t')$  cells that have intensity values that are small compared to their  
 2108 uncertainties, the distributions of the intensity estimates deviate from a Gaussian. This is shown,  
 2109 e.g., in figure 5.12c. As the intensity cannot be negative, the distribution is asymmetric with a tail  
 2110 towards larger intensities. The maximum-likelihood estimate yielded a larger uncertainty than  
 2111 the corresponding Bootstrapping estimate. The intensity value from the maximum-likelihood  
 2112 estimate is close to zero and much smaller than the Bootstrapping mean value. A partial-wave  
 2113 intensity, i.e. a diagonal element of the spin-density matrix, is the sum of the squared real and  
 2114 imaginary parts of the transition amplitude [see equation (5.67) for  $a = b$ ]. This means, that  
 2115 the intensity depends quadratically on the individual fit parameters. Therefore, we expect its  
 2116 distribution to be approximated well by a Gaussian only if its uncertainty is small compared to its  
 2117 value. The deviation of the intensity distribution from a Gaussian is even more pronounced for  
 2118 many waves when using a rank=1 PWD model. An extreme example is shown in figure 5.12d.  
 2119 For a rank=3 model the sum in equation (5.67) has three times more terms than for a rank=1  
 2120 model. Due to the central-limit theorem, we expect the intensity distribution of a rank=3 model  
 2121 to be more similar to a Gaussian.

2122 On average, the maximum-likelihood estimates of the uncertainties are about twice as large as  
 2123 the corresponding Bootstrapping estimates,<sup>[bf]</sup> with a large spread across the  $(m_{K\pi\pi}, t')$  cells.  
 2124 This spread is independent of the  $(m_{K\pi\pi}, t')$  region as shown, for example, in figure 5.13a for the  
 2125 uncertainty on the intensity of the  $1^+ 0^+ \rho(770) K S$  wave in the lowest  $t'$  bin. The bias of the  
 2126 maximum-likelihood estimates of the intensities as defined in equation (5.71) is spread across  
 2127 the  $(m_{K\pi\pi}, t')$  cells as exemplarily shown in figure 5.13b for the intensity of the  $1^+ 0^+ \rho(770) K S$   
 2128 wave in the lowest  $t'$  bin. Typically, this spread is smaller than the intensity's uncertainty. On  
 2129 average, the Bootstrapping means are similar to the maximum-likelihood estimates.

2130 The distributions of the real and imaginary parts of the off-diagonal elements of the spin-density  
 2131 matrix obtained from Bootstrapping are in good agreement with a Gaussian even in cases  
 2132 where the values of the real and imaginary parts are small compared to their uncertainties as  
 2133 shown in figure 5.14. Also, the maximum-likelihood estimate yielded similar results for the  
 2134 values and the uncertainties of the off-diagonal elements. In contrast to the intensities, the  
 2135 real and imaginary parts of the off-diagonal elements of the spin-density matrix are sums of  
 2136 products of real and imaginary parts of different transition amplitudes [see equations (5.67)  
 2137 and (5.68) for  $a \neq b$ ]. Hence, the off-diagonal spin-density matrix elements depend linearly on  
 2138 the individual fit parameters, i.e. they depend linearly on individual fit parameters if keeping  
 2139 the other fit parameters fixed. If the correlations between the fit parameters are weak, this  
 2140 means that the functional dependence of the off-diagonal spin-density matrix elements on all fit  
 2141 parameters is better approximated by a linear function compared to the functional dependence  
 2142 of the intensities. Therefore, the distribution of the off-diagonal spin-density matrix elements  
 2143 is better approximated by a Gaussian. Also, the maximum-likelihood estimates agree better

<sup>[bf]</sup> This is in contrast to rank=1 PWD models, for which the maximum-likelihood estimates of the uncertainties are typically slightly smaller than the corresponding Bootstrapping estimates.

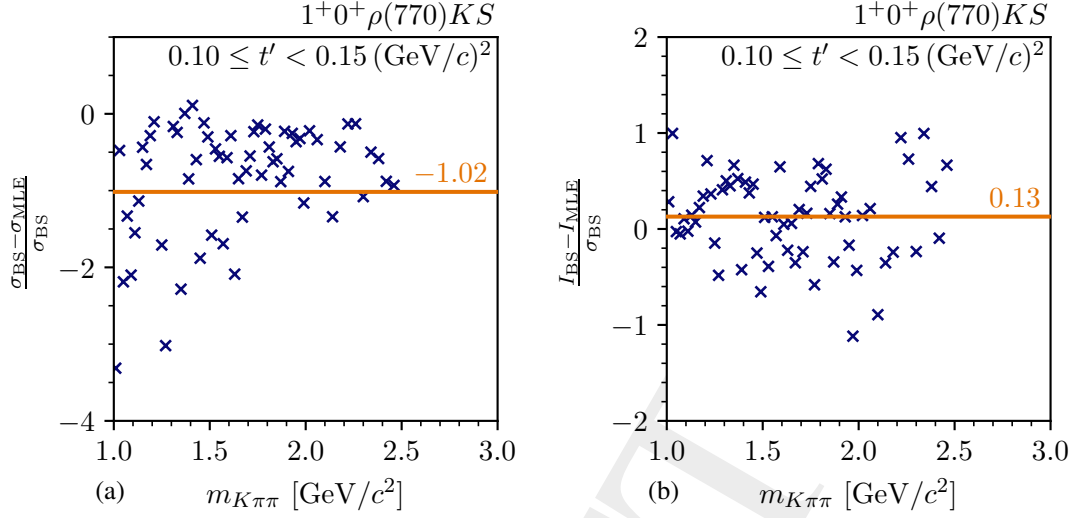


Figure 5.13: Difference between the estimates from Bootstrapping (BS) and the maximum-likelihood estimates (MLE) for the  $1^+ 0^+ \rho(770) K S$  wave as a function of  $m_{K\pi\pi}$  in the lowest  $t'$  bin. (a) shows the relative difference between the uncertainty estimates. (b) shows the bias on the maximum-likelihood estimate of the intensity as defined in equation (5.71) relative to the uncertainty as obtained from Bootstrapping. The orange numbers and horizontal lines represent the corresponding average over all  $m_{K\pi\pi}$  bins.

2144 with the results from Bootstrapping as calculating the maximum-likelihood estimates of the  
 2145 spin-density matrix elements involves linear uncertainty propagation.

2146 According to equation (5.69), Bootstrapping allows us to study the covariance matrix of the  
 2147 spin-density matrix elements, including their linear correlations. Typically, the intensity values  
 2148 exhibit small correlations. For example, the Pearson correlation coefficient [119]

$$\text{Cov}[\lambda_i^{\text{MLE}}, \lambda_j^{\text{MLE}}] \left/ \sqrt{\text{Cov}[\lambda_i^{\text{MLE}}, \lambda_i^{\text{MLE}}] \text{Cov}[\lambda_j^{\text{MLE}}, \lambda_j^{\text{MLE}}]} \right. \quad (5.73)$$

2149 of the intensities of the  $1^+ 0^+ \rho(770) K S$  and the  $2^+ 1^+ \rho(770) K D$  waves obtained from Boot-  
 2150 strapping is only 0.04 for the  $(m_{K\pi\pi}, t')$  cell shown in figure 5.15a. Also, the real and imaginary  
 2151 parts of the spin-density matrix elements show only small correlations, which are, however,  
 2152 typically larger than the correlations between intensities. Figure 5.15b shows as an example the  
 2153 distribution of the real and imaginary parts of a selected spin-density matrix element, which  
 2154 yields a Pearson correlation coefficient of  $-0.13$ . Consistent with our findings for the uncer-  
 2155 tainties, the maximum-likelihood estimate of the covariance matrix of real and imaginary parts,  
 2156 represented by the red uncertainty ellipse in figure 5.15b, agrees well with the corresponding  
 2157 Bootstrapping estimate (orange uncertainty ellipse), while the maximum-likelihood estimate of  
 2158 the full covariance of the intensities in figure 5.15a yielded a larger uncertainty ellipse compared  
 2159 the Bootstrapping estimate. [bg]

[bg] The difference in the positions of the ellipses arises for the same reason as difference between the maximum-likelihood estimates of the intensity values and the Bootstrapping means, also seen in figure 5.12.

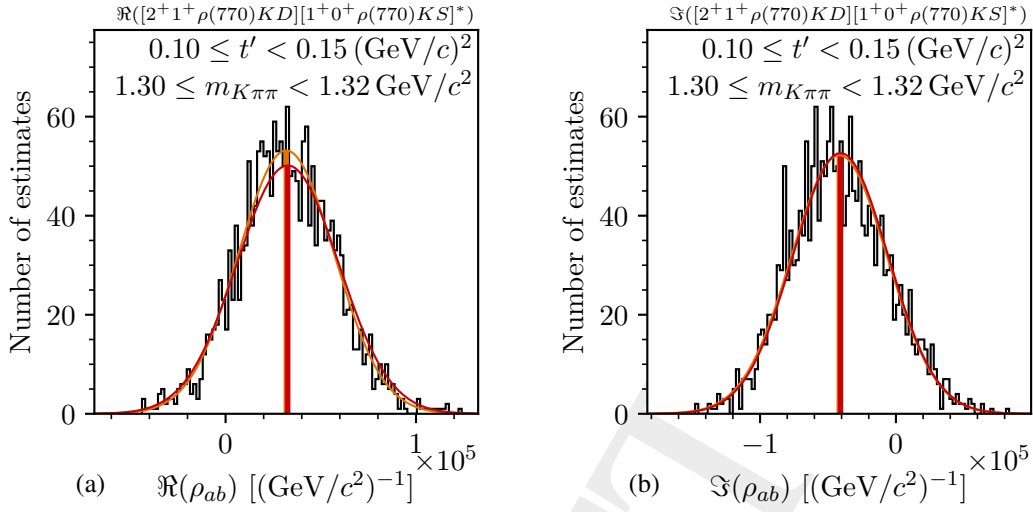


Figure 5.14: Distribution of (a) the real part  $\Re(\rho_{ab})$  and (b) the imaginary part  $\Im(\rho_{ab})$  of the spin-density matrix element for a selected pair of waves as obtained from the Bootstrapping samples (histograms). The orange curves are Gaussian distributions with expectation value and width given by the mean value (vertical orange lines) and the standard deviation of the distributions. The red curves are Gaussian distributions with expectation value and width given by the maximum-likelihood estimate of the intensity value (vertical red lines) and its uncertainty, respectively.

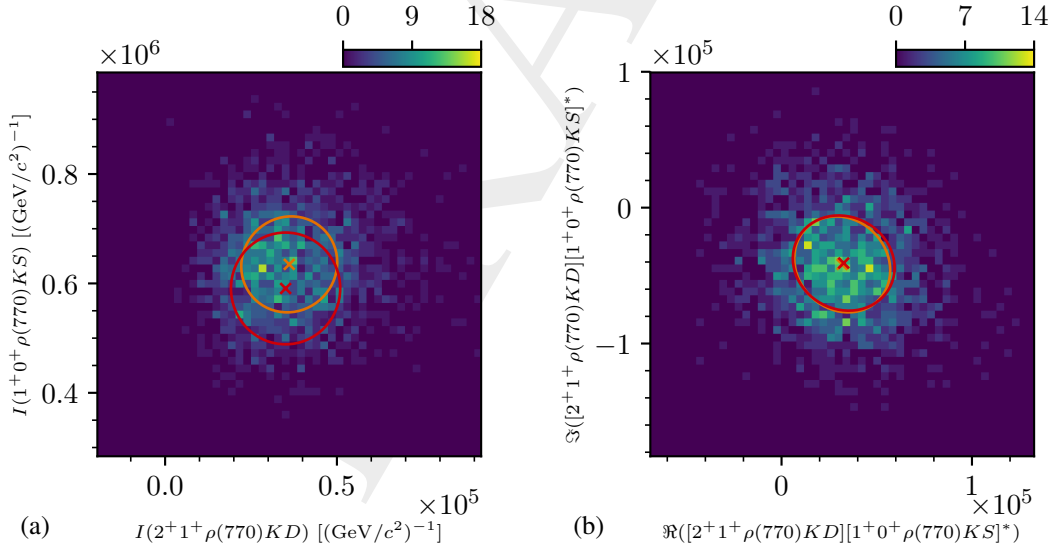


Figure 5.15: Correlations between spin-density matrix elements for the  $(m_{K\pi\pi}, t')$  cells with  $1.30 \leq m_{K\pi\pi} < 1.32 \text{ GeV/c}^2$  and  $0.10 \leq t' < 0.15 \text{ (GeV/c)}^2$  as obtained from the Bootstrapping samples. (a) shows the correlation between the intensities of the  $1^+ 0^+ \rho(770)KS$  and the  $2^+ 1^+ \rho(770)KD$  waves. (b) shows the correlation between the real and imaginary part of the off-diagonal spin-density matrix element of the same two waves. The orange crosses indicate the mean values from Bootstrapping. The orange uncertainty ellipses represent the covariances. The red crosses indicate the maximum-likelihood estimates of the spin-density matrix elements. The red uncertainty ellipses represent the covariances as obtained from the maximum-likelihood estimates.

Using the Bootstrapping method, we were able to estimate the uncertainties and correlations of observables, e.g. spin-density matrix element or data-set fraction parameters, determined from the results of the PWD in a reliable way. Thereby, we took into account non-linearities in the calculation of the observables and we approximated their true distribution with a Gaussian in the best possible way. Thus, we used the Bootstrapping estimates for the uncertainties and correlations in all further analysis steps. Unless stated differently, we show in all figures that present results of a PWD the uncertainties from Bootstrapping. As discussed above, we observe a non-vanishing bias of the maximum-likelihood estimates for the values of observables, e.g. the intensity values. This bias is spread across the  $(m_{K\pi\pi}, t')$  cells as exemplarily shown in figure 5.13b. In order to reduce this bias, we used also the mean values from Bootstrapping defined in equation (5.70) as central values for all data points. Unless state differently, we do this when showing the results of a PWD. Furthermore, we used the Bootstrapping mean values as data points in the RMFs. Although the covariance matrix obtained from Bootstrapping is the covariance of the maximum-likelihood estimates, we used it as an approximation for the covariance of the Bootstrapping mean values.<sup>[bh]</sup> We tested the effect of this approximation in a systematic study that is discussed in section 6.3. For simplicity, we refer to the Bootstrapping mean values of the spin-density matrix elements  $\langle \lambda_i \rangle$  obtained from measured data as measured values and use the symbol  $\lambda_i$  in the rest of the text. We do the same also for other observables, e.g. for the data-set fraction parameters.

## 5.5 A First Glimpse on the Partial-Wave Decomposition Results

Using the formalism described in section 5.1, we performed a PWD of the COMPASS  $K^- \pi^- \pi^+$  data sample. As a model, we used the 238-wave set, which was inferred from data in the wave-set selection procedure described in section 5.2. At the level of the PWD we cannot separate the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  from incoherent backgrounds that are present in the  $K^- \pi^- \pi^+$  sample. Therefore, we effectively modeled these incoherent contributions by using a rank=3 model in the PWD as discussed in section 5.3. Finally, we obtained more accurate estimates for the observables and their uncertainties from the PWD using the Bootstrapping method, which is presented in section 5.4. In this section, we give a general overview over the results of the PWD fit to the  $K^- \pi^- \pi^+$  sample, which is called the 238-wave PWD in the rest of the text. Especially, we focus on the quality of the fit. The physics signals that we observe in the various partial waves are discussed in chapter 7.

For each of the 2000 Bootstrapping samples in each  $(m_{K\pi\pi}, t')$  cell we performed 50 fit attempts with random start-parameter values for the transition amplitudes and data-set fractions. Figure 5.16 shows the result of the 50 fit attempts of one exemplary Bootstrapping sample for each

<sup>[bh]</sup> As the Bootstrapping mean values are estimators of observables, they fluctuate statistically. To obtain an estimate for the covariance matrix of the Bootstrapping mean values, we would need to perform a Bootstrapping of the Bootstrapping. This is computationally prohibitively expensive.

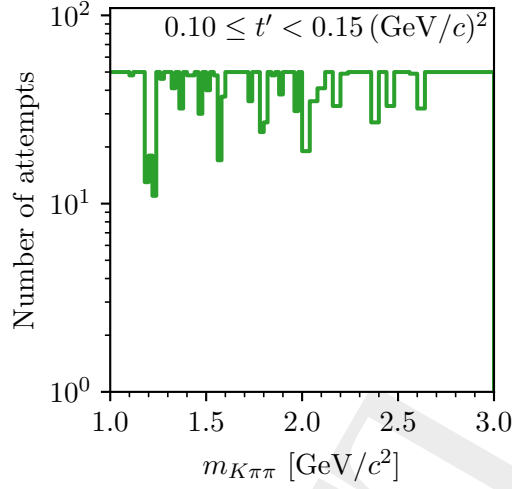


Figure 5.16: Stability of the 50 PWD fit attempts per  $(m_{K\pi\pi}, t')$  cell for an exemplarily selected Bootstrapping sample as a function of  $m_{K\pi\pi}$  in the lowest  $t'$  bin. The green line shows the number of fit attempts that found the best result, i.e. that found a value of  $\ln \mathcal{L}_{\text{PWD}}$  that is at most 0.1 units worse than the largest  $\ln \mathcal{L}_{\text{PWD}}$  value.

2194  $m_{K\pi\pi}$  bin in the lowest  $t'$  bin. In all  $m_{K\pi\pi}$  bins, all of the 50 fit attempts converged<sup>[bi]</sup> and hence  
 2195 yielded a fit result. The best result, i.e. the one with the largest likelihood, was found in more than  
 2196 10 of the 50 fit attempts in all  $m_{K\pi\pi}$  bins as shown by the green histogram in figure 5.16. For most  
 2197 of the  $m_{K\pi\pi}$  bins, it was even found in more than 30 fit attempts. The  $m_{K\pi\pi}$  regions that yielded  
 2198 the best result less than about 20 times, e.g. at about  $1.2 \text{ GeV}/c^2$ , correspond to the  $m_{K\pi\pi}$  regions  
 2199 with a large amount of events (see figure 4.6a). In these regions the higher precision of the data  
 2200 leads to more distinct local minima. The other three  $t'$  bins and all Bootstrapping samples behave  
 2201 similarly. Only in a few Bootstrapping samples the result with the largest value of  $\ln \mathcal{L}_{\text{PWD}}$  was  
 2202 found only once. Hence, we may not have found the best result for these samples. However,  
 2203 these rare occurrences do not influence our final estimates in equations (5.69) and (5.70) from the  
 2204 averages over the Bootstrapping samples.<sup>[bj]</sup> Overall, the large number of fit attempts that found  
 2205 the best solution shows that the PWD fit of the rank=3 model using the 238-wave set is stable. In  
 2206 particular, the fit is much more stable than the wave-set selection fits shown in figure 5.8a. This  
 2207 proves that the fit can reliably find the fit-parameter values that describe the data best.

2208 The fraction of produced events in each of three data sets of the  $K^-\pi^-\pi^+$  sample are represented  
 2209 by the data-set fraction parameters  $\hat{r}^{(i)}(m_{K\pi\pi}, t')$ , which are independent free parameters in each  
 2210  $(m_{K\pi\pi}, t')$  cell as defined in equation (5.25). The estimates for  $\hat{r}^{(i)}(m_{K\pi\pi}, t')$  from the PWD are  
 2211 shown in figure 5.17 for the lowest and highest  $t'$  bins. We expect the data-set fractions to be

<sup>[bi]</sup> We used the low-memory BFGS (LBFGS) [82–84] implementation of the NLOpt package [85] as minimizer, which determines the convergence criteria.

<sup>[bj]</sup> We did two studies in a selected  $(m_{K\pi\pi}, t')$  cell where we performed only one random fit attempt and where we used 500 random fit attempts. Both studies yielded results that are consistent with the main analysis where we used 50 random fit attempts.

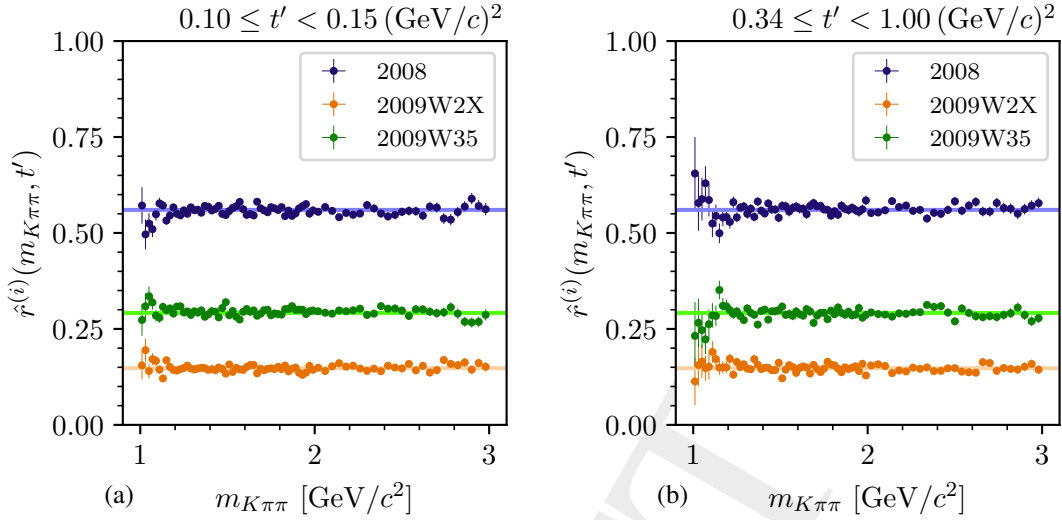


Figure 5.17: Data-set fractions, i.e. the fraction of produced events in each of the three data sets of the  $K^-\pi^-\pi^+$  sample defined in equation (5.25), as a function of  $m_{K\pi\pi}$  (a) in the lowest  $t'$  bin and (b) in the highest  $t'$  bin. The colored horizontal lines show the corresponding average values.<sup>[bk]</sup>

2212 the same in all  $(m_{K\pi\pi}, t')$  cell. This is because the physical distribution of events is the same  
 2213 in each data set and because the data-set fractions represent the fraction of produced events,  
 2214 which are not affected by acceptance effects that depend on  $(m_{K\pi\pi}, t')$ . The data-set fractions in  
 2215 the  $(m_{K\pi\pi}, t')$  cells show no systematic deviation from their corresponding average values,<sup>[bk]</sup>  
 2216 which are represented by the colored horizontal lines in figure 5.17. The average values are 0.56,  
 2217 0.15, and 0.29 for the 2008, 2009W2X, and 2009W35 data sets, respectively. They agree with  
 2218 the fractions of measured events of 0.55, 0.14, and 0.31 as expected, because the experimental  
 2219 acceptance, which may bias the fraction of measured events with respect to fraction of produced  
 2220 events, is similar for the three data sets. This agreement demonstrates, that our estimates of the  
 2221 data-set fraction parameters reliably reproduce the physical quantities they represent. It is a first  
 2222 successful test of the quality of the PWD fit.

2223 A  $\chi^2$  test using the average values as constant hypothesis yielded  $p$ -values of 0.003, 0.080, and  
 2224 0.016 for the 2008, 2009W2X, and 2009W35 data sets, respectively.<sup>[bl]</sup> These  $p$ -values mean  
 2225 that the deviations of the data points from the average are somewhat larger than expected by the  
 2226 statistical uncertainties. As we assume that our estimates of the statistical uncertainties obtained  
 2227 from Bootstrapping are realistic, these deviations indicate systematic effects in the estimates for  
 2228  $\hat{f}^{(i)}(m_{K\pi\pi}, t')$ . However, the obtained  $p$ -values are still reasonably large. Hence, these systematic  
 2229 effects are small. Furthermore, we do not observe an overall systematic deviation from a  
 2230 constant. Thus, we conclude that we obtained realistic estimates for the data-set fractions in each

<sup>[bk]</sup> We determined the average of each data-set fraction over all  $(m_{K\pi\pi}, t')$  cells by calculating the variance-weighted mean (see equation (7.26) in ref. [119]), which uses the uncertainty of the data-set fraction parameter as determined from Bootstrapping. Doing so, we neglected correlations between the data-set fraction parameters.

<sup>[bl]</sup> See sections 4.5 and 4.7 in ref. [119] for details on the  $p$ -value calculation. As for the average, we neglected the correlations between the data-set fractions for the  $p$ -value calculation.



2231 ( $m_{K\pi\pi}, t'$ ) cell. The imperfect statistical consistency that fluctuates from bin to bin indicates that  
 2232 the data-set fractions are affected by systematic effects that are different from bin to bin. For  
 2233 example, such small systematic effects may arise from the wave set. As we individually inferred  
 2234 the wave set from data for each ( $m_{K\pi\pi}, t'$ ) cell as explained in section 5.2, also the wave set is  
 2235 affected by fluctuations from cell to cell. These fluctuations may lead to small systematic effects  
 2236 when using the wave sets in the PWD that is presented here. This is a first indication that the  
 2237 statistical and systematic uncertainties of this analysis are of similar orders of magnitude.

2238 We are mainly interested in the  $m_{K\pi\pi}$  dependencies of the spin-density matrix elements of the  
 2239 partial waves as they provide information about the resonances that decay to the  $K^-\pi^-\pi^+$  final  
 2240 state. Before discussing the individual partial waves, we discuss the  $m_{K\pi\pi}$  dependence of the  
 2241 total model intensity, i.e. the distribution of the predicted number  $\widehat{N}_{\text{ev}}$  of produced events in  
 2242  $m_{K\pi\pi}$  according to equation (5.21). However, as we used a non-equidistant binning in  $m_{K\pi\pi}$ ,  
 2243  $\widehat{N}_{\text{ev}}$  has a jump discontinuity at the  $m_{K\pi\pi}$  position where the bin width changes. In order to take  
 2244 this into account, we show in the following the so-called intensity spectra, which represent the  
 2245 number density in  $m_{K\pi\pi}$ , i.e. the intensity divided by the  $m_{K\pi\pi}$ -bin width as a function of  $m_{K\pi\pi}$ .  
 2246 The intensity spectra are continuous functions in  $m_{K\pi\pi}$ . The blue points in figure 5.18 show  
 2247 the intensity spectrum of the total model intensity summed over the analyzed  $t'$  bins, which  
 2248 is so-called  $t'$ -summed total intensity spectrum. As expected, it exhibits similar features as the  
 2249 measured  $m_{K\pi\pi}$  distribution shown in figure 4.6a,<sup>[bml]</sup> i.e. a double-peak in the mass region of  
 2250 the  $K_1(1270)$  and the  $K_1(1400)$  and a second peak at about  $1.8 \text{ GeV}/c^2$  in the mass region of the  
 2251  $K_2^*(1430)$ .

2252 The PWD enables us to study the contributions from partial waves with given  $J^P$  quantum  
 2253 numbers to the total intensity spectrum. Figure 5.18 gives an overview over these contributions.  
 2254 The orange, green, red, and purple data points show for each  $J^P$  included in the 238-wave set  
 2255 the total intensity of all waves with the given  $J^P$  quantum numbers, i.e. the predicted number  
 2256 of produced events if only these waves are considered in the corresponding calculation in  
 2257 equation (5.21). As expected, the  $1^+$  waves represented by the green points in figure 5.18a  
 2258 dominantly contribute to the double-peak structure at about  $1.4 \text{ GeV}/c^2$ . Also, the  $0^-$  waves  
 2259 (green points in figure 5.18a) strongly contribute to the mass region of the double-peak. Above  
 2260 about  $1.5 \text{ GeV}/c^2$  they have a similar intensity as the  $1^+$  waves. The  $2^-$  waves (green points  
 2261 in figure 5.18b) strongly contribute to the second peak in the total intensity spectrum at about  
 2262  $1.8 \text{ GeV}/c^2$ . This supports our assumption that this peak arises from  $K_2$  resonances in the  
 2263 spectrum. The  $2^+$  waves (orange points in figure 5.18b) show a clear peak in the mass range of  
 2264 the  $K_2^*(1430)$ . Except for this peak, the  $2^+$  waves pick up only little intensity. Similarly, the  $4^+$   
 2265 waves (orange points in figure 5.18c) contribute only little to the data, but they show a clear peak  
 2266 at about  $2 \text{ GeV}/c^2$ , i.e. in the mass region of the  $K_4^*(2045)$  resonance.

2267 The total intensities for waves with  $3^+$ ,  $4^-$ ,  $4^+$ , or  $5^+$  quantum numbers (red points in figure 5.18b  
 2268 and green, orange, and red points in figure 5.18c, respectively) show peaking structures in the

<sup>[bml]</sup> The total intensity spectrum represents the acceptance-corrected  $m_{K\pi\pi}$  distribution, i.e. the underlying physical  
 $m_{K\pi\pi}$  distribution, according to the PWD results. The measured  $m_{K\pi\pi}$  spectrum is distorted with respect to the  
 physical distribution due to the experimental acceptance.

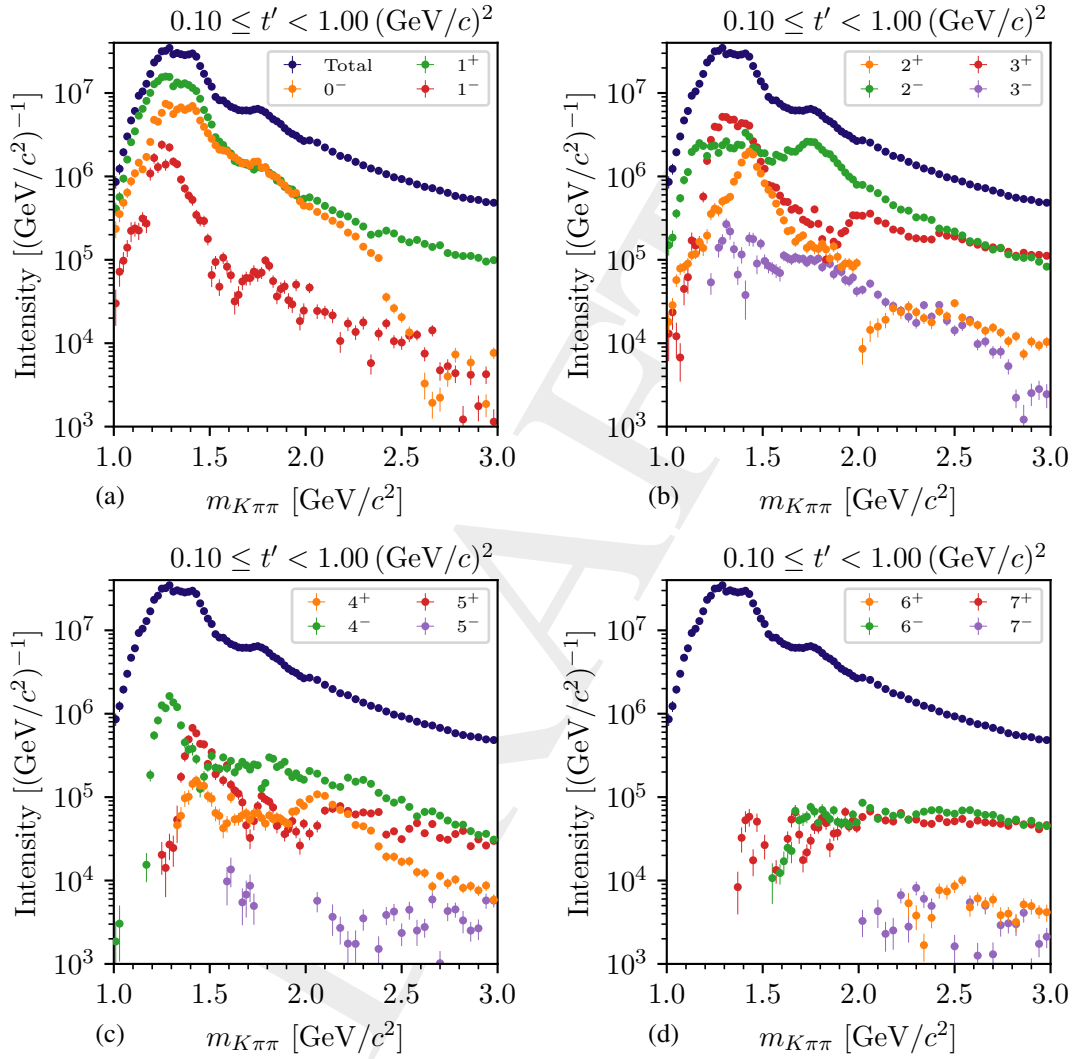


Figure 5.18:  $t'$ -summed spectrum of the total intensity according to equation (5.21) [blue data points in (a) to (d)]. The differently colored data points show for each  $J^P$  included in the 238-wave set the  $t'$ -summed total intensity spectra of all waves with given  $J^P$ .

2269 low-mass region of  $1.2$  to  $1.6 \text{ GeV}/c^2$ . Also, the  $2^-$  waves (green points in figure 5.18b) show  
 2270 intensity in this  $m_{K\pi\pi}$  region. As there are no known or expected resonances with these quantum  
 2271 numbers below about  $1.6 \text{ GeV}/c^2$  (see figure 1.1), these structures require a detailed investigation  
 2272 in systematic and pseudodata studies. The conclusions on this so-called low-mass structures are  
 2273 discussed in section 5.9.

2274 The intensities of partial waves with high spin shown in figure 5.18d exhibit no resonance-like  
 2275 structures. The waves with  $6^+$  (orange points) and  $7^-$  (purple points) quantum numbers do not  
 2276 pick up significant intensity. The  $6^-$  (green points) and  $7^+$  (red points) waves pick up significant  
 2277 intensity only above about  $1.6 \text{ GeV}/c^2$ . Their intensity spectrum is flat. As there are no known  
 2278 or expected strange-meson resonances with such high spins, we suspect the  $J = 6$  and  $7$  waves  
 2279 to be dominated by contributions from non-resonant processes. Especially, Deck-like reactions  
 2280 introduced in section 2.1.1 are known to contribute to partial waves with high spin [11].

2281 Overall, we observe that among waves with odd  $J$ , those with positive parity are enhanced  
 2282 with respect to those with negative parity. For example, the total intensity of  $J^P = 1^+$  waves  
 2283 (green data points in figure 5.18a) is larger than the total intensity of  $1^-$  waves (red data points).  
 2284 For waves with even  $J$  it is vice versa. The waves with enhanced intensity corresponds to  $K_J$   
 2285 states, while those with suppressed intensity correspond to  $K_J^*$  states (see chapter 1). Hence, this  
 2286 observation means that  $K_J$  states contribute more strongly to the  $K^-\pi^-\pi^+$  final state. This can  
 2287 be explained with the fact that many  $K_J^*$  states dominantly decay to the  $K\pi$  final state, while  $K_J$   
 2288 states cannot decay to the  $K\pi$  final state. Hence, assuming that  $K_J^*$  and  $K_J$  states are produced  
 2289 with a similar strength in diffractive scattering, we expect a smaller contribution from  $K_J^*$  states  
 2290 to the  $K^-\pi^-\pi^+$  final state as some of them decay to the  $K\pi$  final state. <sup>[bn]</sup>

2291 We separate in the PWD not only the contributions of intermediate states with given  $J^P$ , but we  
 2292 also distinguish various spin projections  $M^e$  and decay modes when defining the partial waves in  
 2293 equation (5.8). The intensity spectrum of a partial wave is the  $m_{K\pi\pi}$  dependence of its intensity  
 2294 defined equation (5.23). Figures 5.19a, d, and f show the intensity spectra of three selected  
 2295 partial waves. Figure 5.19f shows the intensity spectrum of the  $1^+ 0^+ \rho(770) K S$  partial wave.  
 2296 This wave represents states with  $J^P M^e = 1^+ 0^+$  quantum numbers that decay to the  $\rho(770)$  isobar  
 2297 and the bachelor  $K$  with both in an  $S$ -wave, i.e. with relative orbital angular momentum  $L = 0$ .  
 2298 As the wave-set selection yielded a minimal wave set for each  $(m_{K\pi\pi}, t')$  cell, some waves were  
 2299 selected only in certain  $m_{K\pi\pi}$  regions. For example, the  $1^+ 0^+ \rho(770) K S$  wave was selected only  
 2300 for  $m_{K\pi\pi} \leq 2.5 \text{ GeV}/c^2$  in the second highest  $t'$  bin as shown in figure 5.19f. Furthermore, we do  
 2301 not observe any discontinuity at  $m_{K\pi\pi} = 2 \text{ GeV}/c^2$ , where we doubled the  $m_{K\pi\pi}$  bin width.

2302 The intensity spectrum of the  $1^+ 0^+ \rho(770) K S$  wave exhibits a clear peak at about  $1.3 \text{ GeV}/c^2$ .  
 2303 The PDG lists the well established  $K_1(1270)$  resonance in this mass region. As we expect Breit-  
 2304 Wigner-like resonances to appear as peaks in the intensity spectra (see section 5.1.4), the peak at  
 2305  $1.3 \text{ GeV}/c^2$  is consistent with a  $K_1(1270)$  decaying to  $\rho(770) K$ . In section 7.1 we discuss this  
 2306 signal in detail. Compared to the total intensity spectrum of all  $1^+$  waves shown by the green data

<sup>[bn]</sup>  $K_J^*$  and  $K_J$  states can also decay to other final states, e.g. the  $K\omega$  final state. However, the possibility to decay to the  $K\pi$  final state is the major difference between  $K_J^*$  and  $K_J$  states.

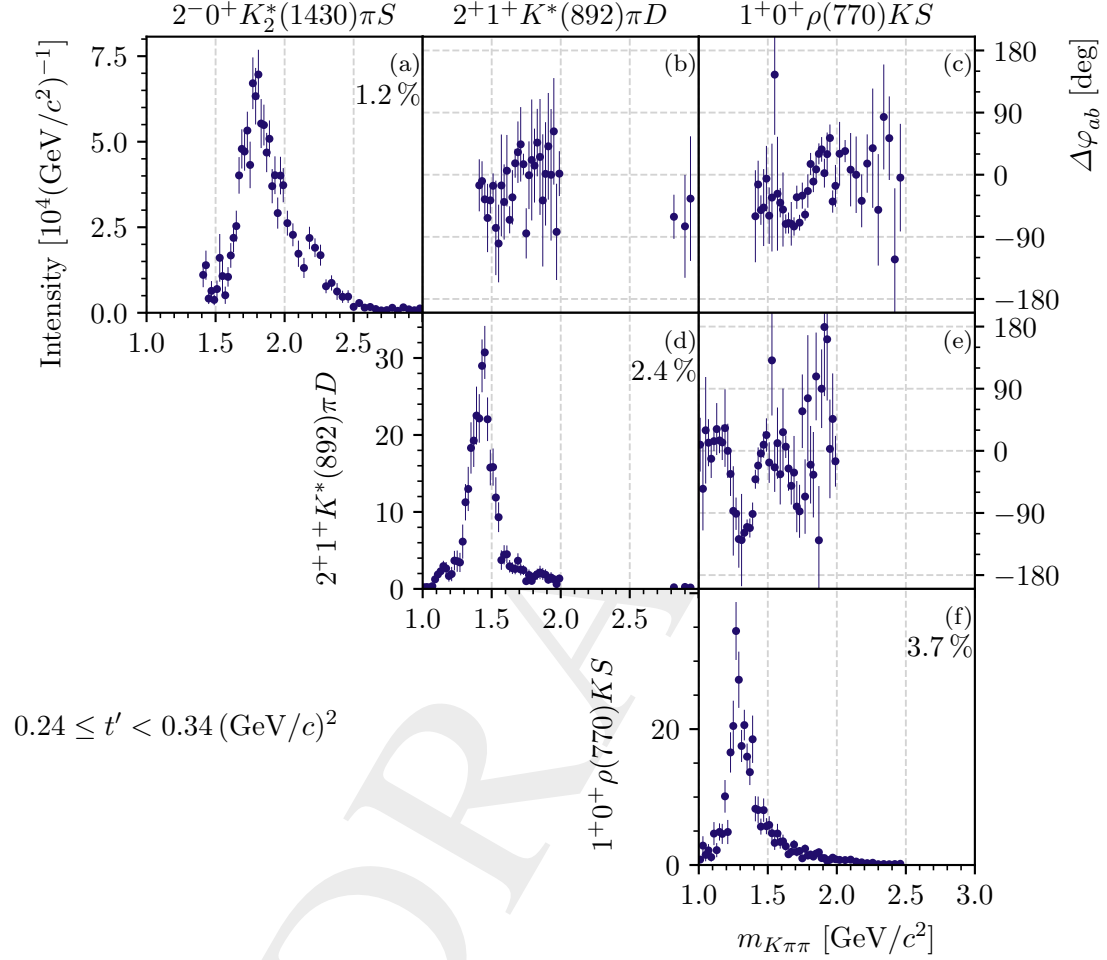


Figure 5.19: Representation of the spin-density matrix for the  $2^- 0^+ K_2^*(1430) \pi S$ ,  $2^+ 1^+ K^*(892) \pi D$ , and  $1^+ 0^+ \rho(770) K S$  waves in the second highest  $t'$  bin. The diagonal elements show the partial-wave intensities as defined in equation (5.23). To account for the different  $m_{K\pi\pi}$  bin widths below and above  $2 \text{ GeV}/c^2$ , the intensities are shown in units of number of events per  $1 \text{ GeV}/c^2$  interval. The off-diagonal elements show the relative phases  $\Delta\varphi_{ab}(m_{K\pi\pi}, t')$  between wave  $a$  (given by the row) and wave  $b$  (given by the column) as defined in equation (5.74). The relative phases represent the interference between partial waves. The percentage number in the upper-right corner of each intensity spectrum is the relative intensity of the corresponding wave as defined in equation (5.76).

2307 points in figure 5.18a, the peak in the  $1^+ 0^+ \rho(770) K S$  wave is more clear. This demonstrates the  
 2308 power of the PWD when studying individual partial waves. The intensity spectrum of the  $2^+ 1^+$   
 2309  $K^*(892) \pi D$  wave shown in figure 5.19d exhibits a clear narrow peak at about  $1.4 \text{ GeV}/c^2$ , i.e. in  
 2310 the mass region of the well-established  $K_2^*(1430)$  resonance. Although the  $2^+$  peak corresponds  
 2311 to only a small fraction of the total intensity (see figure 5.18b), we presumably were able to  
 2312 extract a clean  $K_2^*(1430)$  signal. In section 7.2 we discuss the  $2^+$  waves in detail. The intensity  
 2313 spectrum of the  $2^- 0^+ K_2^*(1430) \pi S$  wave shown in figure 5.19a exhibits a broad peak at about  
 2314  $1.8 \text{ GeV}/c^2$  with a tail towards higher masses. The PDG lists two established resonances with  
 2315  $J^P = 2^-$  in this mass region, the  $K_2(1770)$  and the  $K_2(1820)$ . The high-mass tail might arise  
 2316 from the  $K_2(2250)$  resonance, which is a state that needs further confirmation. The contributions  
 2317 of these resonances can be separated only by modeling the partial-wave amplitudes in the RMF.  
 2318 The results are discussed in section 7.4.

2319 We observe a small backgrounds in the intensity spectra of the partial waves, e.g. below the  
 2320 peak in the intensity spectrum of the  $2^+ 1^+ K^*(892) \pi D$  wave shown in figure 5.19d. These  
 2321 background might arise from background processes that also contribute to the  $K^- \pi^- \pi^+$  sample  
 2322 (see sections 2.1.1 and 5.3). We account of these contributions in the resonance-model fit  
 2323 described in chapter 6. Also, imperfections in the PWD model can bias the estimates, e.g., of the  
 2324 intensity spectra, which might lead to the observed background. We tested such imperfections in  
 2325 the systematic studies presented in section 5.7.

2326 The PWD allows us to study not only the intensity spectra of partial waves but also the interference  
 2327 between them, which is represented by the complex-valued off-diagonal elements of the spin-  
 2328 density matrix. To more clearly see interference effects it is often more instructive to study  
 2329 the phase of a wave  $a$  relative to a reference wave  $b$ , i.e. the relative phase of two partial-waves,  
 2330 which is the phase of the corresponding off-diagonal element of the spin-density matrix:

$$\Delta\varphi_{ab}(m_{K\pi\pi}, t') \equiv \arg \left[ \rho_{ab}(m_{K\pi\pi}, t') \right]. \quad (5.74)$$

2331 The relative phases as a function of  $m_{K\pi\pi}$ , the so-called phase motion, for the selected pairs of  
 2332 waves are shown in figures 5.19b, c, and e. For the rank=3 model employed in this analysis,  
 2333 the relative phases are in general different from the phases of the transition amplitudes of the  
 2334 individual physics processes. In order to interpret the observed relative phases on a qualitative  
 2335 level, we assume that the  $K^- \pi^- \pi^+$  sample is dominated by diffractive scattering into the  $K^- \pi^- \pi^+$   
 2336 final state,<sup>[bo]</sup> which is a coherent process. Inserting equation (5.18) in equation (5.74) yields

$$\begin{aligned} \Delta\varphi_{ab}(m_{K\pi\pi}, t') &= \arg \left[ \sum_z \mathcal{T}_a^z(m_{K\pi\pi}, t') \left[ \mathcal{T}_b^z(m_{K\pi\pi}, t') \right]^* \right] \\ &\approx \arg \left[ \mathcal{T}_a^{z=K\pi\pi}(m_{K\pi\pi}, t') \left[ \mathcal{T}_b^{z=K\pi\pi}(m_{K\pi\pi}, t') \right]^* \right] \\ &= \arg \left[ \mathcal{T}_a^{z=K\pi\pi}(m_{K\pi\pi}, t') \right] - \arg \left[ \mathcal{T}_b^{z=K\pi\pi}(m_{K\pi\pi}, t') \right]. \end{aligned} \quad (5.75)$$

<sup>[bo]</sup> We estimated the incoherent background contributions to be about 10 % (see sections 4.2 and 5.10).

2337 Therefore, the relative phases obtained from the rank=3 PWD can be interpreted in terms of the  
 2338 transition amplitudes of the process  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  on a qualitative level, especially in  
 2339 terms of the amplitudes of resonances decaying to the  $K^- \pi^- \pi^+$  final state. <sup>[bp]</sup>

2340 Figure 5.19e shows the relative phase between the  $a = 2^+ 1^+ K^*(892) \pi D$  wave and the  $b = 1^+ 0^+$   
 2341  $\rho(770) K S$  wave. This phase drops sharply by about  $120^\circ$  around  $1.3 \text{ GeV}/c^2$  and then rises  
 2342 again by about  $120^\circ$  around  $1.4 \text{ GeV}/c^2$ . For Breit-Wigner-like resonances, we expect a rise  
 2343 of the phase of the corresponding amplitude by  $180^\circ$  around the nominal resonance position  
 2344 (see section 5.1.4). The rise around  $1.4 \text{ GeV}/c^2$  is consistent with a dominant contribution of  
 2345 the  $K_2^*(1430)$  resonance to the  $2^+ 1^+ K^*(892) \pi D$  wave. As the  $1^+$  wave enters with a minus  
 2346 sign in equation (5.75), the drop of the phase around  $1.3 \text{ GeV}/c^2$  is consistent with the  $K_1(1270)$   
 2347 resonance dominating the  $1^+ 0^+ \rho(770) K S$  wave. We do not observe full  $180^\circ$  phase motion,  
 2348 because the decreasing phase from the  $K_1(1270)$  is partly compensated by the rising phase of the  
 2349  $K_2^*(1430)$  in the intermediate  $1.35 \text{ GeV}/c^2$  mass region. In addition, non-resonant contributions  
 2350 and incoherent background in the rank=3 PWD model can reduce the height of the phase motion,  
 2351 i.e. can make the relative phases more shallow. The relative phase between the  $2^- 0^+ K_2^*(1430) \pi S$   
 2352 and the  $1^+ 0^+ \rho(770) K S$  wave shown in figure 5.19c rises in the mass region around  $1.8 \text{ GeV}/c^2$ ,  
 2353 where we also observe the peak in the intensity spectrum of the  $2^-$  wave. However, this rise  
 2354 in the relative phase is slower compared to the one in figure 5.19e, which indicates that the  
 2355  $K_2$  states in this mass region have a larger width compared to the  $K_1(1270)$  and the  $K_2^*(1430)$ .  
 2356 This would be consistent with previous observations [9]. As the  $2^- 0^+ K_2^*(1430) \pi S$  wave shows  
 2357 no significant structures below about  $1.6 \text{ GeV}/c^2$  and the  $2^+ 1^+ K^*(892) \pi S$  wave shows no  
 2358 significant structures above about  $1.6 \text{ GeV}/c^2$ , the two waves do not share a mass region where  
 2359 both have large intensities. Therefore, their relative phase shown in figure 5.19b has a large  
 2360 uncertainty. This means, in order to obtain phase information from the PWD, we have to study  
 2361 at least two waves simultaneously. In addition, these waves must have significant intensities in  
 2362 overlapping  $m_{K\pi\pi}$  regions in order to reliably determine their relative phase.

2363 As shown by the red data points in figure 5.18, the  $1^+$  waves contribute most to the total intensity.  
 2364 The  $1^+ 0^+ \rho(770) K S$  wave is one of the largest waves in the 238-wave set. It contributes about  
 2365 4 % to the total intensity. This so-called relative intensity,

$$\frac{\sum_{t', m_{K\pi\pi}} \rho_{aa}(m_{K\pi\pi}, t')}{\sum_{t', m_{K\pi\pi}} \sum_{a,b} \rho_{ab}(m_{K\pi\pi}, t') I_{ab}(m_{K\pi\pi}, t')} = \frac{\sum_{t', m_{K\pi\pi}} \widehat{N}_a(m_{K\pi\pi}, t')}{\sum_{t', m_{K\pi\pi}} \widehat{N}_{\text{ev}}(m_{K\pi\pi}, t')}, \quad (5.76)$$

2366 is the ratio of the intensity of the wave summed over all  $(m_{K\pi\pi}, t')$  cells and the total intensity  
 2367 defined in equation (5.21) summed over all  $(m_{K\pi\pi}, t')$  cells. The latter one takes into account the  
 2368 interference between partial waves. This equals to the ratio of predicted number  $\widehat{N}_a$  of produced

<sup>[bp]</sup> For the expert: We calculated the degree of coherence as defined in equation (H.1) of ref. [72]. For example, in the second highest  $t'$  bin the degree of coherence between the  $2^+ 1^+ K^*(892) \pi D$  and  $1^+ 0^+ \rho(770) K S$  waves shown in figure 5.19 is mainly above 0.6 for  $m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$ , i.e. in the  $m_{K\pi\pi}$  region of the peaks in both waves. This value is sufficiently large to interpret the relative phase between both waves in the  $m_{K\pi\pi}$  region of the peaks in terms of the transition amplitudes of the process  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  on a qualitative level.

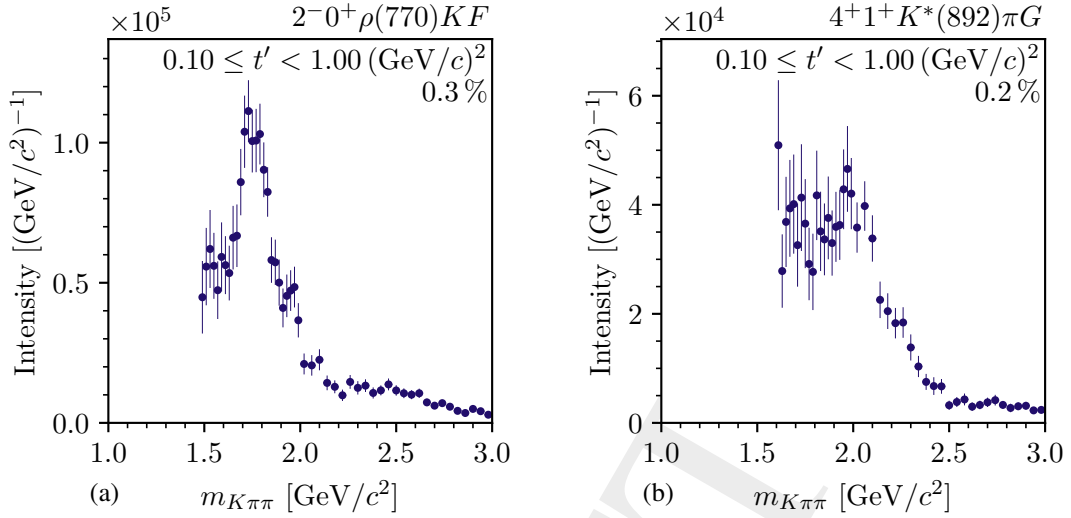


Figure 5.20:  $t'$ -summed intensity spectra, i.e. the partial-wave intensities in each  $m_{K\pi\pi}$  bin summed over the analyzed  $t'$  bins, of (a) the  $2^- 0^+ \rho(770) K F$  wave and (b) the  $4^+ 1^+ K^*(892) \pi G$  wave. To account for the different  $m_{K\pi\pi}$  bin widths below and above  $2 \text{ GeV}/c^2$ , the intensities are shown in units of number of events per  $1 \text{ GeV}/c^2$  interval. The percentage number in the upper-right corner of each intensity spectrum is the relative intensity of the corresponding wave as defined in equation (5.76).

2369 events in all cells if there would be only wave  $a$  and the total predicted number  $\widehat{N}_{\text{ev}}$  of produced  
 2370 events in all cells. <sup>[bq]</sup>

2371 We observe signals not only in comparably large waves at the percent level, e.g. the waves that  
 2372 are shown in figure 5.19, but also in waves at the per-mill level. In figure 5.20 we show the  
 2373  $t'$ -summed intensity spectra, i.e. the intensity of the partial waves according to equation (5.23)  
 2374 summed over the analyzed  $t'$  bins, of two small waves. The  $2^- 0^+ \rho(770) K F$  wave shown in  
 2375 figure 5.20a exhibits a narrow peak at about  $1.8 \text{ GeV}/c^2$ . The peak is in the same mass region as  
 2376 the peak in the  $2^- 0^+ K_2^*(1430) \pi S$  wave shown in figure 5.19a. This is expected, because both  
 2377 waves have the same  $J^P$  quantum numbers and hence the same  $K_2$  states should appear in both  
 2378 waves. However, the two  $2^-$  waves represent different decay modes, i.e. the  $\rho(770) K F$ -wave  
 2379 and the  $K_2^*(1430) \pi S$ -wave decays. The various  $K_2$  states may couple to these two decay modes  
 2380 with different strengths, which can explain the different shapes of the intensity spectra, e.g. the  
 2381 narrower peak in the  $2^- 0^+ \rho(770) K F$  wave compared to the  $2^- 0^+ K_2^*(1430) \pi S$  wave. It is one  
 2382 of the advantages of the  $K^- \pi^- \pi^+$  final state, that we can study the same states in different decay  
 2383 modes in a single consistent analysis.

2384 In contrast to the high-mass tail, the low-mass tail of the intensity spectrum of the  $2^- 0^+$   
 2385  $\rho(770) K F$  wave does become small, as it would be expected, but instead levels out at an  
 2386 intensity of about  $0.5 \times 10^5 / (\text{GeV}/c^2)$  for masses down to about  $1.5 \text{ GeV}/c^2$ . Below  $1.5 \text{ GeV}/c^2$   
 2387 the wave-set selection did not include this wave in the PWD model. We observe similar

<sup>[bq]</sup> Unfortunately, the relative intensities are biased by the so-called leakage effect. The relative intensities can still be used as measure of whether a wave is large or small as discussed in section 5.9.1.

2388 enhanced low-mass tails also for other small partial waves at the per-mill level, e.g. for the  $4^+ 1^+$   
2389  $K^*(892)\pi G$  wave shown in figure 5.20b. The high-mass tail of a potential signal from the  
2390 well-known  $K_4^*(2045)$  resonance above  $2 \text{ GeV}/c^2$  is clearly visible, but below  $2 \text{ GeV}/c^2$  the  
2391 intensity is almost constant down to a mass of about  $1.6 \text{ GeV}/c^2$ , below which the wave-set  
2392 selection did not select this wave. As the  $K_4^*(2045)$  is the lightest known  $4^+$  state, we would  
2393 expect the intensity of the  $4^+ 1^+ K^*(892)\pi G$  wave to become small below the nominal  $K_4^*(2045)$   
2394 mass of about  $2 \text{ GeV}/c^2$ . Furthermore, the amplitude of this wave is suppressed at low masses,  
2395 because of the additional energy needed to produced its high spin of  $J = 4$  and its large orbital  
2396 angular momentum of  $L = 4$ .<sup>[br]</sup> Similar arguments hold for the enhanced low-mass tail in the  
2397  $2^- 0^+ \rho(770) K F$  wave. Therefore, we suspect these enhanced low-mass tails to be artifacts of  
2398 our analyses. They may arise from the incoherent background in our data, which is studied in  
2399 section 5.10 or from imperfections in the analysis model, which are tested in various systematic  
2400 studies discussed in section 5.7. Furthermore, the enhanced low-mass tails are less pronounced  
2401 when using a rank=1 PWD model of the 238-wave set, which has about three times fewer free fit  
2402 parameters than the used rank=3 model. As the 238-wave set was constructed using a rank=1  
2403 model (see section 5.2), the rank=3 model may contain more parameters than can be reliably  
2404 determined from data. This additional freedom of the rank=3 model might be misused by the  
2405 fit to account for imperfections of the PWD model, e.g. by leading to destructive interference,  
2406 and thereby causing such enhanced low-mass tails. Apart from the enhanced low-mass tails, we  
2407 do not observe any signs that would indicate a too large PWD model. For example, too large  
2408 models typically suffer from multimodality, but we reliably found the best fit result as discussed  
2409 at the beginning of this section. In contrast to the low-mass structures observed e.g. in the  $3^+$   
2410 waves as discussed above, the enhanced low-mass tails do not show any peaking resonance-like  
2411 signals. In addition, the enhanced low-mass tails are only a small effect. They only affect small  
2412 partial waves at the per-mill level. In this analysis, we focus mostly on large partial waves.

2413 In our data, the  $K_4^*(2045)$  is only a small signal at the per-mill level that is potentially affected by  
2414 model imperfection as discussed above. However, in general it is a well-established resonance  
2415 observed by various previous experiments and its mass and width are known [28, 120–122].  
2416 Therefore, we use the  $K_4^*(2045)$  as a kind of standard candle in our analysis. It allows to test the  
2417 reliability of our results. Our results for the  $K_4^*(2045)$  resonance are discussed in section 7.3.

2418 From this first glimpse of the results of the PWD we conclude that the fits yielded stable and  
2419 consistent results. We observe resonance-like signals in various partial waves in  $m_{K\pi\pi}$  regions  
2420 of well known strange-meson resonances. We also observe potential signals of excited states  
2421 that need further confirmation such as the  $K_2(2250)$ . Before modeling these signals in the  
2422 resonance-model fit presented in chapter 6 and interpreting them in chapter 7, we further study  
2423 the reliability of the results of the PWD. To do so, we compare in section 5.6 the predictions  
2424 of the PWD model with optimized parameters for kinematic distributions to the corresponding  
2425 measured distributions. In section 5.7 we study the influence of systematic effects from the  
2426 event selection and the PWD. In section 5.8 we study the consistency of the PWD based on a  
2427 pseudodata sample for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . Finally, in section 5.10, we study the  
2428 influence of incoherent background from the reaction  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  on our results.

<sup>[br]</sup> In the PWD model described in section 5.1, this effect is modeled by the angular-momentum barrier factors.



## 2429 5.6 Agreement between Partial-Wave Model and Data

2430 The goal of the construction of the 238-wave set presented in section 5.2 was to find a minimal  
 2431 set of waves that is sufficient to describe the data. In this section, we study how well the result of  
 2432 the PWD fit using the 238-wave set describes the  $K^-\pi^-\pi^+$  sample. The maximum-likelihood  
 2433 formalism presented in section 5.1.3 does not directly yield a goodness-of-fit criterion. Therefore,  
 2434 we compare the predictions of the PWD model for the kinematic distributions of the measured  
 2435 final-state particles according to equation (5.30) using the parameter estimates from the 238-wave  
 2436 PWD, <sup>[bs]</sup>the so-called PWD predictions, to the corresponding measured distributions.

2437 The five-dimensional phase space of the  $K^-\pi^-\pi^+$  final state can be represented by four angles  
 2438 and the invariant mass of one of the three two-body subsystems as discussed in section 5.1.1.  
 2439 Hence, different representations of the same  $K^-\pi^-\pi^+$  kinematics are possible, depending on  
 2440 which two final-state particles are in the two-body isobar system. We consider here the  $K^-\pi^+$   
 2441 and  $\pi^-\pi^+$  isobar systems. The five phase-space variables are the decay angles  $\cos\theta_{GJ}$  and  $\phi_{GJ}$  of  
 2442 the isobar in the decay  $X^- \rightarrow \xi^0 b^-$  defined in the Gottfried-Jackson rest frame of  $X^-$ ; the decay  
 2443 angles  $\cos\theta_{HF}$  and  $\phi_{HF}$  of the  $K^-$  or  $\pi^-$  in the decay  $\xi^0 \rightarrow K^-\pi^+$  or  $\xi^0 \rightarrow \pi^-\pi^+$ , respectively,  
 2444 defined in the helicity rest frame of the  $\xi^0$ ; and the invariant mass  $m_{K^-\pi^+}$  or  $m_{\pi^-\pi^+}$ , respectively,  
 2445 of the two-body isobar system.

2446 In order to visualize the five-dimensional phase-space distribution, we show one- and two-  
 2447 dimensional projection in the following. Figure 5.21 shows exemplarily the measured  $K^-\pi^-\pi^+$   
 2448 distribution (blue data points) and the corresponding PWD predictions (orange histograms),  
 2449 in the  $m_{K\pi\pi}$  region of the  $K_1$  double-peak in the five phase-space variables defined for the  
 2450  $\pi^-\pi^+$  isobar system. The distributions of all analyzed  $m_{K\pi\pi}$  regions and for both, the  $\pi^-\pi^+$  and  
 2451 the  $K^-\pi^+$  isobar systems can be found in appendix D.2 in figures D.36 to D.47. Overall, the  
 2452 PWD predictions agree well with the corresponding measured distributions. The PWD model  
 2453 reproduces the features of the angular distributions of the  $X^-$  decay, exemplarily shown in  
 2454 figures 5.21a and 5.21b, and of the isobar decay, exemplarily shown in figures 5.21c and 5.21d.  
 2455 As the angular distributions represent the spin and orbital angular momentum of the contributing  
 2456 partial waves, this agreement suggests that we do not miss important waves with certain  $J$  and  $L$   
 2457 in the wave set, i.e. limiting ourselves to  $J \leq 7$  and  $L \leq 7$  when constructing the wave pool was  
 2458 sufficient; and that the wave-set selection selected the significant waves. The structures observed  
 2459 in the angular distributions in figures 5.21a to 5.21d are hard to interpret directly, because they  
 2460 arise not only from waves with  $\pi^-\pi^+$  isobars, but also from waves with  $K^-\pi^+$  isobars. The latter  
 2461 ones have a complicated distribution in the phase-space variables defined for the  $\pi^-\pi^+$  isobar  
 2462 system. Figure 5.21e shows the  $m_{\pi^-\pi^+}$  spectrum, which exhibits a clear peak from the  $\rho(770)$   
 2463 resonances at about  $0.8 \text{ GeV}/c^2$  and two shoulders: one in the mass region of the  $f_0(980)$  at about  
 2464  $1 \text{ GeV}/c^2$  and one in the mass region of the  $f_2(1270)$  at about  $1.3 \text{ GeV}/c^2$ . The  $m_{K^-\pi^+}$  spectrum  
 2465 shown in figure 5.22a exhibits a clear  $K^*(892)$  signal at about  $0.9 \text{ GeV}/c^2$  and a second peak in  
 2466 the mass region of the  $K_0^*(1430)$  and  $K_2^*(1430)$  resonances. All these structures are reproduced

<sup>[bs]</sup> We determined the histograms that show the PWD predictions by weighting a reconstructed phase-space pseudodata sample using weights that are proportional to the model intensity in equation (5.16) using the parameter estimates from the 238-wave PWD. See appendix C.3 for details.

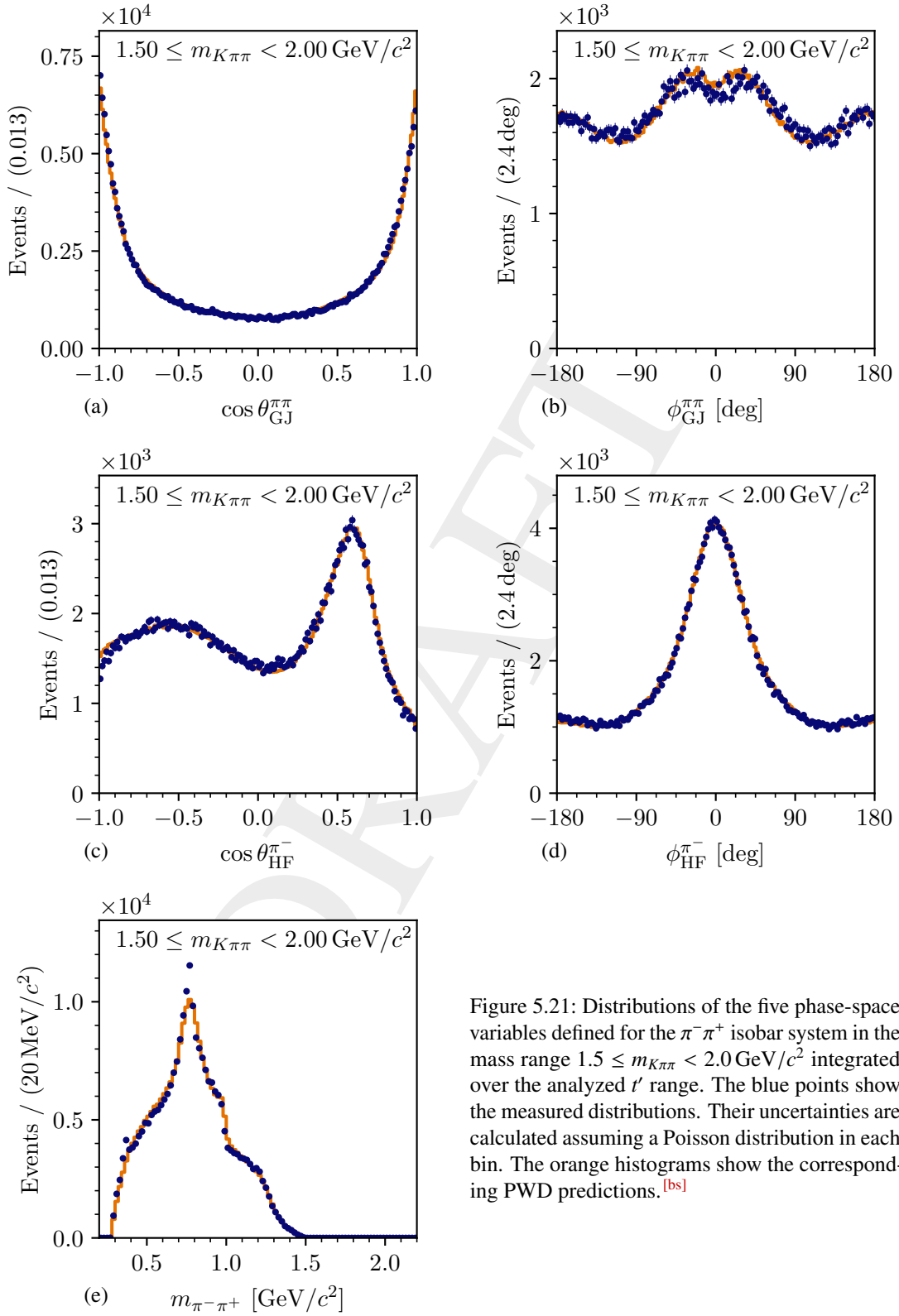


Figure 5.21: Distributions of the five phase-space variables defined for the  $\pi^- \pi^+$  isobar system in the mass range  $1.50 \leq m_{K\pi\pi} < 2.00 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. Their uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD predictions.<sup>[bs]</sup>

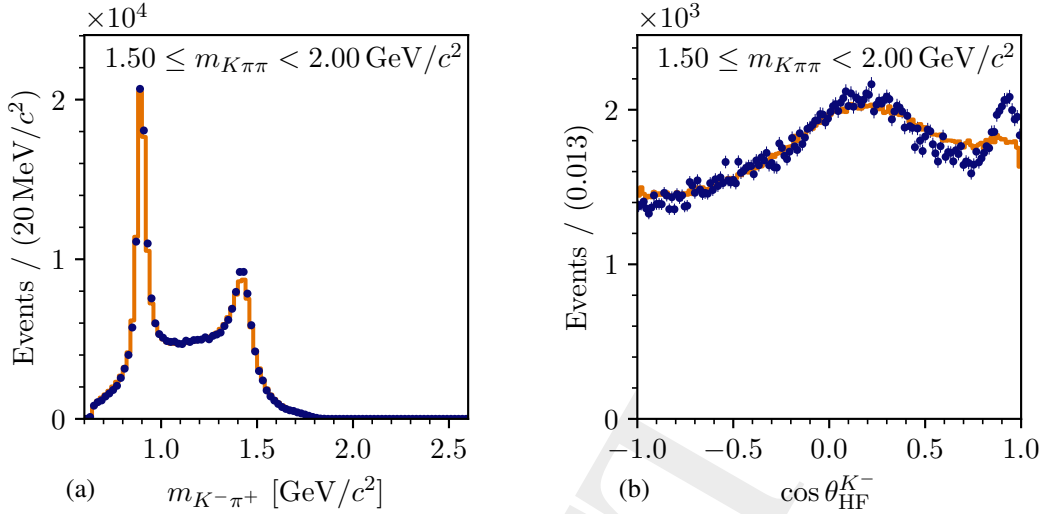


Figure 5.22: Distributions of two phase-space variables defined for the  $K^-\pi^+$  isobar system in the mass range  $1.5 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD predictions. (a) shows the distribution in  $m_{K^-\pi^+}$ . (b) shows the distribution in  $\cos \theta_{\text{HF}}^{K^-}$  of the decay  $\xi_{K^-\pi^+}^0 \rightarrow K^-\pi^+$ .

2467 well by the PWD model; which suggest that we do not miss isobar resonances that contribute  
 2468 significantly to the data, i.e. that the list of isobar resonances considered when constructing the  
 2469 wave pool was sufficient (see table 5.2).

2470 However, we also observe regions where the PWD model does not perfectly reproduce the  
 2471 measured distributions. The angular distributions of the  $X^-$  decay are not perfectly described as  
 2472 shown, e.g. in figure 5.21b. This imperfection becomes more apparent in the 2D distribution of the  
 2473 Gottfried-Jackson angles, i.e. when not marginalizing over  $\cos \theta_{\text{GJ}}^{\pi\pi}$  or  $\phi_{\text{GJ}}^{\pi\pi}$ . The difference between  
 2474 the measured distribution in the Gottfried-Jackson angles and the corresponding PWD prediction  
 2475 is shown in figure 5.23a relative to the expected standard deviation in each  $(\cos \theta_{\text{GJ}}^{\pi\pi}, \phi_{\text{GJ}}^{\pi\pi})$  cell  
 2476 according to a Poisson distribution. We observe a band (blue region) where the PWD model  
 2477 underestimates the measured number of events. This band coincides with the kinematic region  
 2478 where the acceptance changes most and practically vanishes as shown by the dark blue region  
 2479 in figure 5.23b. This strong modulation of the acceptance is caused by the limited momentum  
 2480 range of the final-state particle identification by the RICH detector (see section 3.2.2). The  
 2481 imperfection in the description of the measured distributions by the PWD model may indicate  
 2482 that the treatment of acceptance effects caused by the RICH is not complete (see appendix C.2.3  
 2483 for details on how we modeled the RICH acceptance). We studied the robustness of the PWD  
 2484 results against incompleteness in the treatment of the RICH acceptance in the systematic studies  
 2485 described in section 5.7. The acceptance for the reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  is discussed in  
 2486 appendix D.2.

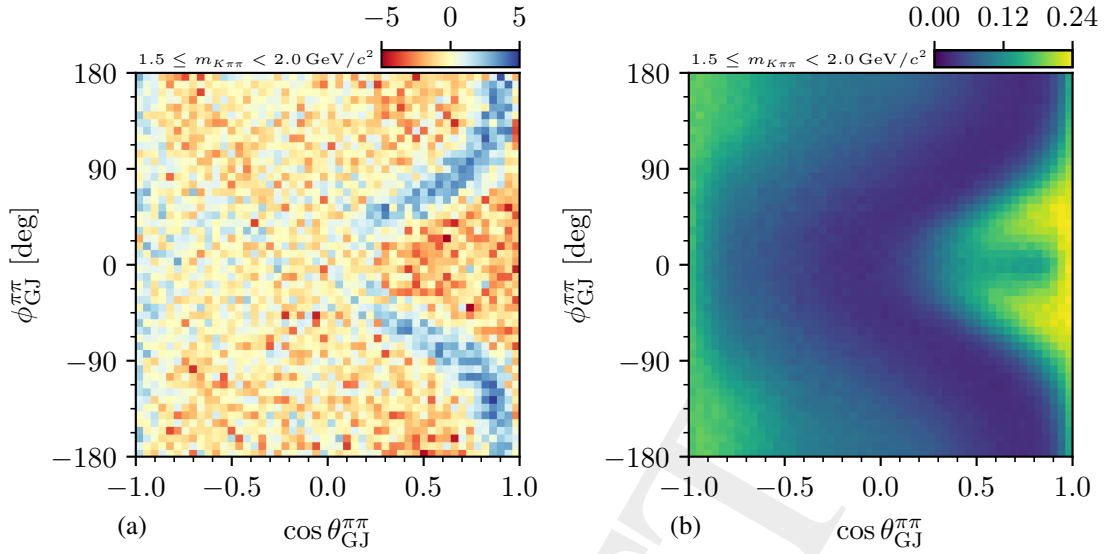


Figure 5.23: Distribution of the two two-body decay angles for the decay  $X^- \rightarrow \xi_{\pi\pi^+}^0 K^-$  in the mass range  $1.5 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. (a) shows the difference between the measured number of events and the corresponding PWD prediction<sup>[bs]</sup> divided by the square root of the PWD prediction. (b) shows the acceptance.

2487 As discussed in section 4.2, we expect about 4 % background from events of the reaction  $K^- + p \rightarrow$   
 2488  $K^- K^- K^+ + p$  in the  $K^- \pi^- \pi^+$  sample. A part of these background events, where the  $K^- K^- K^+$   
 2489 subsystem arises from a  $\phi(1020)$  decay, manifests itself in a narrow peak at about  $0.38 \text{ GeV}/c^2$   
 2490 in the  $m_{\pi^- \pi^+}$  spectrum observed in the measured data (blue data points in figure 5.21e). As  
 2491 expected, this  $\phi(1020)$  peak is not reproduced by the PWD model as the 238-wave set is not  
 2492 able to effectively describe such a narrow signal. Furthermore, the background from  $\phi(1020)$   
 2493 decays is more pronounced at  $m_{K\pi\pi}$  above  $2 \text{ GeV}/c^2$  than in the low- $m_{K\pi\pi}$  region (compare  
 2494 figures D.36e and D.40e). The  $K^- K^- K^+$  background should be also visible in the phase-space  
 2495 variables defined for the  $K^- \pi^+$  isobar system. For example, we observe an enhancement at  
 2496  $\cos \theta_{\text{HF}}^{K^-} \approx 0.9$  as shown in figure 5.22b, which is not reproduced by the PWD model, similar to  
 2497 the  $\phi(1020)$  peak in the  $m_{\pi^- \pi^+}$  spectrum. This enhancement accounts for about 2 % of the total  
 2498 distribution. We expect this enhancement to mainly arise from part of the about 4 %  $K^- K^- K^+$   
 2499 background, because the angular distribution as predicted from a simplified model for the reaction  
 2500  $K^- + p \rightarrow K^- \phi(1020) + p$  with  $\phi(1020) \rightarrow K^- K^+$  strongly peaks at  $\cos \theta_{\text{HF}}^{K^-} \approx 0.95$ , similar  
 2501 to the enhancement observed in our data.<sup>[bt]</sup> Hence, the discrepancies between the measured  
 2502 distribution and the PWD prediction discussed in this paragraph are mainly due to the non-  
 2503 description of part of the  $K^- K^- K^+$  background. The other part of the  $K^- K^- K^+$  background  
 2504 is effectively taken into account by using a rank=3 PWD model as discussed in section 5.3.  
 2505 We do not expect that this small non-description biases significantly the physics results of this  
 2506 analysis, i.e. the measurement of the resonance parameters discussed in chapter 6. The  $K^- K^- K^+$   
 2507 background belongs to a different coherent sector than the  $K^- \pi^- \pi^+$  resonance contribution that we

<sup>[bt]</sup> We generated a pseudodata sample of the reaction  $K^- + p \rightarrow K^- \phi(1020) + p$  with  $\phi(1020) \rightarrow K^- K^+$ , because the events from  $\phi(1020)$  decays are a significant contribution to the total  $K^- K^- K^+$  background. We used a simplified model based on the findings in ref. [37] and analyzed this pseudodata sample applying the  $K^- \pi^- \pi^+$  hypothesis.

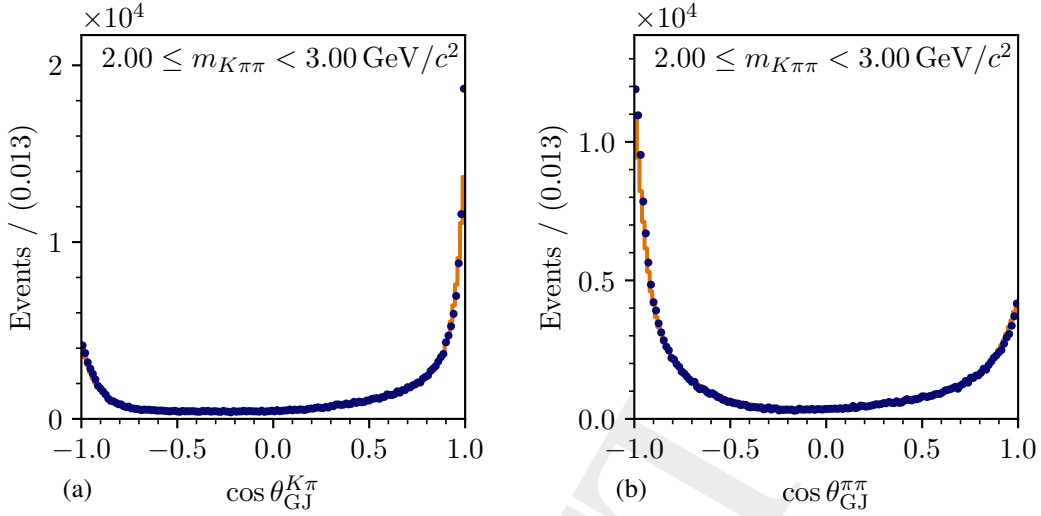


Figure 5.24: Agreement between PWD model and data in the mass range  $2.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD predictions. (a) shows the distribution in  $\cos \theta_{\text{GJ}}^{K\pi}$  of the decay  $X^- \rightarrow \xi_{K^- \pi^+}^0 \pi^-$ . (b) shows the distribution in  $\cos \theta_{\text{GJ}}^{\pi\pi}$  of the decay  $X^- \rightarrow \xi_{\pi^- \pi^+}^0 K^-$ .

2508 are interested in. Furthermore, we tested the robustness of the PWD results against the influence  
 2509 of the  $K^- K^- K^+$  background contributions in the systematic studies of the final-state particle  
 2510 identification discussed in section 5.7.1, because weaker or more restrictive particle-identification  
 2511 cuts change the fraction of the  $K^- K^- K^+$  background in the  $K^- \pi^- \pi^+$  sample.

2512 Figure 5.24 shows the  $\cos \theta_{\text{GJ}}$  distributions for the  $X^-$  decay in the  $m_{K\pi\pi}$  region above  $2 \text{ GeV}/c^2$ .  
 2513 The distribution for the decay to the  $K^- \pi^+$  isobar system shown in figure 5.24a peaks strongly  
 2514 towards  $\cos \theta_{\text{GJ}}^{K\pi} = +1$ , i.e. we observe an enhancement of events where the  $K^- \pi^+$  system goes  
 2515 in forward direction with respect to the direction of the beam  $K^-$  in the  $K^- \pi^- \pi^+$  center-of-  
 2516 momentum frame. The distribution for the decay to the  $\pi^- \pi^+$  isobar system shown in figure 5.24b  
 2517 peaks strongly towards  $\cos \theta_{\text{GJ}}^{\pi\pi} = -1$ , i.e. we observe an enhancement of events where the  $\pi^- \pi^+$   
 2518 system goes backwards in the  $K^- \pi^- \pi^+$  center-of-momentum frame. This behavior is consistent  
 2519 with models for non-resonant production. In Deck-like reactions, the  $K^- \pi^+$  system is produced  
 2520 at the upper vertex by exchanging a virtual pion (see figure 2.2a), so that the  $K^- \pi^+$  system goes  
 2521 mainly in the direction of the beam  $K^-$  leading to a peak at  $\cos \theta_{\text{GJ}}^{K\pi} = +1$ . Kinematically, this  
 2522 peak becomes sharper at higher  $m_{K\pi\pi}$  [123]. In central-production reactions (see figure 2.3a),  
 2523 the beam  $K^-$  scatters elastically and a  $\pi^- \pi^+$  system is produced approximately at rest in the  
 2524 overall  $K_{\text{beam}}^- p_{\text{target}}$  center-of-momentum frame. In the Gottfried-Jackson angles defined in the  
 2525  $K^- \pi^- \pi^+$  center-of-momentum frame, this translates to  $\cos \theta_{\text{GJ}}^{\pi\pi} \approx -1$ . At high  $m_{K\pi\pi}$ ,  $\cos \theta_{\text{GJ}}^{\pi\pi}$   
 2526 is kinematically anti-correlated with  $\cos \theta_{\text{GJ}}^{K\pi}$ . Therefore, we attribute both peaks at  $\cos \theta_{\text{GJ}}^{K\pi} = +1$   
 2527 and  $\cos \theta_{\text{GJ}}^{\pi\pi} = -1$  in our data to both, Deck-like and central-production reactions. Based only  
 2528 on the angular distributions we cannot separate the two processes.<sup>[bu]</sup> The narrow peaks in the

<sup>[bu]</sup> Deck-like reactions with pion exchange exhibit structures from  $K^- \pi^+$  resonances in the  $m_{K^- \pi^+}$  distribution and

2529 measured angular distributions can be described fairly well by the PWD model mainly by using  
 2530 partial waves with high spin  $J \gtrsim 5$  shown in figures 5.18c and 5.18d. The description of the  
 2531 non-resonant processes in terms of partial waves requires in principle infinitely high spins [124],  
 2532 but including waves with  $J \gg 7$  in the wave pool would significantly increase its size. Thus, we  
 2533 decided to consider only waves with  $J \leq 7$  when constructing the wave pool in section 5.2.1, at  
 2534 the expense of small imperfections in the description of the  $\cos \theta_{\text{GJ}}$  distribution for  $\cos \theta_{\text{GJ}}^{K\pi} \approx +1$   
 2535 and accordingly  $\cos \theta_{\text{GJ}}^{\pi\pi} \approx -1$  at high  $m_{K\pi\pi}$ .<sup>[bv]</sup>

2536 Overall, the PWD model describes the kinematic distributions of the  $K^-\pi^-\pi^+$  sample well.  
 2537 Therefore, we conclude that the PWD fit yielded reliable results that can be interpreted in terms  
 2538 of physics signals. The small remaining imperfections can be attributed to non-resonant and  
 2539 incoherent background contributions, for which the  $K^-\pi^-\pi^+$  partial waves were not constructed,  
 2540 or to potential imperfections of the detector model used to estimate the acceptance. We test the  
 2541 influence of these imperfections in the systematic studies discussed in the following section 5.7.

## 2542 5.7 Systematic Studies

2543 Given the increasing size of data samples from high-precision experiments, the statistical uncer-  
 2544 tainties become smaller and uncertainties imposed by systematic effects play a more important  
 2545 role. This underlines the importance of performing detailed systematic studies to test the influ-  
 2546 ence of systematic effects on the analysis results. For example, the systematic uncertainties of  
 2547 measured masses and widths of isovector light-meson resonances observed in the COMPASS  
 2548  $\pi^-\pi^-\pi^+$  analysis are more than a factor 10 larger compared to the corresponding statistical  
 2549 uncertainties [41].

2550 Acceptance effects were taken into account in the PWD fits as explained in section 5.1.3.  
 2551 Nonetheless, the model for the acceptance may be imperfect, which may introduce systematic  
 2552 effects in the results of the PWD. This holds especially for analyses where the acceptance is  
 2553 strongly modulated in the kinematic variables in which the analysis is performed, as it is the case  
 2554 in this work (see figure 5.23b and appendix D.2). The strongest acceptance effect in the  $K^-\pi^-\pi^+$   
 2555 sample arises from the limited kinematic range of the final-state particle identification by the  
 2556 RICH detector. Also, the misidentification of final-state particles by the RICH is the largest  
 2557 source of background events in the  $K^-\pi^-\pi^+$  sample. Therefore, we present in section 5.7.1 three  
 2558 systematic studies that test the influence of the final-state particle identification on the results of  
 2559 the PWD.

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a continuous spectrum in the  $m_{\pi^-\pi^+}$  distribution, while central-production reactions with a centrally produced  $\pi^-\pi^+$  system exhibit structures from  $\pi^-\pi^+$  resonances in the  $m_{\pi^-\pi^+}$  distribution and a continuous spectrum in the  $m_{K^-\pi^+}$  distribution. Still, based only on kinematics the two processes cannot be separated completely, because their kinematic distributions overlap.

<sup>[bv]</sup> In the COMPASS  $\pi^-\pi^-\pi^+$  analysis, first studies were performed of including models for Deck and central-production amplitudes into the PWD model to account for non-resonant contributions [43, 125]. In these studies, the description of the data by the model improved. However, these studies did not yield a convincing description of all non-resonant contributions yet [125].

Another important source of systematic effects are assumptions entering the PWD model. The most critical of these assumptions is the used wave set. In order to minimize systematic effects caused by the chosen wave set, we inferred the wave set from data using the model-selection techniques discussed in section 5.2. Nonetheless, the employed wave-set selection method may induce systematic effects in the selected wave set and thereby in the PWD results. To test for such effects, we present in section 5.7.2 an alternative approach for the wave-set selection.

In order to estimate the systematic effects, we compare in the following the results from the studies to those from the 238-wave PWD of the main analysis shown in section 5.5. In particular, we compare intensity spectra of partial waves, representative for the results of the PWD. However, performing a Bootstrapping of the PWD fit as done in the main analysis (see section 5.4) is computationally too expensive and cannot be done for the systematic studies. Thus, we show in sections 5.7.1 and 5.7.2 the maximum-likelihood estimates of the partial-wave intensities. As for the main analysis, we expect the bias from using the maximum-likelihood estimates to be small on average (see figure 5.13b). As the maximum-likelihood estimates of the uncertainties are strongly biased towards larger values (see section 5.4), we do not show error bars for the results of the systematic studies. For the results of the main analysis, we show the estimates from Bootstrapping for the values and uncertainties as in the rest of the text.

### 5.7.1 Final-State Particle Identification

In order to test for systematic effects introduced by the final-state particle identification, we performed three systematic studies where we changed the acceptance and the misidentification probability of the final-state particle identification in three different ways. We accounted for the different acceptances by adjusting our acceptance model accordingly in the PWD fits. We used the 238-wave set for the PWD, which is also used in the main analysis. In these RICH studies we tested three aspects: (i) can the acceptance model reproduce the corresponding change in the RICH acceptance; (ii) are the results of the PWD sensitive to the shape of the acceptance; and (iii) is the PWD result robust with respect to bias caused by misidentified final-state particles?

The probabilities to identify and misidentify a final-state particle are functions of the particle momentum that change when changing the RICH likelihood-ratio threshold  $\mathcal{T}_R$  as shown in figure 3.13. Especially, the region between 30 and 60 GeV/c, where the efficiency drops, is sensitive to the choice of  $\mathcal{T}_R$ . We performed two systematic studies in which we changed  $\mathcal{T}_R$ .

In one study, we used a weaker RICH threshold of  $\mathcal{T}_R = 1.05$  instead of 1.15, which is used in the main analysis. Using a lower RICH threshold increases the fraction of misidentified  $K^-$  and  $\pi^-$  in the final state to about 8 %, which is a factor of 4 larger than in the main analysis (see figure 3.14). In addition, the size of the data sample in this study is about 17 % larger than in the main analysis. Also, the momentum range, in which the RICH identifies a particle efficiently, is slightly enlarged when using the weaker RICH threshold (see figure 3.13a). Thus, we have access to a larger fraction of the  $K^- \pi^- \pi^+$  phase-space in this study, which adds more information to the PWD fit, at the expense of a reduced purity of the sample.

2598 In the second study, we used a more restrictive RICH threshold of  $\mathcal{T}_R = 1.30$  instead of 1.15.  
 2599 This reduces the misidentification probability only marginally, while it introduces much stronger  
 2600 acceptance effects. In this study, the size of the data sample is about 30 % smaller than in the  
 2601 main analysis. One should note, that for such a significantly reduced data sample the 238-wave  
 2602 set, which was selected based on the larger  $K^-\pi^-\pi^+$  sample of the main analysis, might be too  
 2603 large. This might introduce artifacts from overfitting in the PWD.

2604 As presented in section 5.6, we observe imperfections in the description of the data by the PWD  
 2605 model in kinematic regions where the acceptance decreases rapidly. These imperfections may  
 2606 be caused by imperfections of the employed acceptance model in these regions. Therefore, we  
 2607 excluded in the third RICH study the region in the final-state particle momenta, in which the  
 2608 identification probability decreases most rapidly, i.e. we limited the RICH particle identification  
 2609 to momenta below 40 GeV/c instead of 60 GeV/c, which was used in the main analysis. This  
 2610 hard cut in the particle momenta can be perfectly reproduced by the acceptance model in this  
 2611 study, while modeling the momentum dependence of the particle-identification probability as  
 2612 done in the main analysis (see appendix C.2.3) implicates some approximations. For example,  
 2613 the dependence of the particle-identification probability on other kinematic variables, such as the  
 2614 position at which the particle traverses the RICH detector, is neglected.<sup>[bw]</sup> Applying the more  
 2615 restrictive RICH momentum cut reduces the sample size by about 10 % compared to the main  
 2616 analysis.

2617 Figure 5.25 compares the results of the PWD from the three RICH studies to those from the  
 2618 main analysis for four exemplary selected partial waves. Overall, we find good agreement of  
 2619 the results from the three RICH studies and from the main analysis for most partial waves. For  
 2620 example, the intensity spectrum of the  $1^+ 0^+ \rho(770) K S$  wave shown in figure 5.25a exhibits the  
 2621 same peak at about 1.3 GeV/c<sup>2</sup> in all studies and in main analysis. Also, the shoulder at about  
 2622 1.5 GeV/c<sup>2</sup> and the high-mas tail of the intensity spectrum agrees among all results. Only for  
 2623 the small plateau between about 1.0 and 1.2 GeV/c<sup>2</sup>, the study with a more restrictive RICH  
 2624 threshold (red data points) yielded slightly higher intensities compared to the main analysis,  
 2625 while the studies with a weaker RICH threshold (green data points) and with a more restrictive  
 2626 momentum limit (orange data points) yielded a slightly lower intensity. Therefore, we conclude,  
 2627 that this small plateau is an artifact from imperfections in our analysis.

2628 Such artifacts may arise from overfitting or from destructive interferences, because both are  
 2629 sensitive also to small systematic effects. Such artifacts are visible especially in small partial  
 2630 waves at the per-mill level, e.g. in the  $4^+ 1^+ K^*(892)\pi G$  wave shown in figure 5.25b. In the  
 2631  $m_{K\pi\pi}$  region above 2 GeV/c<sup>2</sup>, where we expected the high-mass tail of the  $K_4^*(2045)$  resonance,  
 2632 the RICH studies yielded results that are similar to those from the main analysis, except for the  
 2633 study with a more restrictive RICH threshold, which yielded slightly different results. However,  
 2634 this difference can be explained by the 30 % smaller amount of data in this study, which may

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<sup>[bw]</sup> The dependence of the particle-identification probability on other kinematic variables, except for the momentum and the track angle of the particle, is assumed to be small. This assumption is supported by a first study of the  $\pi^\pm$  identification probability as a function of the position at which the particle traverses the RICH. This study revealed only a weak dependence of the particle-identification probability on the position at which the particle traverses the RICH.



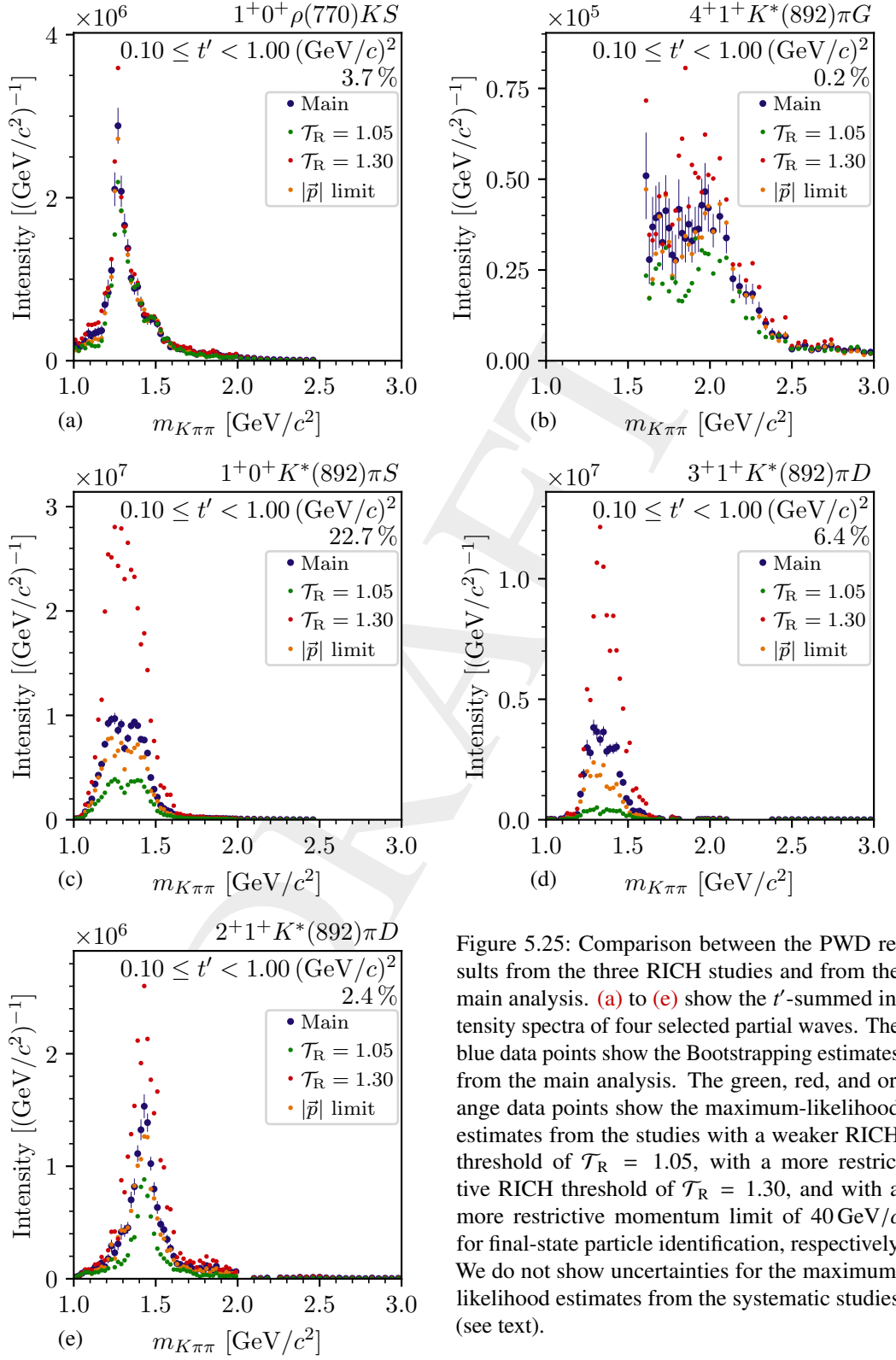


Figure 5.25: Comparison between the PWD results from the three RICH studies and from the main analysis. (a) to (e) show the  $t'$ -summed intensity spectra of four selected partial waves. The blue data points show the Bootstrapping estimates from the main analysis. The green, red, and orange data points show the maximum-likelihood estimates from the studies with a weaker RICH threshold of  $\mathcal{T}_R = 1.05$ , with a more restrictive RICH threshold of  $\mathcal{T}_R = 1.30$ , and with a more restrictive momentum limit of 40 GeV/c for final-state particle identification, respectively. We do not show uncertainties for the maximum-likelihood estimates from the systematic studies (see text).

2635 lead to artifacts from overfitting in addition to the statistical fluctuations. The enhancement  
 2636 in the intensity below about  $2 \text{ GeV}/c^2$  is sensitive to systematic effects. Especially, the study  
 2637 with weaker RICH threshold yields a smaller enhancement. We observe similar results for other  
 2638 partial waves that exhibit such enhanced low-mass tails such as the  $2^- 0^+ \rho(770) K F$  wave shown  
 2639 in figure 5.20a. These observations support our assumption that these enhanced low-mass tails  
 2640 are mainly analysis artifacts. They become smaller when adding information to the PWD fit as  
 2641 done in the study with weaker RICH threshold.

2642 Given the good agreement between the various systematic RICH studies and the main analysis  
 2643 for most partial waves, we observe surprisingly large effects in some other waves. Two of these  
 2644 waves are shown as an example in figures 5.25c and 5.25d. As expected, we observe in the main  
 2645 analysis a double-peak structure in the intensity spectrum of the  $1^+ 0^+ K^*(892) \pi S$  wave, which  
 2646 presumably originates from the known  $K_1(1270)$  and  $K_1(1400)$  resonances. The RICH studies  
 2647 yielded similar shapes, but with intensities that are different by a factor more than 2. Especially  
 2648 the study with a more restrictive RICH threshold yielded an about 2.6 times larger intensity and  
 2649 the study with a weaker RICH threshold yielded an about 2.5 times smaller intensity. Above  
 2650 about  $1.6 \text{ GeV}/c^2$ , we find again good agreement of the results from the RICH studies with the  
 2651 main analysis. As already discussed for the total intensity distribution of waves with  $J^P = 3^+$  in  
 2652 section 5.5, we observe a peak-like structure in the intensity spectrum of the  $3^+ 1^+ K^*(892) \pi D$   
 2653 wave in the mass range between about 1.2 and  $1.6 \text{ GeV}/c^2$  (see figure 5.25d). However, there  
 2654 is no known or expected  $K_3$  state in this mass region (see figure 1.1). Furthermore, this low-  
 2655 mass structure is very sensitive to systematic effects, similar to the double-peak in the  $1^+ 0^+$   
 2656  $K^*(892) \pi S$  wave. The structure in the  $3^+ 1^+ K^*(892) \pi D$  wave nearly vanishes in the study  
 2657 with a weaker RICH threshold, while it becomes almost a factor 3 larger in the study with a  
 2658 more restrictive RICH threshold. Interestingly, the mass range of about 1.0 to  $1.6 \text{ GeV}/c^2$ , in  
 2659 which we observe the large systematic effects described above, coincided with the mass range of  
 2660 the low-mass structure seen in the  $3^+ 1^+ K^*(892) \pi D$  wave. Also, the  $2^+ 1^+ K^*(892) \pi D$  wave  
 2661 shown in figure 5.25e is sensitive to systematic effects. While the shape of its intensity spectrum  
 2662 is similar in the RICH studies and in the main analysis, its intensity becomes larger in the study  
 2663 with a more restrictive RICH threshold and smaller in the study with a weaker RICH threshold,  
 2664 analogously to the two waves discussed above. However, in the  $2^+ 1^+ K^*(892) \pi D$  wave these  
 2665 systematic effects are much weaker compared to the  $1^+ 0^+ K^*(892) \pi S$  and  $3^+ 1^+ K^*(892) \pi D$   
 2666 waves. Before being able to conclude on the origin of this effect in section 5.9, we add another  
 2667 piece of information obtained from the pseudodata studies presented in section 5.8.

## 2668 5.7.2 Alternative Approach for Wave-Set Selection

2669 The potentially largest sources of systematic effects in the wave-set selection are the regularization  
 2670 term used to suppress insignificant waves in equation (5.53) and the term in equation (5.57)  
 2671 designed to impose continuity. In the main analysis, we chose a certain form for these terms based  
 2672 on experience from previous analyses and based on tests using other forms (see sections 5.2.2  
 2673 and 5.2.3). Also, the choice of the parameter values for  $\Gamma$  and  $\lambda$  appearing in the regularization  
 2674 and continuity terms may introduce systematic effects.

2675 Therefore, we used in this study an alternative approach for the wave-set selection fit based  
 2676 on information field theory (IFT) [126]. IFT is a Bayesian probability theory. It allows us to  
 2677 apply regularization and to impose continuity as a function of  $m_{K\pi\pi}$  consistently using a common  
 2678 formalism. The regularization and continuity conditions are formulated in terms of the prior  
 2679 probability. The so-called hyperparameters of the prior probability are inferred from data by  
 2680 formulating hyperpriors for these parameters. Thereby, this approach potentially reduces the  
 2681 bias in the wave-set selection that originates from the choice of these parameters. We present in  
 2682 appendix G.1.1 the IFT model used in this study, which was developed in close collaboration with  
 2683 the information field theory group at the Max Planck institute for Astrophysics [127, 128]. In the  
 2684 IFT model, we formulated a prior probability that favors small partial-wave intensities and thus  
 2685 suppresses insignificant waves. Continuity of the transition amplitudes in  $m_{K\pi\pi}$  is represented in  
 2686 terms of the correlations between the transition amplitudes at different  $m_{K\pi\pi}$  locations. Continuity  
 2687 is imposed by requiring a strong correlation between nearby  $m_{K\pi\pi}$  locations in the prior term,  
 2688 while allowing for weaker correlations between  $m_{K\pi\pi}$  locations that are far apart. A detailed  
 2689 introduction to IFT is given in ref. [126].

2690 In the IFT study, we follow the same strategy as outlined in section 5.2: Based on the same  
 2691 wave pool as used in the main analysis (see section 5.2.1) and applying the same thresholds for  
 2692 sub-threshold decays of heavy isobar resonances (see section 5.2.4), we performed wave-set  
 2693 selection fits that use the IFT approach to suppress insignificant waves and to impose continuity  
 2694 in the wave set. As in the main analysis, we used a rank=1 model for the wave-set selection fits.  
 2695 Based on the results of these wave-set selection fits, we constructed a wave set in each  $(m_{K\pi\pi}, t')$   
 2696 cell by requiring a minimal intensity for a partial wave to be selected, similar as in the main  
 2697 analysis discussed in section 5.2.5.<sup>[bx]</sup> Finally, we performed a PWD fit using equation (5.38)  
 2698 with these selected wave sets, which yielded the final results of the IFT study.

2699 We used the Python framework NIFTy [129] to implement the IFT model in equation (G.15),  
 2700 together with the likelihood of the PWD for a single data set given in equation (5.33). Fitting  
 2701 of multiple data sets is not yet developed for this framework. Hence, we used only the  $K^-\pi^-\pi^+$   
 2702 sample from the 2008 diffraction data set for the wave-set selection fits in this study, which  
 2703 corresponds to about 56 % of the full  $K^-\pi^-\pi^+$  sample. The reduced amount of data in this study  
 2704 might lead to smaller wave sets, because small signals may become insignificant with respect  
 2705 to the reduced precision. Employing the continuity condition as imposed by the IFT approach  
 2706 required us to include the full analyzed  $m_{K\pi\pi}$  range in a single IFT wave-set selection fit, while  
 2707 in the main analysis we considered only small  $m_{K\pi\pi}$  ranges of 15 bins in one fit. This prohibits  
 2708 using an  $m_{K\pi\pi}$ -dependent binning in  $m_{K\pi\pi}$ . Hence, we used 20 MeV/ $c^2$  wide  $m_{K\pi\pi}$  bins over the  
 2709 full analyzed  $m_{K\pi\pi}$  range. For the final PWD with the selected wave set we used the 2008 and  
 2710 2009 sample, and we used 40 MeV/ $c^2$  wide bins for  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$  as in the main analysis.

2711 Figure 5.26 shows selected results from the IFT study. The size of the wave sets from the  
 2712 IFT wave-set selection fits as a function of behaves similar  $m_{K\pi\pi}$  as in the main analysis (cf.

<sup>[bx]</sup> The IFT method does not produce jump discontinuities in the ordered partial-wave intensities. Thus, we used a constant intensity threshold of 3, which is the same value as used in the main analysis for  $(m_{K\pi\pi}, t')$  cells where the automatic threshold detection failed (see appendix D.1.1).

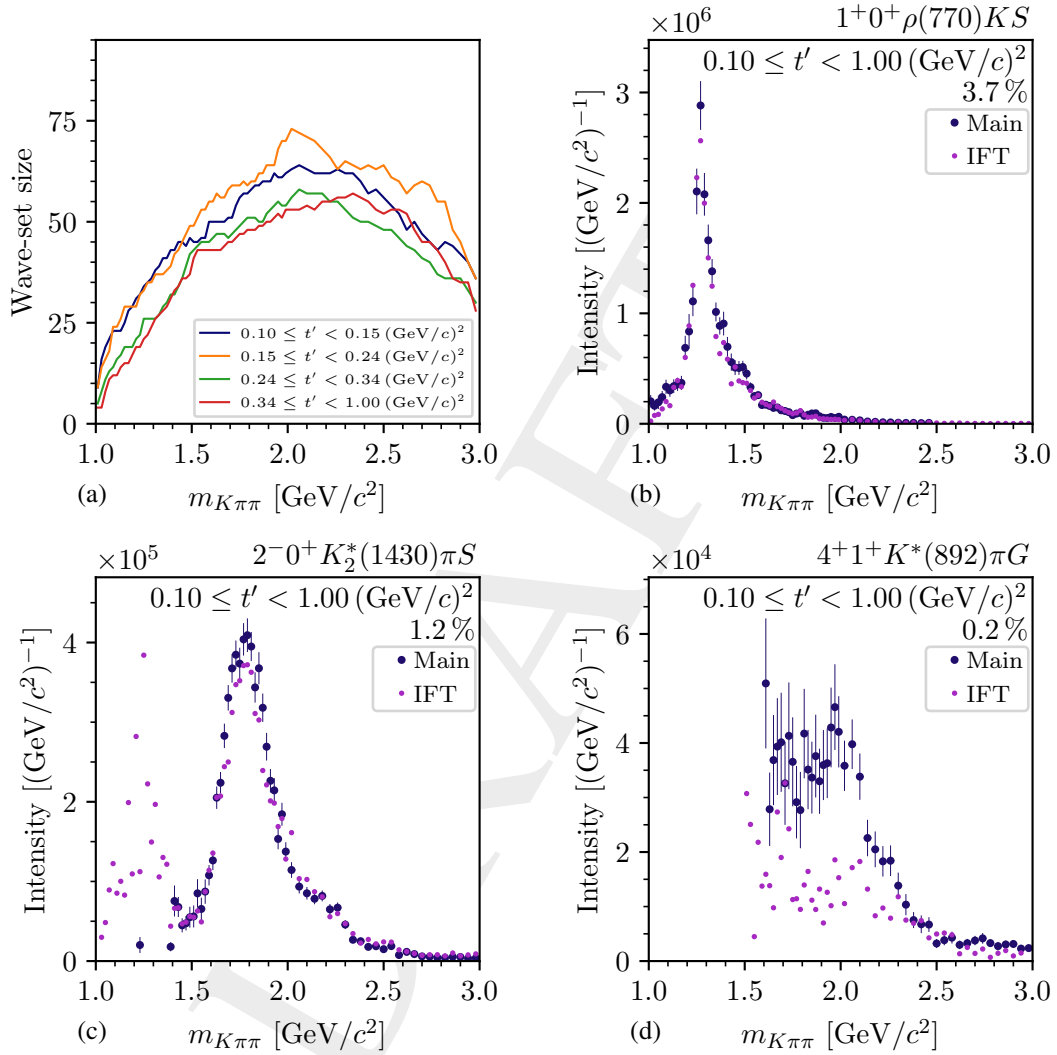


Figure 5.26: Results from the study using a wave set that was selected using IFT. (a) shows the size of the wave sets obtained in the IFT study as a function of  $m_{K\pi\pi}$  in the four  $t'$  bins. (b) to (d) show the  $t'$ -summed intensity spectra of three selected partial waves. The blue data points show the Bootstrapping estimates from the main analysis. The violet data points show the maximum-likelihood estimates from the study using the wave set constructed from the IFT wave-set selection fits. We do not show uncertainties for the maximum-likelihood estimates from the systematic study (see text).

2713 figures 5.10 and 5.26a). Only the jump of the wave-set size at  $2 \text{ GeV}/c^2$  is not visible in the IFT  
 2714 study as we did not change the  $m_{K\pi\pi}$  binning here. The  $t'$  dependence of the wave-set size is  
 2715 also consistent with the main analysis. Given the potentially reduced bias in the IFT study by  
 2716 inferring the prior hyperparameters from data, this good agreement between the IFT study and  
 2717 the main analysis suggests that our choice for the regularization parameters was appropriate. This  
 2718 means that the regularization in the main analysis was strong enough to suppress insignificant  
 2719 waves so that the wave sets did not become too large and this means also the regularization in the  
 2720 main analysis was not too strong so that significant waves were not suppressed.

2721 Considering all  $(m_{K\pi\pi}, t')$  cells, the wave set from the IFT study consists of 104 partial waves. [by]  
 2722 This is significantly smaller than the 238-wave set selected in the main analysis. However, about  
 2723 90 of the 238 partial waves contain only noise as discussed in section 5.2.6, while we find only six  
 2724 noisy waves in the IFT wave set. That these noisy waves were not included in the IFT wave-set  
 2725 demonstrates that IFT is a superior approach to impose continuity. One reason for this is that the  
 2726 whole analyzed  $m_{K\pi\pi}$  range could be considered in a single IFT wave-set selection fit.

2727 Figures 5.26b to 5.26d compare the result of the PWD using the IFT wave set (violet data  
 2728 points) to those from the main analysis (blue data points). For most partial waves, we find good  
 2729 agreement between the IFT study and the main analysis, exemplarily shown in figure 5.26b  
 2730 for the  $t'$ -summed intensity spectrum of the  $1^+ 0^+ \rho(770) K S$  wave. Thus, we expect no large  
 2731 systematic effects from the wave-set selection in the main analysis.

2732 For some partial waves, we find low-mass enhancements in the IFT study. For example, the  
 2733  $2^- 0^+ K_2^*(1430) \pi S$  wave shown in figure 5.26c is practically not selected in the main analysis in  
 2734  $m_{K\pi\pi}$  bins below about  $1.4 \text{ GeV}/c^2$ , while it was selected in the IFT study also below  $1.4 \text{ GeV}/c^2$   
 2735 resulting in a low-mass enhancement that peaks about  $1.3 \text{ GeV}/c^2$ . As there are no known or  
 2736 expected  $K_2$  states in this mass region, we assume this low-mass enhancement to be a model  
 2737 artifact. The continuity of the wave set imposed by the IFT wave-set selection extends over the  
 2738 full analyzed  $m_{K\pi\pi}$  range. This leads to a wider  $m_{K\pi\pi}$  range in which the  $2^- 0^+ K_2^*(1430) \pi S$  wave  
 2739 was selected. However, in the  $m_{K\pi\pi}$  region below about  $1.4 \text{ GeV}/c^2$ , the  $2^- 0^+ K_2^*(1430) \pi S$  wave  
 2740 may destructively interference with other waves, which can case such low-mass enhancements  
 2741 as discussed for sub-threshold waves in section 5.2.4. For  $m_{K\pi\pi} > 1.4 \text{ GeV}/c^2$ , the results from  
 2742 the IFT study agree well with those from the main analysis.

2743 For some partial waves at the per-mill level such as the  $4^+ 1^+ K^*(892) \pi G$  wave shown in  
 2744 figure 5.26d, the IFT study disagrees with the main analysis. In contrast to the main analysis, the  
 2745 result of the IFT study does not exhibit a potential intensity peak from the  $K_4^*(2045)$  resonance,  
 2746 which is expected to be observed in this partial wave at about  $2 \text{ GeV}/c^2$ . Partial waves with such  
 2747 small intensities are most sensitive to bias from the selected wave set. Also the IFT method  
 2748 has some parameters that must be chosen a priori, e.g. the parameters of the hyper-priors in  
 2749 equations (G.13) and (G.14). As those parameters were not yet fine-tuned in the IFT study, their  
 2750 choice might lead to some bias in small waves from the IFT wave-set selection.

[by] In addition to the 104 partial waves, we also included the incoherent flat wave in the PWD fits.

2751 Finally, we observe large systematic effects in those waves that exhibit low-mass structures and  
 2752 that already showed large systematic effects in the RICH studies discussed in section 5.7.1. Such  
 2753 a wave is, for example the  $3^+ 1^+ K^*(892)\pi D$  partial wave shown in figure G.3g.

2754 Overall, the wave-set selection using IFT yielded very promising results. However, there are  
 2755 some caveats such as the missing  $K_4^*(2045)$  signal, which have to be resolved before the IFT  
 2756 wave-set selection can be used in the main analysis.

2757 Reviewing all studies presented in this section 5.7, the systematic studies and the main analysis  
 2758 agree well for most partial waves. From this we conclude that we expect no large systematic  
 2759 effects on the results of the PWD for these waves. appendix G.1, we present an overview over  
 2760 all systematic studies for those partial waves that are discussed in this work. However, for  
 2761 some partial waves, we observe large systematic effects in the mass region below  $1.6 \text{ GeV}/c^2$   
 2762 together with unexpected low-mass structures in this mass region. These effects demand further  
 2763 clarification, and we will conclude on them in section 5.9.

## 2764 5.8 Pseudodata Studies using the $K^-\pi^-\pi^+$ PWD Model

2765 To further test the consistency of our PWD results, we studied our analysis in an environment  
 2766 where we controlled the input, i.e. where we knew the distribution from which the events  
 2767 were produced, how the measurement process distorted these distributions, and what values of  
 2768 the spin-density matrix elements we expect. These input-output studies were carried out by  
 2769 generating pseudodata samples. Hence, we call them pseudodata studies. What we will call  
 2770 produced pseudodata samples are simulated samples of events that are distributed according to  
 2771 a given physics model. In this section, we discuss samples that were generated according to  
 2772 a PWD model as given in equation (5.16). In order to study apparatus effects, i.e. resolution  
 2773 and acceptance effects, the produced pseudodata events are processed through the COMPASS  
 2774 detector Monte Carlo simulation and the event reconstruction algorithm.<sup>[bz]</sup> Then we applied  
 2775 the same event selection criteria as for the measured data. This procedure yields so-called  
 2776 reconstructed pseudodata samples, which resemble the distribution of measured events. A de-  
 2777 tailed description of how we generated these samples is given in appendix C.

2778 In this section, we discuss pseudodata samples for the reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$ , which  
 2779 were generated according to three different PWD models. All three models are based on the  
 2780 results of a PWD fit of the 238-wave set to the measured  $K^-\pi^-\pi^+$  sample, which is called  
 2781 the 238-wave pseudodata model in the text below.<sup>[ca]</sup> We applied the same procedure to the

<sup>[bz]</sup> We used the Monte Carlo simulation of the experimental setup of the 2008 diffraction data taking for all pseudodata studies. The 2009 setup is nearly identical to the 2008 setup. Thus, the conclusions drawn from the pseudodata studies using the 2008 setup can be applied to the main analysis of the measured  $K^-\pi^-\pi^+$  sample from 2008 and 2009.

<sup>[ca]</sup> We generated the pseudodata samples by applying equation (5.16) with the maximum-likelihood estimates of the parameters from a PWD fit using a rank=1 model and the 238-wave set without applying table D.1. This model is called the 238-wave pseudodata model. This was done, because historically, we generated the pseudodata samples

2782 pseudodata samples as in the main analysis; i.e. we applied the same event selection, which is  
 2783 discussed in section 4.1, and we performed a PWD using a rank=3 model and the 238-wave  
 2784 set.<sup>[cb]</sup> As for the systematic studies presented in section 5.7, performing a Bootstrapping of the  
 2785 PWD for all pseudodata studies was computationally too expensive. Thus, we present in this  
 2786 section the maximum-likelihood estimates from the PWD of the pseudodata samples, and we do  
 2787 not show the corresponding uncertainties. In section 6.4, we present pseudodata studies where  
 2788 we also performed a Bootstrapping.

### 2789 5.8.1 Pseudodata Sample based on the 238-Wave Pseudodata Model

2790 We generated a pseudodata sample of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  that is as similar  
 2791 as possible to the measured  $K^- \pi^- \pi^+$  sample. To this end, we used the 238-wave pseudodata  
 2792 model. In total, we generated  $50 \times 10^6$  produced events in the analyzed  $m_{K\pi\pi}$  and  $t'$  range.  
 2793 About  $3.18 \times 10^6$  events of all produced events were reconstructed, i.e. passed all event-selection  
 2794 criteria.<sup>[cc]</sup>

2795 Figure 5.27 shows the  $t'$ -summed intensity spectra of four exemplary selected partial waves from  
 2796 the PWD of this pseudodata sample. The results of the PWD of the produced pseudodata sample  
 2797 (cyan data points), i.e. the pseudodata sample without acceptance and resolution effects,<sup>[cd]</sup> agree  
 2798 well with the reference model (blue crosses), i.e. the expectation from the 238-wave pseudodata  
 2799 model. This demonstrates that the PWD formalism presented in section 5.1 works in the ideal  
 2800 case with perfect acceptance and with a perfect PWD model, which by construction is able to  
 2801 describe the data.

2802 The results of the PWD of the reconstructed pseudodata sample are shown by the green data  
 2803 points. The reconstructed pseudodata sample is afflicted with the same acceptance affects,  
 2804 resolution effects, and misidentification of the final-state particles as the measured data. Thus,  
 2805 we test in this pseudodata study whether our analysis is robust with respect to these apparatus  
 2806 effects. The results of this study agree with the reference model for most partial waves. We  
 2807 find good agreement for relatively large partial waves such as the  $1^+ 0^+ \rho(770) K S$  wave shown  
 2808 in figure 5.27a as well as for small waves at the per-mill level such as the  $4^+ 1^+ K^*(892) \pi G$   
 2809 wave shown in figure 5.27b. In figure 5.25e we show that the intensity of the  $2^+ 1^+ K^*(892) \pi D$

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before deciding to switch to a rank=3 spin-density matrix in the PWD, before extending the wave set from the  
 wave-set selection fits according to table D.1, and before using Bootstrapping. As all three changes in the PWD  
 resulted in a similar agreement between the PWD model and the measured data, the pseudodata samples based on  
 the 238-wave pseudodata model reproduce the measured  $K^- \pi^- \pi^+$  sample. As generating these pseudodata samples  
 is computationally very expensive, we did not regenerate the pseudodata samples after changing the analysis.

<sup>[cb]</sup> We used the 238-wave set without applying table D.1 to be consistent with the 238-wave pseudodata model.

<sup>[cc]</sup> The fraction of reconstructed events corresponds to an average acceptance of 6.44 %. However, this estimate is  
 strongly biased by the leakage effect as discussed in section 5.9.1. Based on the findings shown there, we estimated  
 an actual average acceptance of about 12 %. This comparably low acceptance is mainly due to the limited kinematic  
 range of the final-state particle identification.

<sup>[cd]</sup> As the produced pseudodata sample is not affected by acceptance effects, we used a perfect-acceptance model in  
 the corresponding PWD fit, i.e. we used  $\eta^{(i)}(\tau, m_{K\pi\pi}, t') = 1$  in equation (5.27).

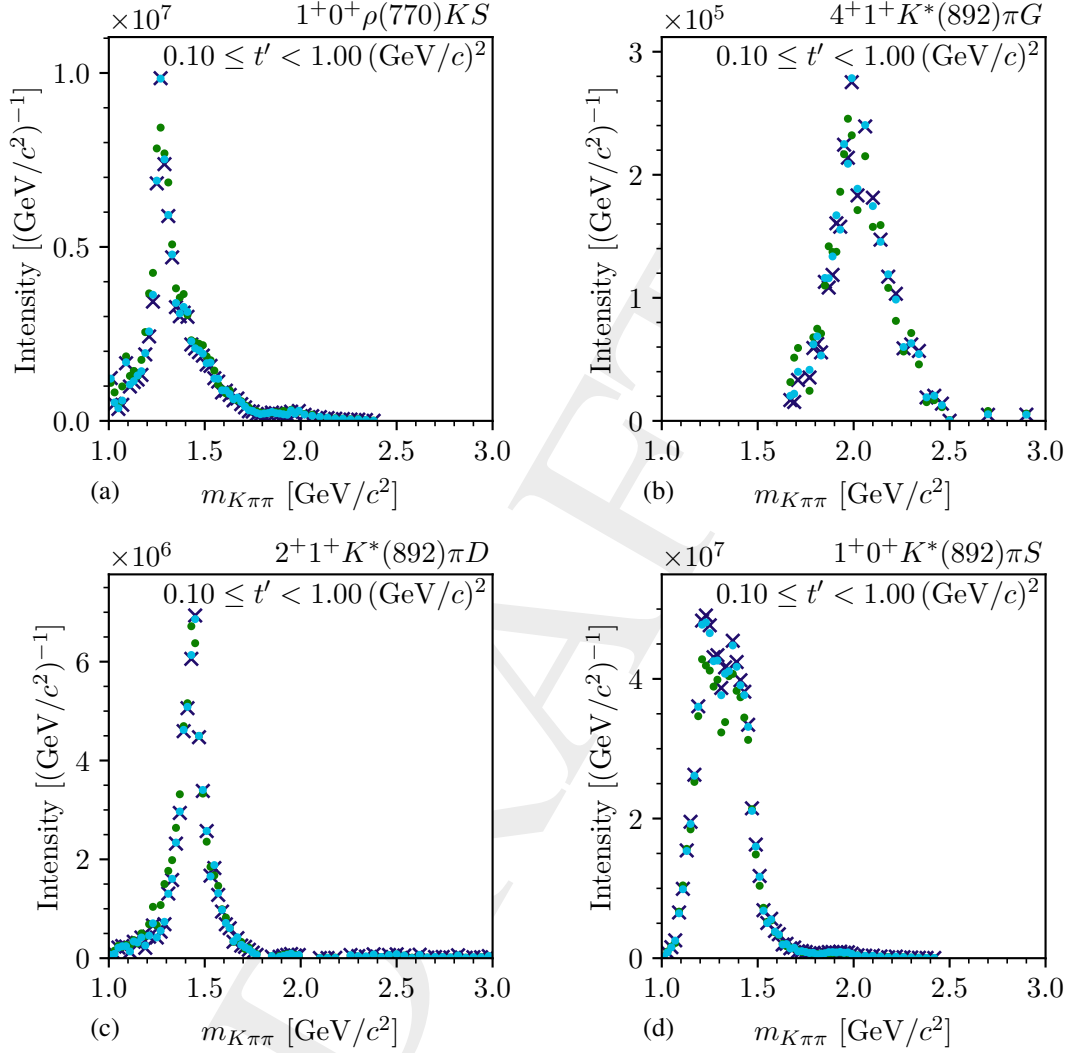


Figure 5.27:  $t'$ -summed intensity spectra of four selected partial waves as obtained from the PWD of the pseudodata sample that was generated using the full 238-wave pseudodata model. The cyan data points represent the PWD of the produced pseudodata sample. The green data points represent the PWD of the reconstructed pseudodata sample. The blue crosses represent the expected values, i.e. the values from the 238-wave pseudodata model scaled such that its prediction for the total number of produced events is equal to the number of produced pseudodata events. We show the maximum-likelihood estimates of the intensities obtained from the pseudodata. The corresponding maximum-likelihood estimates of the uncertainties are not shown (see text).



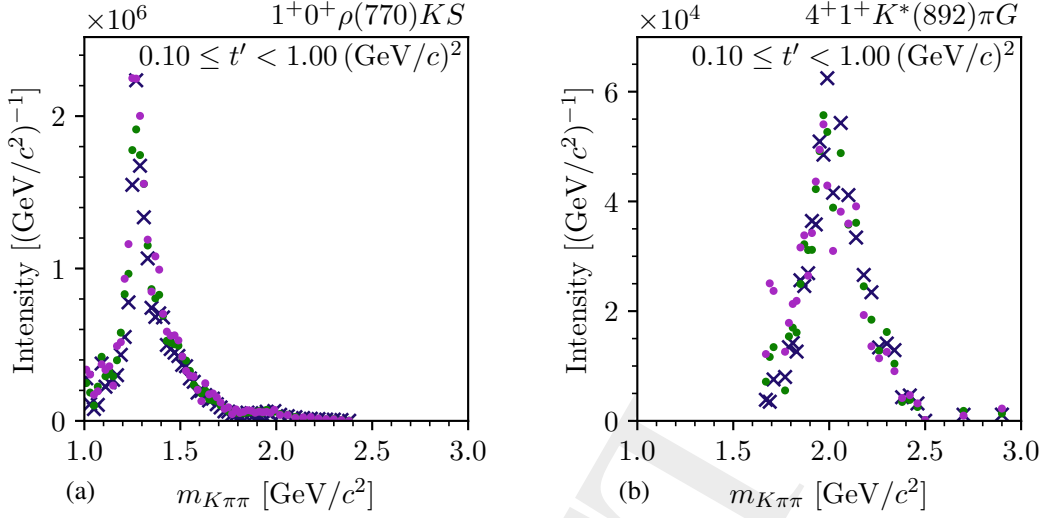


Figure 5.28: Same as figure 5.27, but showing in addition to the results of the PWD of a subset of  $720 \times 10^3$  events of the reconstructed pseudodata sample (violet data points).

2810 wave exhibits a modest sensitivity to systematic effects. In contrast, we find here consistent  
 2811 results for the intensity spectrum of the  $2^+ 1^+ K^*(892)\pi D$  wave in figure 5.27c. Hence, the  
 2812  $2^+ 1^+ K^*(892)\pi D$  wave is interpreted in terms of physics signals as discussed in section 7.2.  
 2813 From the findings discussed in this paragraph we conclude that the signals in most of the partial  
 2814 waves are robust with respect to these apparatus effects.

2815 As expected, we observe larger fluctuations of the results from the reconstructed pseudodata  
 2816 sample compared to those from the produced pseudo data samples because the size of the  
 2817 reconstructed pseudodata sample is about 20 times smaller. Still, the reconstructed pseudodata  
 2818 sample is about 4.3 times larger than the measured  $K^- \pi^- \pi^+$  sample and thus more precise. To test  
 2819 whether the sample size biases the results of the PWD, we performed a PWD where we used only  
 2820 a sub-sample of  $720 \times 10^3$  events of the reconstructed pseudodata sample, which hence has the  
 2821 same size as the measured  $K^- \pi^- \pi^+$  sample. The violet data points in figure 5.28 show the results  
 2822 of this study for two exemplary selected waves. The results are similar to those using the full  
 2823 reconstructed pseudodata sample (green data points) and to the 238-wave pseudodata reference  
 2824 model (blue crosses), even for waves at the per-mill level such as the  $4^+ 1^+ K^*(892)\pi G$  wave  
 2825 shown in figure 5.28b. Thus, we conclude, that our analysis is robust with respect to statistical  
 2826 fluctuations, e.g. that we do not expect large artifacts from overfitting in most partial waves.

2827 However, there is a certain set of partial waves for which the results from the reconstructed  
 2828 pseudodata sample do not agree well with the 238-wave pseudodata reference model. For  
 2829 example, the intensity spectrum of the  $1^+ 0^+ K^*(892)\pi S$  wave obtained from the reconstructed  
 2830 pseudodata sample (green points in figure 5.27d) is slightly but systematically smaller compared  
 2831 to the reference model in the  $m_{K\pi\pi}$  region below about  $1.6 \text{ GeV}/c^2$ . Interestingly, we observe  
 2832 these discrepancies only in the PWD of the reconstructed pseudodata sample, while the results  
 2833 obtained from the produced pseudodata sample agree with the reference. As the difference

2834 between both pseudodata samples are acceptance effects, this suggests that this discrepancy  
2835 is related to effects from the experimental acceptance.<sup>[ce]</sup> Understanding these discrepancies  
2836 requires further investigations, which will be summarized in section 5.9.

### 2837 5.8.2 Introducing Imperfections into the Pseudodata

2838 In this section we test the robustness of our PWD with respect to imperfections in the analysis  
2839 model. To this end, we used the reconstructed pseudodata sample based on the 238-wave  
2840 pseudodata model, but performed a PWD fit using a detuned acceptance model. Instead of  
2841 using the acceptance model of the main analysis, which would be the correct one, we used the  
2842 acceptance model from the systematic study with a more restrictive momentum limit for the  
2843 RICH final-state particle identification (see section 5.7.1). This means we identified final-state  
2844 pions and kaons up to 60 GeV/c in the reconstructed pseudodata sample, but when fitting the  
2845 PWD model to this pseudodata sample, we wrongly set the probability to identify final-state  
2846 particles to zero in the range  $40 \leq |\vec{p}| < 60$  GeV/c in the acceptance model. This introduced a  
2847 modest but not negligible imperfection in the PWD fit. In particular, the introduced imperfection  
2848 is located in a kinematic region where the acceptance in the main analysis strongly changes  
2849 and where we observe some deviations between the PWD model predictions and the measured  
2850 data in this kinematic region as discussed in section 5.6. Thus, we expect the PWD fit to be  
2851 sensitive to imperfections especially in this kinematic region. As we modeled the acceptance  
2852 in this kinematic region in the acceptance model used in the main analysis, we assume that the  
2853 imperfections in the measured data are not larger than the imperfections introduced in this study.  
2854 Hence, the study using the detuned acceptance model is suited well to test the robustness of the  
2855 PWD.

2856 The orange data points in figure 5.29 represent the results of the PWD using the detuned  
2857 acceptance model. Given the introduced imperfection, we still find good agreement between the  
2858 results of this study and the 238-wave pseudodata reference model (blue crosses) for most of  
2859 the waves as exemplarily shown in figures 5.29a and 5.29b. Only in the low-mass tail of the  
2860  $1^+ 0^+ \rho(770) K S$  wave shown in figure 5.29a, i.e. in the  $m_{K\pi\pi}$  region below about 1.3 GeV/c<sup>2</sup>,  
2861 this study yielded intensities slightly larger than the reference model. This might indicate that  
2862 the imperfections due to the detuned acceptance model lead to small artifacts in the low-mass  
2863 region, similar to the low-mass enhancements discussed in section 5.5. Nonetheless, from the  
2864 good agreement found in most of the partial waves we conclude that our analysis model and  
2865 analysis procedure is robust with respect to such modest imperfections in the description of the  
2866 acceptance.

---

<sup>[ce]</sup> In addition to acceptance effects, the reconstructed pseudodata sample is also affected by resolution effects. We excluded that the observed discrepancies are caused by resolution effects in a study, where we used the true physical values of the kinematic variables, i.e. the values with which the event was produced, in the PWD of the reconstructed pseudodata sample instead of using the reconstructed values. Hence, in this study the PWD fit is free of resolution effects. The results of this study show similar discrepancies as those observed when using the reconstructed quantities.

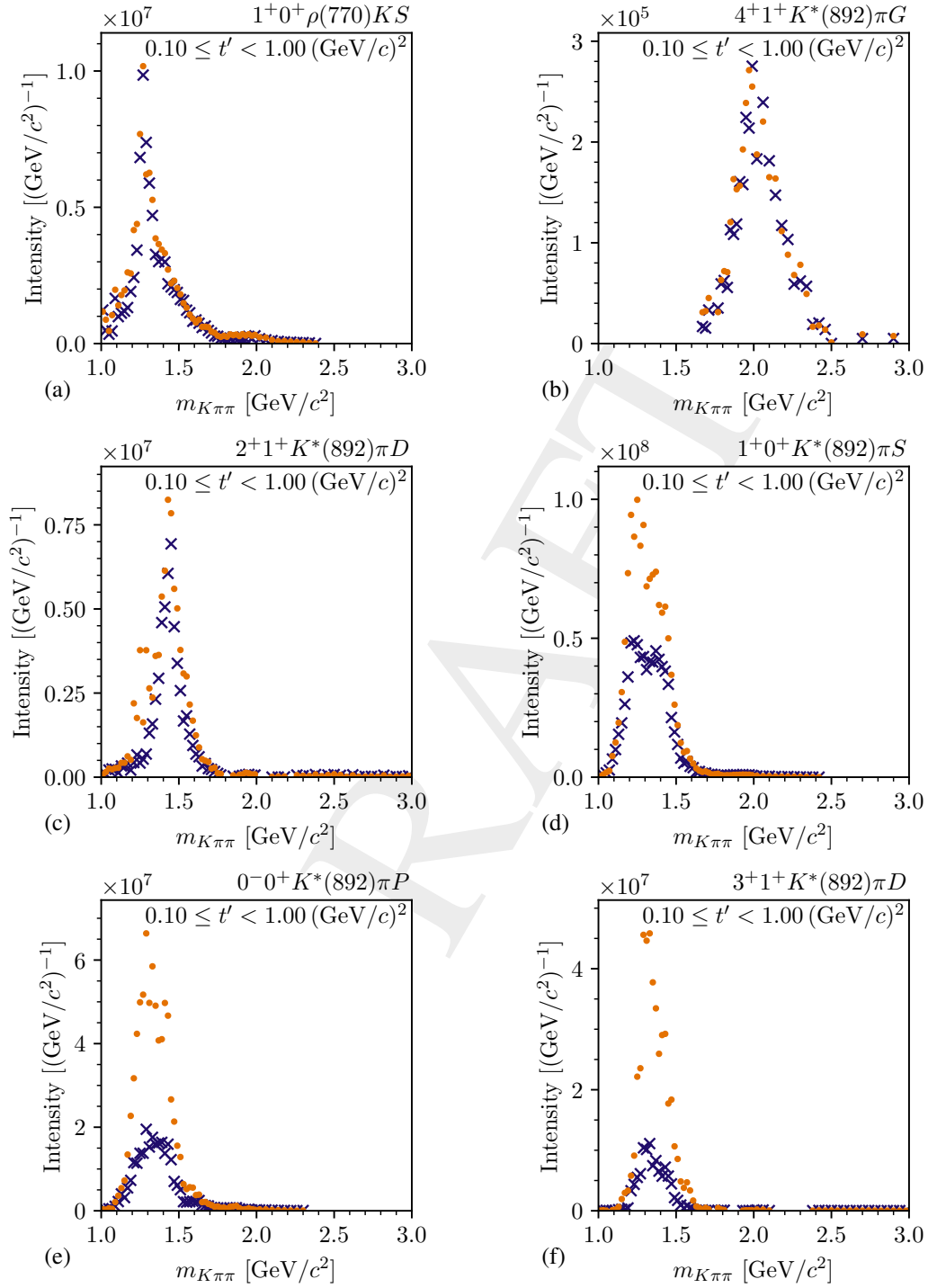


Figure 5.29: Same as figure 5.27, but showing the result of the PWD of the reconstructed pseudodata using the detuned acceptance model (orange data points).

2867 Using the detuned acceptance model yielded a slightly larger intensity of the  $2^+ 1^+ K^*(892) \pi D$   
 2868 wave compared to the 238-wave pseudodata reference model as shown in figure 5.29c, while  
 2869 the shape remains similar. This is consistent with our finding that the  $2^+ 1^+ K^*(892) \pi D$  wave  
 2870 from the measured  $K^- \pi^- \pi^+$  sample is only modestly sensitive to systematic effects as discussed  
 2871 in section 5.7.1. Only in about four  $m_{K\pi\pi}$  bins at about  $1.3 \text{ GeV}/c^2$ , the intensity is much larger  
 2872 than in the reference model. We do not observe such a deviation if we use the correct model  
 2873 for the acceptance. Thus, the discrepancy may arise due to destructive interference of the  $2^+ 1^+$   
 2874  $K^*(892) \pi D$  wave with other partial waves that were selected only in those  $m_{K\pi\pi}$  bins. The  
 2875 resulting, typically small, effect on the total model intensity from such a destructive interference  
 2876 may be misused by the fit to partly account for the introduced imperfection.

2877 Finally, we find large deviations for a certain set of partial waves when using the detuned  
 2878 acceptance model. Among these waves are the  $1^+ 0^+ K^*(892) \pi S$ , the  $0^- 0^+ K^*(892) \pi P$ , and  
 2879 the  $3^+ 1^+ K^*(892) \pi D$  waves shown in figures 5.29d, 5.29e, and 5.29f; respectively. In all waves,  
 2880 the intensity obtained using the detuned acceptance model is much larger than the reference  
 2881 model. However, this discrepancy is limited to the  $m_{K\pi\pi}$  region below about  $1.6 \text{ GeV}/c^2$ . Most  
 2882 of these waves have the  $K^*(892)$  isobar. As shown e.g. in figure 5.27d, we find discrepancies  
 2883 in a similar set of waves also when using the correct model for the acceptance. However, these  
 2884 discrepancies are much smaller. Interestingly, we find these small deviations in the same partial  
 2885 waves for which we observe large systematic effects (see section 5.7) and in many of these waves  
 2886 we observe unexpected low-mass structures (see section 5.5). In section 5.9, we will conclude on  
 2887 this effect.

### 2888 5.8.3 Pseudodata without the $1^+ 0^+ \rho(770) K S$ or $2^+ 1^+ K^*(892) \pi D$ Waves

2889 In order to study artifacts due to wrongly assigned intensity in individual partial waves in more  
 2890 detail, we generated pseudodata samples based on the 238-wave pseudodata model, but we  
 2891 omitted in each study a single wave, i.e. we set the amplitude of this wave to zero. Thus,  
 2892 the PWD of such a pseudodata sample should yield zero intensity for the omitted wave. Any  
 2893 significant deviation from zero intensity would indicate artifacts in the omitted wave.

2894 We generated a pseudodata sample where we omitted the  $1^+ 0^+ \rho(770) K S$  wave.<sup>[cf]</sup> Figure 5.30a  
 2895 shows the  $t'$ -summed intensity spectrum of the  $1^+ 0^+ \rho(770) K S$  wave as obtained from this  
 2896 pseudodata sample using the correct model for the acceptance (green data points) or using  
 2897 the detuned acceptance model (orange data points). We used the same detuned acceptance  
 2898 model as in section 5.8.2. Overall, the intensity of the  $1^+ 0^+ \rho(770) K S$  wave obtained in  
 2899 this study is small compared to the intensity observed in the measured  $K^- \pi^- \pi^+$  sample (blue  
 2900 crosses).<sup>[cg]</sup> We obtained similar results when using the correct and the detuned acceptance

<sup>[cf]</sup> We generated  $40 \times 10^6$  pseudodata events.

<sup>[cg]</sup> We determined the scale factor for the full 238-wave pseudodata model, such that the prediction for the number of produced events from the 238-wave pseudodata model without the  $1^+ 0^+ \rho(770) K S$  wave is equal to the number of produced pseudodata events in this study. The scaled 238-wave pseudodata model gives the expected spin-density matrix elements for all waves except for the  $1^+ 0^+ \rho(770) K S$  wave, for which the expectation is zero.

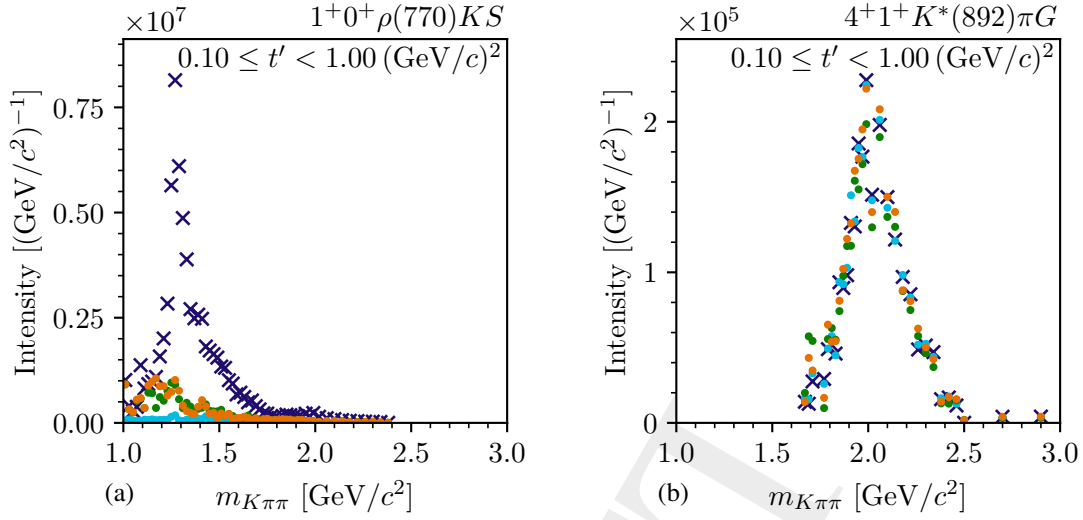


Figure 5.30: Results from the PWD of the pseudodata sample that was generated from the 238-wave pseudodata model, but with the  $1^+0^+\rho(770)KS$  amplitudes set to zero. The  $t'$ -summed intensity spectra of two selected partial waves are shown. The cyan data points represent the PWD of the produced pseudodata. The green data points represent the PWD of the reconstructed pseudodata using the correct model for the acceptance. The orange data points represent the PWD of the reconstructed pseudodata using the detuned acceptance model. The blue crosses represent the full 238-wave pseudodata model scaled accordingly.<sup>[cgl]</sup> We show the maximum-likelihood estimates of the intensities obtained from the pseudodata. The corresponding maximum-likelihood estimates of the uncertainties are not shown.

2901 model. However, the intensity is not zero as expected. Especially, in the  $m_{K\pi\pi}$  region below about  
 2902  $1.3 \text{ GeV}/c^2$  we observe small artificial intensities in this partial wave. The PWD of the produced  
 2903 pseudodata sample (cyan data points) yielded practically zero intensity in the  $1^+0^+\rho(770)KS$   
 2904 wave. Thus, we conclude that the small artifacts observed in the  $1^+0^+\rho(770)KS$  wave arise  
 2905 from the limited acceptance, which is mainly caused by the limited range of the RICH final-state  
 2906 particle identification. These artifacts are not sensitive to imperfections in the analysis model.  
 2907 As discussed in section 5.7.1, we also observe small systematic effects in this  $m_{K\pi\pi}$  region in  
 2908 the  $1^+0^+\rho(770)KS$  wave obtained from the PWD of the measured  $K^-\pi^-\pi^+$  sample. The other  
 2909 partial waves are not affected when omitting the  $1^+0^+\rho(770)KS$  wave as exemplarily shown in  
 2910 figure 5.30b. In all pseudodata and systematic studies discussed so far, most of the partial waves  
 2911 behave similar to the  $1^+0^+\rho(770)KS$  wave. Thus, we expect the conclusions drawn here for  
 2912 the  $1^+0^+\rho(770)KS$  wave to hold also for most of the other waves.

2913 One of the exceptions is the  $2^+1^+K^*(892)\pi D$  wave, which is affected by small systematic effects  
 2914 (see figure 5.25e). Thus, we performed another pseudodata study using a pseudodata sample  
 2915 where we omitted the  $2^+1^+K^*(892)\pi D$  wave.<sup>[ch]</sup> In the highest  $t'$  bin shown in figure 5.31b,  
 2916 we observe only little intensity in the  $2^+1^+K^*(892)\pi D$  wave, as expected. Only in two  $m_{K\pi\pi}$   
 2917 bins at about  $1.3 \text{ GeV}/c^2$  and only when we used the detuned acceptance model (orange data  
 2918 points), the  $2^+1^+K^*(892)\pi D$  wave picked up some intensity. We observe larger intensities in

<sup>[ch]</sup> We generated again  $40 \times 10^6$  pseudodata events.

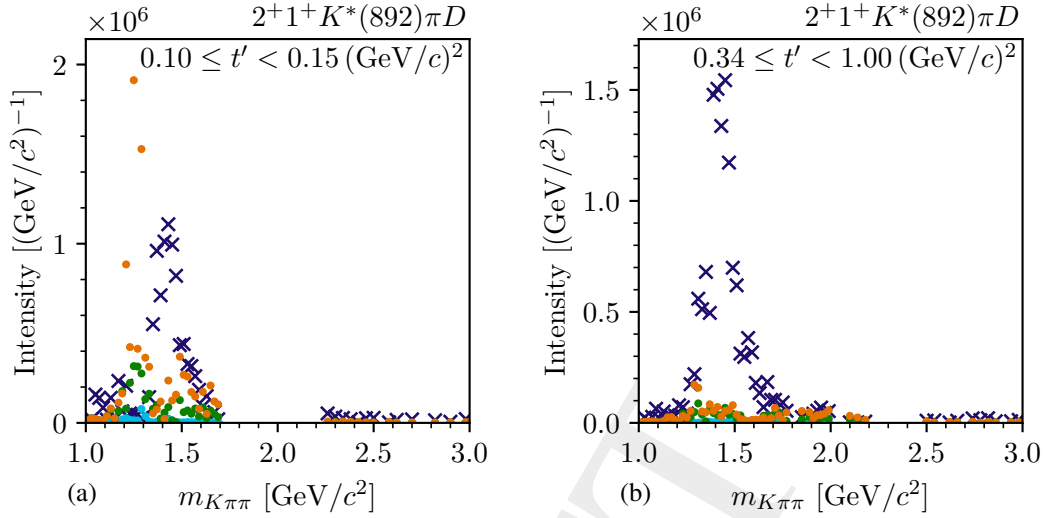


Figure 5.31: Same as figure 5.30 but for the pseudodata study based on the 238-wave pseudodata model without the  $2^+ 1^+ K^*(892)\pi D$  wave component.

2919 the lowest  $t'$  bin shown in figure 5.31a. The intensity obtained using the correct model for the  
 2920 acceptance (green data points) peaks at about  $1.3 \text{ GeV}/c^2$ . This peak becomes larger when using  
 2921 the detuned acceptance model (orange data points). It is even larger than the intensity obtained  
 2922 from the measured  $K^-\pi^-\pi^+$  sample (blue crosses). Such a large artificial intensity is typical  
 2923 for destructive interferences, which become enhanced when introducing imperfections, because  
 2924 they are misused by the fit to account for the imperfections. The intensity obtained from the  
 2925 PWD of the produced pseudodata sample (cyan data points) is practically zero, in agreement  
 2926 with the reference model. From this pseudodata study, we expect modest artifacts in the  $2^+ 1^+$   
 2927  $K^*(892)\pi D$  wave obtained from the PWD of the measured  $K^-\pi^-\pi^+$  sample mainly in the low- $t'$   
 2928 and low- $m_{K\pi\pi}$  region, which is consistent with the findings in the systematic studies. The results  
 2929 for the other waves (not shown) are not biased when omitting the  $2^+ 1^+ K^*(892)\pi D$  wave.

2930 Reviewing all studies presented in this section 5.8 we conclude that for most of the partial waves  
 2931 we expect no considerable artifacts in our analysis caused by e.g. an imperfect acceptance model.  
 2932 We find indications for modest artificial intensities in the  $2^+ 1^+ K^*(892)\pi D$  wave mainly in the  
 2933 low- $t'$  and low- $m_{K\pi\pi}$  region. However, there is a certain set of partial waves, e.g. the  $1^+ 0^+$   
 2934  $K^*(892)\pi S$  wave, whose results are very sensitive to imperfections in the analysis model, e.g. to  
 2935 a detuned acceptance model. We discuss this set of waves in the following section 5.9.

## 2936 5.9 The Leakage Effect

2937 As discussed in section 5.7, there is a certain set of partial waves, for which we observe large  
 2938 systematic effects, e.g. for which the various systematic studies yielded different intensity spectra.  
 2939 In the PWD pseudodata studies discussed in section 5.8, we find a similar set of partial waves,  
 2940 for which we obtained results that differ from the reference model, especially when using the  
 2941 detuned acceptance model. Among these waves are the  $1^+ 0^+ K^*(892) \pi S$ ,  $0^- 0^+ K^*(892) \pi P$ ,  
 2942 and  $3^+ 1^+ K^*(892) \pi D$  waves, for which the discrepancies are largest. The deviations are limited  
 2943 to the region  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$ . In the same  $m_{K\pi\pi}$  region, we observe in the measured  
 2944 data an unexpected peaking structure in the  $3^+ 1^+ K^*(892) \pi D$  wave (see blue data points in  
 2945 figure 5.25d), while there is no known or expected  $K_3$  state in this mass region. The peaking  
 2946 structure dominates this wave, which contributes a surprisingly large fraction of 6.4 % to the total  
 2947 intensity. Also, the  $1^+ 0^+ K^*(892) \pi S$  and  $0^- 0^+ K^*(892) \pi P$  waves exhibit peaking structures  
 2948 in the low-mass region, which depend strongly on the details of the analysis procedure, e.g. on  
 2949 the RICH threshold as shown in figure 5.25c. In contrast to the  $3^+ 1^+ K^*(892) \pi D$  wave, there  
 2950 are known resonances, which may contribute to these structures, i.e. the  $K_1(1270)$ , the  $K_1(1400)$ ,  
 2951 and the  $K(1460)$ . In the rest of the text, we denote such unexpected low-mass structures that  
 2952 have large systematic uncertainties and correspond to deviations in the PWD pseudodata studies  
 2953 by the term leakage artifacts.

2954 We observe leakage artifacts only in a limited set of partial waves, the so-called leakage waves.  
 2955 The other partial waves are called non-leakage waves. Thus, the leakage artifacts must be linked  
 2956 to the distributions of events in the phase-space variables as predicted for the leakage waves. The  
 2957 distribution in the phase-space variables of a wave is characteristic for this wave and is given by  
 2958 the corresponding decay amplitude defined in equation (5.10). In order to study the properties  
 2959 of the decay amplitudes we study the phase-space integral matrix defined in equation (5.22).  
 2960 Figure 5.32a shows the magnitude of the elements of this matrix. The phase-space integral matrix  
 2961 can be interpreted as the Gram matrix [130] of the decay amplitudes. It is also similar to the  
 2962 matrix of overlap integrals used in quantum chemistry [131]. The diagonal elements have a value  
 2963 of one by construction. The off-diagonal elements called overlaps in this work are a measure for  
 2964 the orthogonality of the decay amplitudes as a function of the phase-space variables. If  $|I_{ab}| = 0$ ,  
 2965 the decay amplitudes of waves  $a$  and  $b$  are orthogonal. If  $|I_{ab}| = 1$ , the decay amplitudes of  
 2966 waves  $a$  and  $b$  are linearly dependent, i.e. the distribution of events in the phase-space variables  
 2967 is identical for both waves. Overall, we observe very small overlaps (dark blue off-diagonal  
 2968 cells in figure 5.32a). For example, the overlaps between waves with different  $J^P$  are practically  
 2969 zero as expected, because the Wigner  $D$ -functions are orthogonal. There are a few exceptions  
 2970 of waves with larger overlaps (green and yellow off-diagonal cells in figure 5.32a), which are  
 2971 understood as discussed in appendix D.3. They do not cause issues in the main analysis and are  
 2972 not related to the leakage waves. In summary, the phase-space integral matrices do not give a  
 2973 hint to understand the leakage artifacts.

2974 However, we observe the leakage artifacts only in data affected by detector acceptance effects.  
 2975 The phase-space integral matrix provides a measure of the orthogonality of waves in the full  
 2976 phase space. However, the phase-space is non-uniformly covered by the detector acceptance. In

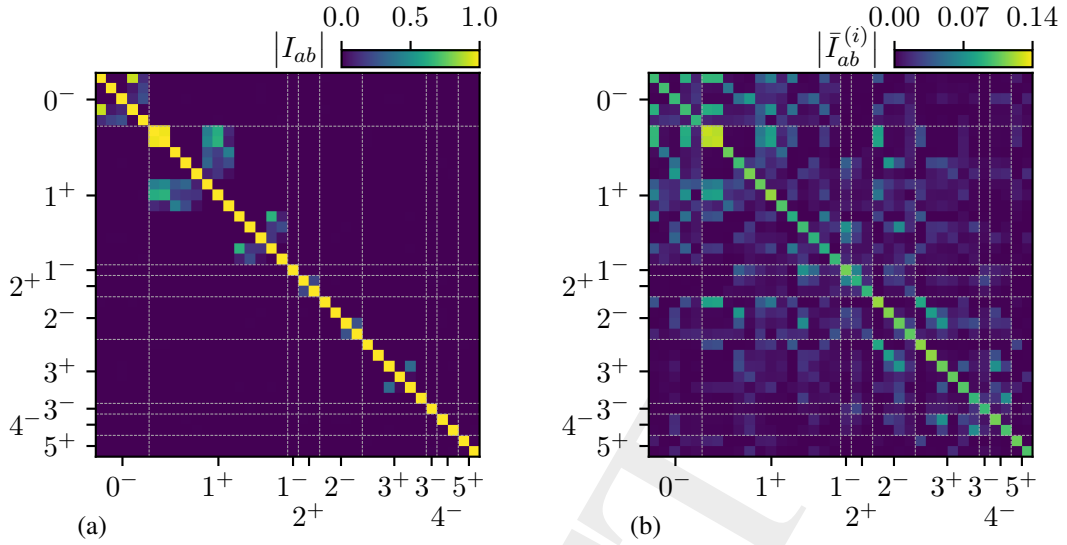


Figure 5.32: Magnitude of the integral-matrix elements for the waves that were selected in the kinematic cell at  $m_{K\pi\pi} = 1.31 \text{ GeV}/c^2$  in the lowest  $t'$  bin. (a) shows the phase-space integral matrix given in equation (5.22). (b) shows the acceptance-integral matrix given in equation (5.29) for the acceptance of the  $i = 2008$  setup. The incoherent flat wave is not shown.

2977 particular, there are parts of the phase-space that are experimentally not accessible in measured  
 2978 data, which is mainly caused by the limited kinematic range of the RICH final-state particle  
 2979 identification (see figure 5.23b). This leads to a loss of information, i.e. there is no information  
 2980 about a part of the phase-space distribution in the measured data. These acceptance effects are  
 2981 taken into account in the acceptance-integral matrix defined in equation (5.29), which can be  
 2982 interpreted as the Gram matrix of the decay amplitudes in the experimentally accessible part of  
 2983 the phase space.<sup>[ci]</sup> Figure 5.32b shows the magnitude of the acceptance-integral matrix elements  
 2984 in the  $m_{K\pi\pi}$  region of the leakage artifacts. The acceptance-integral matrix exhibits completely  
 2985 different features compared to the phase-space integral matrix in figure 5.32a. The diagonal  
 2986 elements are smaller than one, because they represent the average acceptance of the corresponding  
 2987 wave, i.e. the average acceptance if the data would contain only this wave. Particularly noteworthy  
 2988 are the large overlaps with respect to the diagonal elements between almost all waves in the wave  
 2989 set,<sup>[ci]</sup> also between waves with different  $J^P$ . These large overlaps show a none-orthogonality  
 2990 of the decay amplitudes that is caused by the loss of information due to the limited acceptance.  
 2991 However, this does not mean that the partial waves cannot be distinguished at all in the PWD,  
 2992 but the large overlaps indicate that the decay amplitudes are more similar in the experimentally  
 2993 accessible region of the phase space. Thus, they are harder to distinguish and more sensitive to  
 2994 systematic effects.

<sup>[ci]</sup> To be precise, the acceptance does not just select certain regions of the phase space, i.e. is not just zero or one, but is a continuous function in the phase-space variables with values between zero and one (neglecting resolution effects). When interpreting the acceptance-integral matrix as the Gram matrix of the decay amplitudes, we take into account the limitation and distortion of the phase-space by the acceptance.

<sup>[cj]</sup> The magnitudes of the off-diagonal elements of  $\bar{I}_{ab}^{(i)}$  are not limited to the range  $0 \leq \bar{I}_{ab}^{(i)} \leq 1$ . Still, the color scale allows us to interpret off-diagonal elements that are green or yellow as large and those that are dark blue as small.



2995 In order to identify waves with large overlaps, we performed an eigenvalue decomposition of the  
2996 acceptance-integral matrix, i.e. <sup>[ck]</sup>

$$\bar{I}_{ab} = \sum_h e^h v_a^h [v_b^h]^* . \quad (5.77)$$

2997 Here,  $e^h$  are the eigenvalues of the acceptance-integral matrix labeled by  $h$  and  $v_a^h$  is the element  
2998 of the eigenvector of  $e^h$  that belongs to the partial wave  $a$ . In the eigenvalue basis, the PWD  
2999 prediction for the total number of measured events in a given  $(m_{K\pi\pi}, t')$  cell as defined in  
3000 equation (5.28) reads <sup>[ck]</sup>

$$\widehat{N}_{ev} = \sum_{a,b \in \mathbb{W}} \rho_{ab} \bar{I}_{ab} = \sum_h e^h \sum_{a,b \in \mathbb{W}} \rho_{ab} v_a^h [v_b^h]^* . \quad (5.78)$$

3001 As the contribution of each eigenvector to  $\widehat{N}_{ev}$  is multiplied by the corresponding eigenvalue,  
3002 eigenvectors of vanishing eigenvalues, i.e. eigenvalues close to zero, do not strongly influence  
3003  $\widehat{N}_{ev}$ . This means that the corresponding partial waves, i.e. partial waves with large corresponding  
3004  $v_a^h$ , may destructively interfere such that even large intensities in the individual partial waves  
3005 lead to only a small change in the description of the measured sample by the PWD model. <sup>[cl]</sup>  
3006 Hence, these waves are only loosely constrained by the data. This may be an explanation for  
3007 the leakage effect. We therefore searched for vanishing eigenvalues and studied which partial  
3008 waves contribute to the eigenvectors that correspond to vanishing eigenvalues, i.e. we searched  
3009 for waves with large  $v_a^h$ , while the corresponding  $e^h$  is vanishing.

3010 We find vanishing eigenvalues of the acceptance-integral matrix shown in figure 5.32b. The  
3011 smallest eigenvalue, which has a value of 0.0010, mainly arises from waves with  $[K\pi]_S^{K\pi}$ ,  
3012  $[K\pi]_S^{K\eta}$ , and  $[\pi\pi]_S^{\text{AMPK}}$  isobars as discussed in appendix D.3. Those waves exhibit similarly  
3013 large overlaps already in the phase-space integral matrix in figure 5.32a. Hence, the smallest  
3014 eigenvalue is not driven by acceptance effects. Since the leakage artifacts only appear in data  
3015 affected by acceptance effects, this smallest eigenvalue is not related to the leakage artifacts. The  
3016 second smallest eigenvalue, which has a value of 0.0021, arises from large contributions of the  
3017  $0^- 0^+ K^*(892) \pi S$ ,  $3^+ 1^+ K^*(892) \pi D$ ,  $2^- 0^+ K^*(892) \pi P$ ,  $1^- 1^+ K^*(892) \pi P$ ,  $1^+ 1^+ K^*(892) S$ ,  
3018 and  $1^+ 0^+ K^*(892) \pi S$  waves; ordered by the corresponding  $|v_a^h|$  value; and other waves with  
3019 smaller  $|v_a^h|$ . We find large contributions of similar partial waves to the two next largest eigenvalues  
3020 with values of 0.0027 and 0.0032. The fifth smallest eigenvalues becomes quickly larger with  
3021 a value of about 0.0068. Hence, the fifth and all other remaining eigenvalues are not further  
3022 interest here. With increasing  $m_{K\pi\pi}$ , the smallest eigenvalues become significantly larger. For  
3023 example at  $m_{K\pi\pi} \approx 1.6 \text{ GeV}/c^2$ , the smallest eigenvalue has a value of 0.16. Thus, at higher  
3024 masses even the smallest eigenvalues do not vanish and contribute to the total model intensity.

<sup>[ck]</sup> Here, we drop the data-set label ( $i$ ) for simplicity, because we want to demonstrate a general feature of the acceptance-integral matrix.

<sup>[cl]</sup> The PWD model describes the distribution in the phase-space variables and not only  $\widehat{N}_{ev}$ . Nonetheless, combinations of waves that correspond to vanishing eigenvalues do not strongly contribute to the model predictions for the phase-space distributions in equation (5.28). For example, if an eigenvalue is exactly zero, the corresponding linear combination of decay amplitudes is exactly zero everywhere in phase space.

3025 This set of waves that mainly contributes to vanishing eigenvalues of the acceptance-integral  
 3026 matrix agrees with the leakage waves observed in the systematic and pseudodata studies. Fur-  
 3027 thermore, the vanishing eigenvalues become larger and the leakage artifacts become smaller at  
 3028 a similar  $m_{K\pi\pi}$  of about  $1.6 \text{ GeV}/c^2$ . Thus, we conclude that the leakage artifacts are related  
 3029 to the vanishing eigenvalues, i.e. they are related by the loss of information due to the limited  
 3030 acceptance. This acceptance-induced effect is called leakage effect in the rest of the text. How-  
 3031 ever, the eigenvalues that correspond to the leakage effect are not exactly zero, which means  
 3032 that the leakage waves can be distinguished in principle. This is supported by our finding that  
 3033 the leakage artifacts are small in the PWD pseudodata studies in section 5.8 where we used the  
 3034 correct model for the acceptance and where we fitted a pseudodata sample that is much larger  
 3035 than the measured  $K^-\pi^-\pi^+$  sample. However, in the measured  $K^-\pi^-\pi^+$  sample, where we have  
 3036 only a limited amount of data available and where the analysis model is not perfect, e.g. due to  
 3037 background in the sample, the leakage waves may easily be misused by the PWD fit to account  
 3038 for imperfections in the model. This is strongly supported by our finding that the leakage artifacts  
 3039 are much more pronounced in the pseudodata study where we used a detuned acceptance model  
 3040 (see section 5.8.2).

### 3041 5.9.1 Reproducing the Leakage Effect in Pseudodata

3042 Having identified the cause of the leakage effect, we further studied it using additional pseudodata  
 3043 samples. As the  $1^+ 0^+ K^*(892)\pi S$  wave is the largest wave in our analysis with an intensity of  
 3044 about 23 % of the total intensity and as this wave contributes strongly to the leakage effect, we  
 3045 generated a pseudodata sample of  $50 \times 10^6$  events according to only the  $1^+ 0^+ K^*(892)\pi S$  wave  
 3046 from the 238-wave pseudodata model.

3047 The results of the PWDs of the produced pseudodata sample and of the reconstructed pseudodata  
 3048 sample using the correct model for the acceptance (not shown) do not exhibit artifacts from the  
 3049 leakage effect in any of the waves in the produced pseudodata and in any of the non-leakage  
 3050 waves in the reconstructed pseudodata. They are consistent with the findings in the previous  
 3051 pseudodata studies discussed in section 5.8. In the leakage waves we observe only small artifacts  
 3052 from the leakage effect in the reconstructed pseudodata when using the correct model for the  
 3053 acceptance.

3054 The results of the PWD of the reconstructed pseudodata using the detuned acceptance model are  
 3055 shown by the orange data points in figure 5.33. The intensity of the  $1^+ 0^+ K^*(892)\pi S$  wave is  
 3056 larger than the reference model, which is expected from the previous studies due to the leakage  
 3057 effect. However, we observe surprising results for some of the leakage waves. For example,  
 3058 although the reference model is zero for the  $3^+ 1^+ K^*(892)\pi D$  wave, we find a peaking structure  
 3059 in the corresponding intensity spectrum at about  $1.3 \text{ GeV}/c^2$  (orange data points in figure 5.33b),  
 3060 which is similar to the 238-wave pseudodata model (blue crosses), which was obtained from the  
 3061 measured  $K^-\pi^-\pi^+$  sample. Also, the intensity spectrum of the  $0^- 0^+ K^*(892)\pi P$  wave (orange  
 3062 data points figure 5.33c) is surprisingly similar to the one obtained from measured data in the  
 3063 mass region below about  $1.6 \text{ GeV}/c^2$ , although it is expected to vanish.

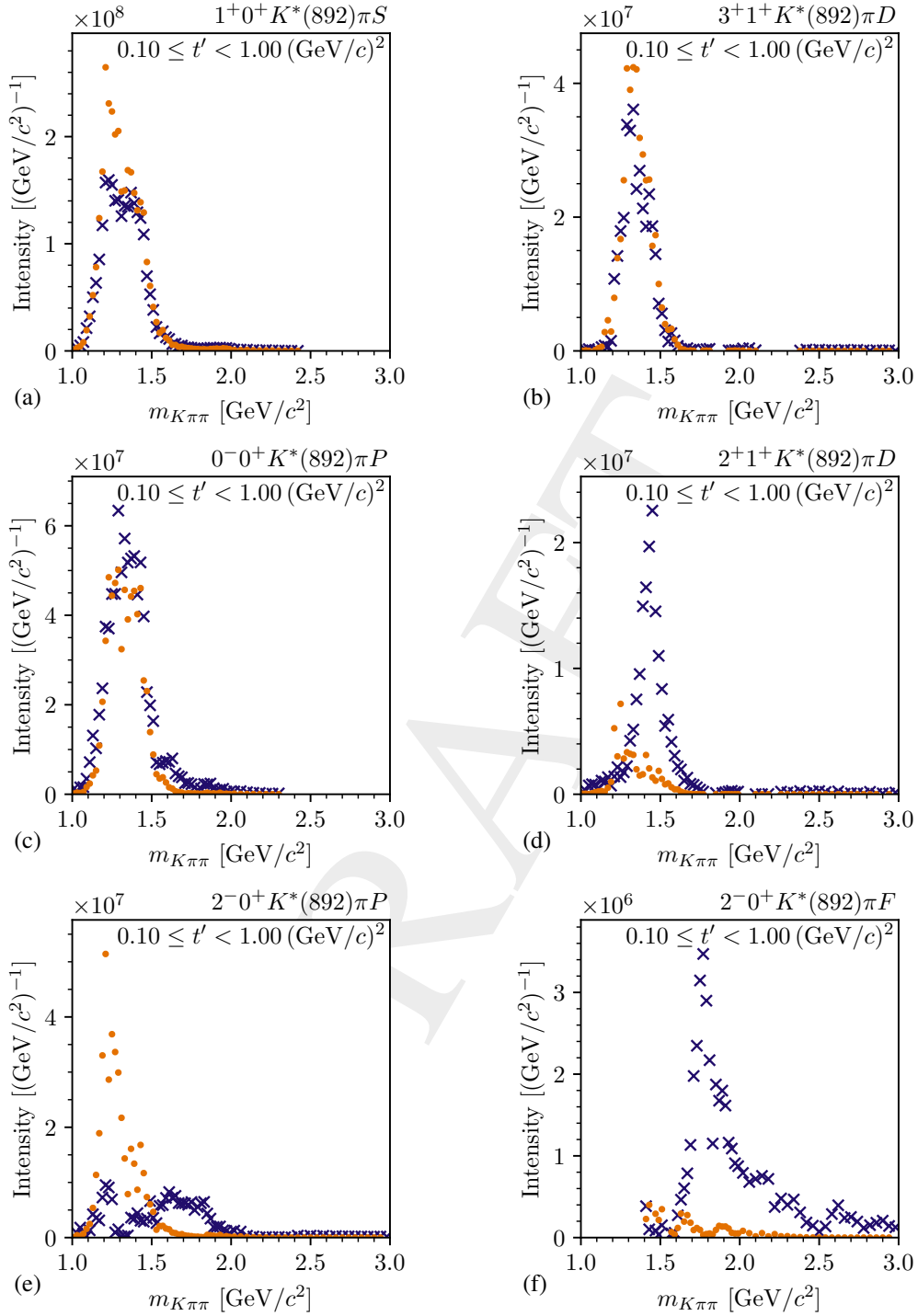


Figure 5.33: Results from the PWD using the detuned acceptance model of the reconstructed pseudodata sample that was generated using only the  $1^+0^+K^*(892)\pi S$  wave from the 238-wave pseudodata model (orange data points). The blue crosses represent the full 238-wave pseudodata model scaled accordingly (see figure 5.30). We show the maximum-likelihood estimates of the intensities obtained from the pseudodata. The corresponding maximum-likelihood estimates of the uncertainties are not shown (see section 5.8).

3064 As the intensity of the reference model of those  $3^+$  and  $0^-$  waves is zero, the low-mass structures  
 3065 in this pseudodata study are artifacts that are generated by our analysis procedure. As these  
 3066 artifacts appear only in the PWD of the reconstructed pseudodata and only when using the  
 3067 detuned acceptance model; and as these artifacts appear only in leakage waves, we conclude  
 3068 that these artifacts arise from the leakage effect. This supports our conclusion, that the leakage  
 3069 artifacts observed in the measured  $K^- \pi^- \pi^+$  sample are an acceptance-induced effect.

3070 The low-mass structures observed e.g. in the  $3^+$  and  $0^-$  waves in this pseudodata study are  
 3071 similar to the low-mass structures observed in the measured  $K^- \pi^- \pi^+$  sample in the same waves.  
 3072 Hence, we conclude that these low-mass structures observed in the measured  $K^- \pi^- \pi^+$  sample  
 3073 are dominantly caused by the leakage effect. For example, for the  $3^+ 1^+ K^*(892) \pi D$  wave  
 3074 this is also consistent with the fact that there is no known or expected  $K_3$  state in this  $m_{K\pi\pi}$   
 3075 region. Furthermore, when adding information to the PWD fit and thereby potentially weakening  
 3076 the leakage effect, as done in the systematic study with a less restrictive RICH threshold, the  
 3077 low-mass structure in the  $3^+ 1^+ K^*(892) \pi D$  wave becomes much smaller (green data points in  
 3078 figure 5.25d).<sup>[cm]</sup> When removing information and thereby potentially enhancing the leakage  
 3079 effect, as done in the systematic study with more restrictive RICH threshold, the low-mass  
 3080 structure in the  $3^+ 1^+ K^*(892) \pi D$  wave becomes even larger (red data points in figure 5.25d).  
 3081 Both observations are consistent with the assumption that the low-mass structure in the  $3^+ 1^+$   
 3082  $K^*(892) \pi D$  wave arises mainly from the leakage effect. We find similar effects also in other  
 3083 leakage waves, e.g. in the  $0^- 0^+ K^*(892) \pi P$  wave.

3084 Fortunately, the leakage effect affects only a limited and identifiable subset of the partial waves.  
 3085 Most of them have a  $K^*(892)$  isobar. In general, waves with  $\pi^- \pi^+$  isobar are not affected by the  
 3086 leakage effect.<sup>[cn]</sup> In some cases, a different orbital angular momentum is already sufficient to  
 3087 suppress artifacts from the leakage effect. For example, we observe large artifacts in the  $2^- 0^+$   
 3088  $K^*(892) \pi P$  wave shown in figure 5.33e, which are even larger than the 238-wave pseudodata  
 3089 model representing the measured data;<sup>[co]</sup> while the artifacts in the  $2^- 0^+ K^*(892) \pi F$  wave shown  
 3090 in figure 5.33f are negligibly small, i.e. they are two orders of magnitude smaller than in the  
 3091  $2^- 0^+ K^*(892) \pi P$  wave. The  $2^+ 1^+ K^*(892) \pi D$  wave shown in figure 5.33d exhibits modest  
 3092 artifacts from the leakage effect. They are mainly focused in the low-mass tail of the peak. This  
 3093 is consistent with the modest systematic effects observed in this wave (see section 5.7). Hence,  
 3094 an interpretation of the  $2^+ 1^+ K^*(892) \pi D$  wave in terms of physics signals is possible.

<sup>[cm]</sup> In the study with a less restrictive RICH threshold, the intensity in the low-mass region of the  $3^+ 1^+ K^*(892) \pi D$  wave is drastically reduced, but there is a non-negligible remaining low-mass intensity, which indicates a remaining bias from the leakage effect. As this study uses already a very low RICH threshold, we conclude that we cannot circumvent the leakage effect. As such a very low RICH threshold leads to larger misidentification, it may cause other systematic effects in our analysis. Thus, we kept the RICH threshold of the main analysis.

<sup>[cn]</sup> Only the  $1^+ 0^+ [\pi\pi]_S^{\text{AMPK}} K P$  wave shows artifacts for  $m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$ . However, this wave is not discussed in this work as it shows no physics signals. Furthermore, these artifacts may also arise from other effects than from the leakage effect, e.g. from destructive interference with the  $1^+ 0^+ f_0(980) K P$  wave.

<sup>[co]</sup> The fact that the pseudodata study yielded even larger artifacts in the  $2^- 0^+ K^*(892) \pi P$  wave than the leakage artifacts observed in measured data indicates that we do not exactly reproduce the leakage artifacts in this pseudodata study, especially in small waves such as the  $2^- 0^+ K^*(892) \pi P$  wave. This is expected, because the imperfection that we introduced in this pseudodata study by using the detuned acceptance model is different and probably larger than the imperfections in the analysis of the measured data and because the leakage artifacts are triggered by imperfections in our analysis.

3095 The appearance of the leakage effect in this pseudodata study allows us to also investigate its  
 3096 footprint in the kinematic distributions. Figure 5.34 shows the distribution in the two-body  
 3097 decay angles of the decay  $X^- \rightarrow \xi_{K^-\pi^+}^0 \pi^-$  in the Gottfried-Jackson frame (GJ). As expected, the  
 3098 prediction of the reconstructed distribution from the PWD fit to the reconstructed pseudodata  
 3099 using the detuned acceptance model (see figure 5.34b) agrees with the actual reconstructed  
 3100 distribution of the pseudodata sample (see figure 5.34a).<sup>[cp]</sup> Figure 5.34c shows the distribution  
 3101 of the produced pseudodata sample, i.e. without acceptance effects. The distribution is flat in  
 3102 the Gottfried-Jackson angles as expected.<sup>[cq]</sup> However, the PWD prediction for the produced  
 3103 distribution shown in figure 5.34d drastically deviates from the actual distribution in figure 5.34c.  
 3104 The PWD model overestimates the distribution by more than a factor of six in the region where  
 3105 the acceptance is practically zero (see dark blue regions in figure 5.34e). This large deviation  
 3106 is caused by the leakage effect, which artificially predicts produced events in the region of  
 3107 practically zero acceptance, i.e. in the region where we are blind experimentally. Hence, the  
 3108 leakage effect has only little influence on the prediction for the reconstructed distributions, which  
 3109 in the PWD fit is compared to the measured distribution (cf. figures 5.34a and 5.34b). Thus, the  
 3110 leakage waves are only weakly constrained by the data.

3111 The leakage effect biases not only the PWD prediction of the distribution of produced events, but  
 3112 the PWD model also overestimates the total number of produced events  $\widehat{N}_{\text{ev}}$ . In the pseudodata  
 3113 study that is based on the full 238-wave pseudodata model in section 5.8.1, which is most  
 3114 similar to the measured  $K^-\pi^-\pi^+$  sample, the PWD model overestimates the total number of  
 3115 produced events by about a factor two. This also leads to a bias of the relative intensities defined  
 3116 in equation (5.76), because  $\widehat{N}_{\text{ev}}$  enters the denominator. Especially the relative intensities of  
 3117 non-leakage waves are affected as the nominator in equation (5.76) is not biased by the leakage  
 3118 effect. Assuming that the leakage effect appears with a similar strength also in the PWD of  
 3119 the measured  $K^-\pi^-\pi^+$  sample, the relative intensities of non-leakage waves are underestimated  
 3120 by about a factor 2 in the 238-wave PWD. Hence, the relative intensities cannot directly be  
 3121 interpreted in terms of how much a wave contributes to the measured data. Nonetheless, the  
 3122 relative intensities can be compared among non-leakage waves as the bias from the leakage effect  
 3123 is the same for all of them. Thus, the relative intensities can still be used as a measure of whether  
 3124 a wave is large or small.

3125 In the pseudodata study discussed above, we showed that if the pseudodata contain only the  
 3126  $1^+ 0^+ K^*(892) \pi S$  wave with an amplitude that is similar to the one obtained from the measured  
 3127  $K^-\pi^-\pi^+$  sample, we reproduce the leakage effect with a similar shape and strength as in the  
 3128 measured  $K^-\pi^-\pi^+$  sample for most of the leakage waves. To study whether this is also the case  
 3129 for other partial waves, we produced a pseudodata sample containing only the  $3^+ 1^+ K^*(892) \pi D$

<sup>[cp]</sup> The pseudodata distribution is less noisy than the corresponding distribution from the PWD prediction. The samples to generate both distributions contain a similar number of events. While the events in the reconstructed pseudodata sample are already distributed accordingly, we used reconstructed events that are phase-space distributed and weighted them to obtain the PWD prediction for the reconstructed distribution (see appendix C.3). Given the same number of events, the first sample contains more information. Therefore, the distribution of the pseudodata sample is less noisy.

<sup>[cq]</sup> The pseudodata sample was generated based on the decay amplitude of the  $1^+ 0^+ K^*(892) \pi S$  wave. We expect a flat distribution in the Gottfried-Jackson angles as this wave has  $M = 0$  and  $L = 0$  [132].

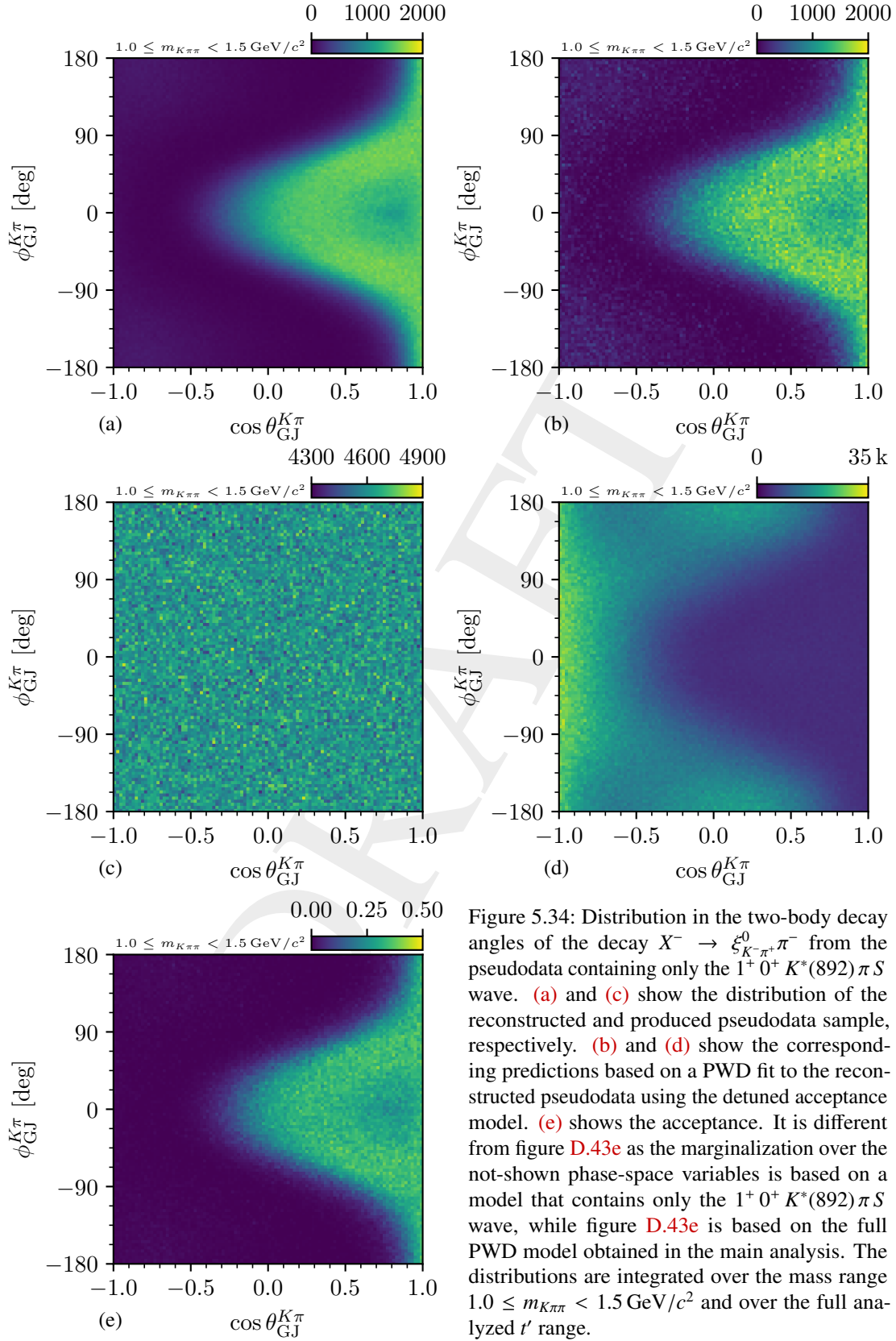


Figure 5.34: Distribution in the two-body decay angles of the decay  $X^- \rightarrow \xi_{K\pi^+}^0 \pi^-$  from the pseudodata containing only the  $1^+ 0^+ K^*(892) \pi S$  wave. (a) and (c) show the distribution of the reconstructed and produced pseudodata sample, respectively. (b) and (d) show the corresponding predictions based on a PWD fit to the reconstructed pseudodata using the detuned acceptance model. (e) shows the acceptance. It is different from figure D.43e as the marginalization over the not-shown phase-space variables is based on a model that contains only the  $1^+ 0^+ K^*(892) \pi S$  wave, while figure D.43e is based on the full PWD model obtained in the main analysis. The distributions are integrated over the mass range  $1.0 \leq m_{K\pi\pi} < 1.5 \text{ GeV}/c^2$  and over the full analyzed  $t'$  range.

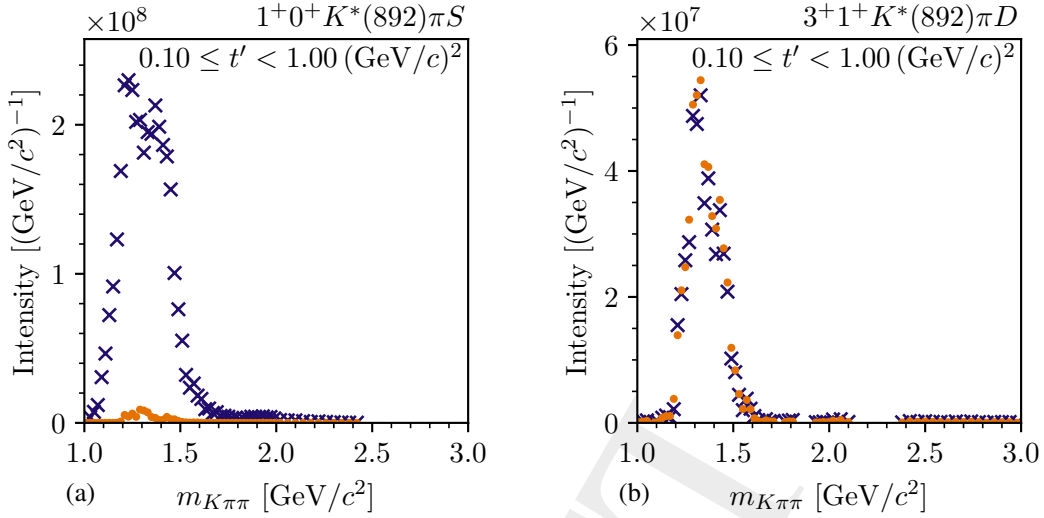


Figure 5.35: Same as figure 5.33, but showing the PWD using the detuned acceptance model of the reconstructed pseudodata sample that was generated using only the  $3^+ 1^+ K^*(892) \pi D$  wave from the 238-wave pseudodata model.

3130 wave from the 238-wave pseudodata model. Figure 5.35 shows the results of a PWD of these  
 3131 pseudodata. The intensity spectrum of the  $3^+ 1^+ K^*(892) \pi D$  wave obtained using the detuned  
 3132 acceptance model (orange data points) agrees with the reference model (blue crosses). The other  
 3133 partial waves exhibit only negligibly small artifacts from the leakage effect as exemplarily shown  
 3134 for the  $1^+ 0^+ K^*(892) \pi S$  wave in figure 5.35a. Thus, the  $3^+ 1^+ K^*(892) \pi D$  wave alone does not  
 3135 lead to a leakage effect similar to the one observed in the measured  $K^- \pi^- \pi^+$  sample.

3136 In another pseudodata study, we tested whether the combination of all waves except for the  $1^+ 0^+$   
 3137  $K^*(892) \pi S$  wave can reproduce the leakage artifacts. Therefore, we generated a pseudodata  
 3138 sample using the 238-wave pseudodata model without the  $1^+ 0^+ K^*(892) \pi S$  wave. Figure 5.36  
 3139 shows the results from this study. Using the detuned acceptance model causes artifacts in the  
 3140 leakage waves exemplarily shown in figures 5.36a and 5.36b. As we expect the low-mass  
 3141 structure in the  $3^+ 1^+ K^*(892) \pi D$  wave in the reference model obtained from the measured  
 3142  $K^- \pi^- \pi^+$  sample (blue crosses) to be dominantly produced by the leakage effect and as we  
 3143 obtained in this study a low-mass structure (orange data points), which is about twice as large as  
 3144 the reference model, we conclude that the leakage artifacts in this study are of similar strength as  
 3145 in the measured  $K^- \pi^- \pi^+$  sample.

3146 From these pseudodata studies we conclude that the strength of the artifacts caused by the leakage  
 3147 effect depends on the data. The leakage effect itself is given by the decay amplitudes of the  
 3148 leakage waves and the acceptance and corresponds to an approximate ambiguity in the PWD  
 3149 model. The amount by which this ambiguity creates artifacts in the partial waves is given by how  
 3150 much the leakage waves actually contribute to the data sample. The  $1^+ 0^+ K^*(892) \pi S$  wave is  
 3151 the dominant contribution.

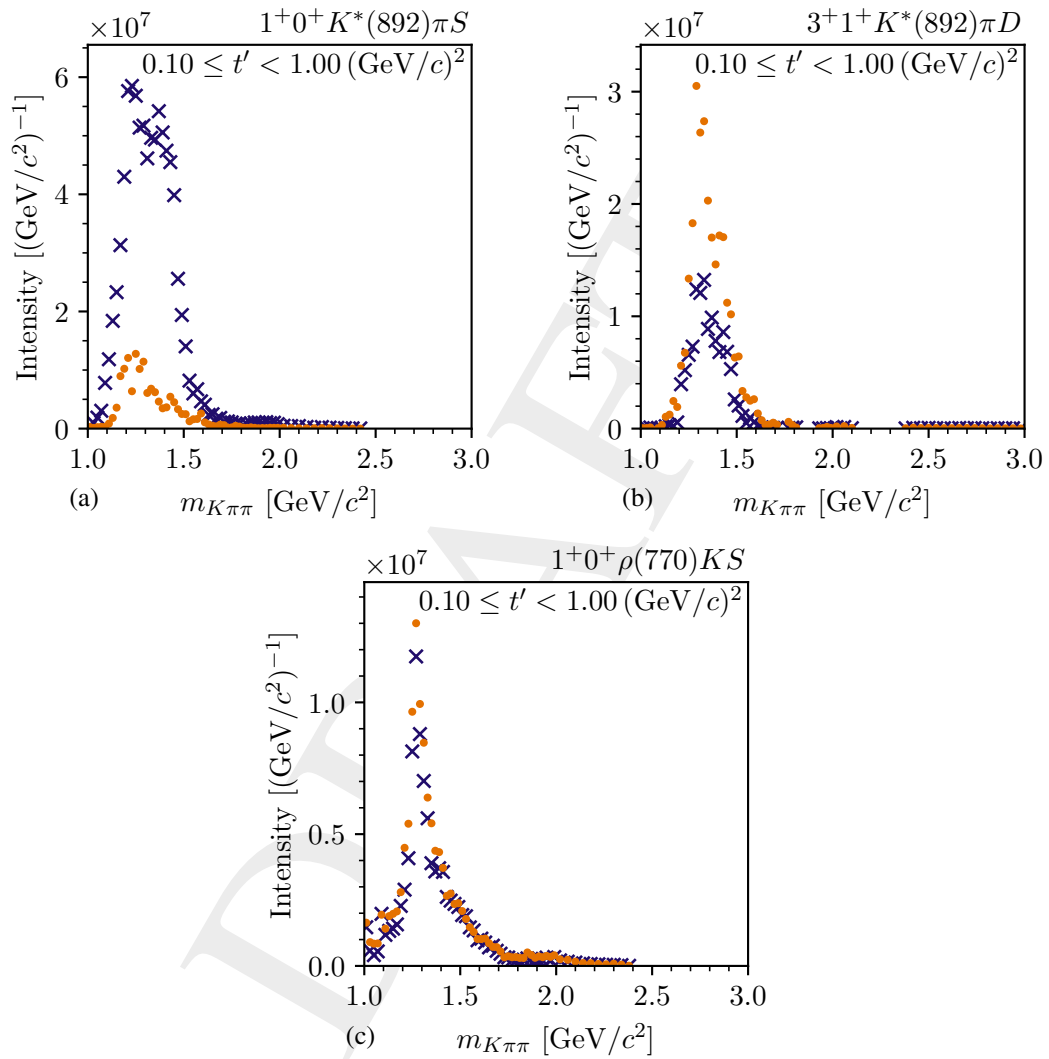


Figure 5.36: Same as figure 5.33, but showing the PWD using the detuned acceptance model of the reconstructed pseudodata sample that was generated using the 238-wave pseudodata model without the  $1^+0^+ K^*(892)\pi S$  wave.



## 3152 5.9.2 Robustness of Non-Leakage Waves with respect to the Leakage Effect

3153 As discussed in sections 5.7 and 5.8, the non-leakage waves are in general robust with respect  
 3154 to systematic effects and imperfections in the analysis model. Having identified the cause of  
 3155 the leakage effect, we performed further studies to explicitly test for a potential influence of the  
 3156 leakage effect on the non-leakage waves. In the pseudodata studies discussed in section 5.9.1, in  
 3157 which we reproduced the leakage effect, the non-leakage waves exhibited only small artifacts,  
 3158 which are negligible compared to the physics signals in these waves, as shown e.g. in figures 5.33f  
 3159 and 5.36c.

3160 As the  $3^+ 1^+ K^*(892)\pi D$  wave is one of the major waves affected the leakage effect and as we  
 3161 assume the low-mass structure in this wave to be predominantly a leakage artifact, we performed a  
 3162 PWD of the measured  $K^-\pi^-\pi^+$  sample using the 238-wave set but omitting the  $3^+ 1^+ K^*(892)\pi D$   
 3163 wave for  $m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$ . Figure 5.37 shows the results from this systematic study (light  
 3164 red data points) compared to the main analysis (blue data points). The intensity spectra of the  
 3165 leakage waves obtained from this study deviate from the main analysis as shown in figures 5.37a  
 3166 and 5.37b. This is expected, because by omitting the  $3^+ 1^+ K^*(892)\pi D$  wave from the wave  
 3167 set, we changed the eigenvalue decomposition of the acceptance-integral matrix and thereby  
 3168 altered the leakage effect.<sup>[cr]</sup> The results of the non-leakage waves agree with the main analysis  
 3169 as exemplarily shown in figure 5.37c. Even the  $2^+ 1^+ K^*(892)\pi D$  wave shown in figure 5.37d,  
 3170 which exhibits modest systematic effects and modest artifacts from the leakage effect in the  
 3171 previous studies, is robust when omitting the  $3^+ 1^+ K^*(892)\pi D$  wave. This is another indication  
 3172 for the robustness of the non-leakage waves with respect to the leakage effect.

3173 Reviewing our findings presented in this section 5.9, we can explain the large systematic effects  
 3174 observed for some partial waves in section 5.7 and the deviations observe in the same waves in  
 3175 the PWD pseudodata studies in section 5.8 in terms of the leakage effect. The leakage effect is  
 3176 caused by the loss of information due to the limited detector acceptance, which is dominated  
 3177 by the limited kinematic range of the RICH final-state particle identification. This effect is  
 3178 visible in the acceptance-integral matrix. We identified those waves that are affected by the  
 3179 leakage effect using three different approaches: (i) waves that exhibit unstable intensities in the  
 3180 systematic studies, (ii) waves with deviations from the corresponding reference model in the  
 3181 PWD pseudodata studies, and (iii) waves with large overlaps in the acceptance-integral matrix.  
 3182 All three approaches yield a consistent set of leakage waves. Figure G.3 shows the intensity  
 3183 distribution of all leakage waves that are discussed in this work. Furthermore, we identified the  
 3184  $m_{K\pi\pi}$  range that is affected by the leakage effect to be  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$ . An interpretation  
 3185 of the leakage waves in this  $m_{K\pi\pi}$  region in terms of physics signals is possible only to a very  
 3186 limited extend and only on a qualitative level. The leakage effect also strongly biases the PWD  
 3187 model predictions for the distribution of produced events. The non-leakage waves are robust  
 3188 with respect to the leakage effect. Thus, they can be interpreted in terms of physics signals as  
 3189 done in the RMF introduced in chapter 6. The physics signals in the individual partial waves are  
 3190 discussed in chapter 7.

<sup>[cr]</sup> However, as the leakage effect is caused by several leakage waves, we still expect the results from this study to be biased by the leakage effect.

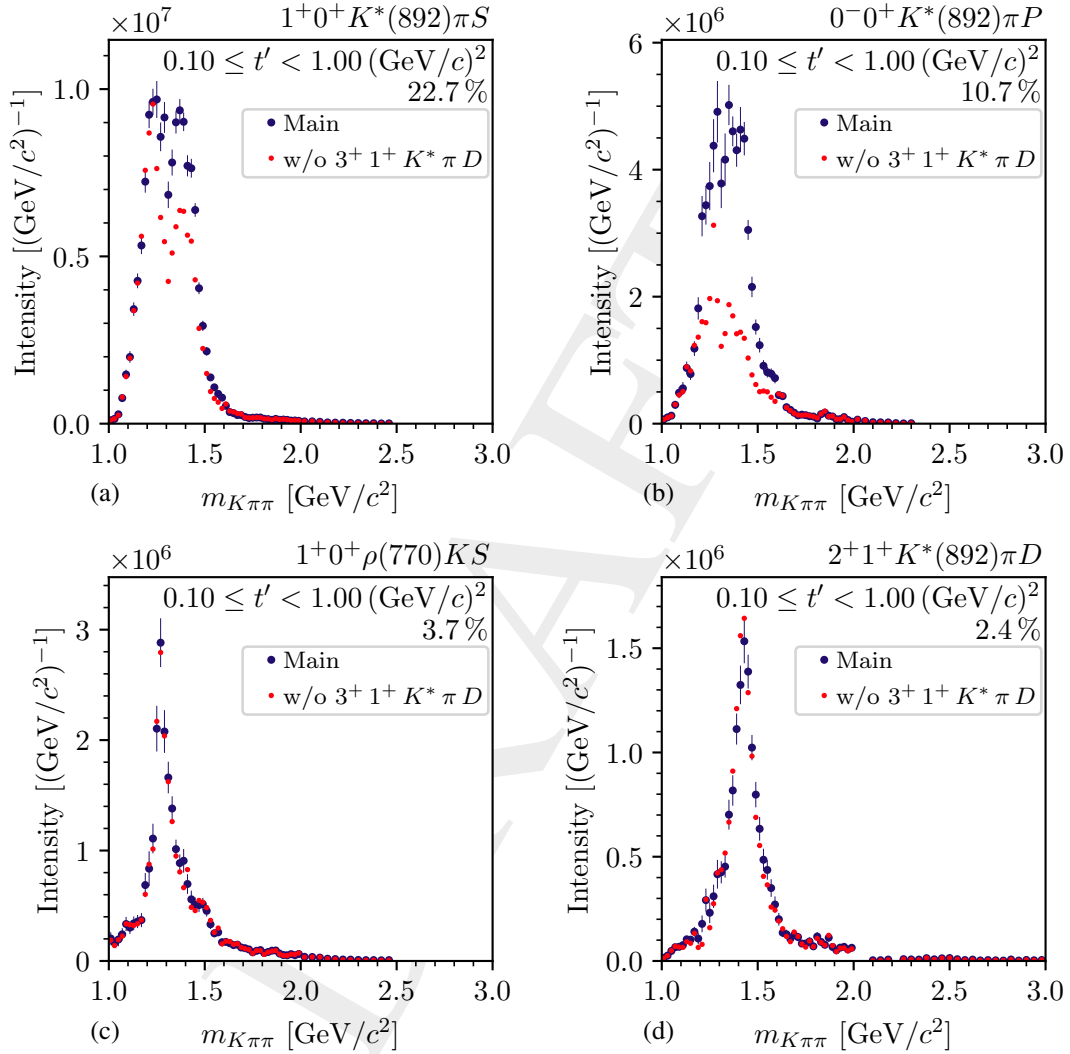


Figure 5.37: Comparison between the results of the PWD of the measured  $K^- \pi^- \pi^+$  sample omitting the  $3^+ 1^+ K^*(892) \pi D$  wave for  $m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$  (maximum-likelihood estimates; light red data points) and the main analysis (Bootstrapping estimates; blue data points). We do not show uncertainties for the maximum-likelihood estimates (see section 5.7).

3191 **5.10  $\pi^-\pi^-\pi^+$  Pseudodata Studies**

3192 The treatment of incoherent background processes is an important task in the analysis of the  
 3193 reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$ , as discussed in section 5.3. We expect the largest background  
 3194 from events of the reaction  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$ , where the beam pion that was erroneously  
 3195 identified as a kaon and where one of the final-state pions was wrongly assumed to be a kaon.  
 3196 This background is called  $\pi^-\pi^-\pi^+$  background. Since the pion component in the beam is 36  
 3197 times larger than the kaon component, this leads to a non-negligible  $\pi^-\pi^-\pi^+$  background in the  
 3198  $K^-\pi^-\pi^+$  sample, even considering the excellent misidentification probability for beam particle  
 3199 identification of only 1%. The final-state particle identification can suppress this background  
 3200 only to a very limited extend, because we required only one of the two negative final-state particle  
 3201 to be identified either as a  $K^-$  or a  $\pi^-$  and the  $K^-\pi^-\pi^+$  and the  $\pi^-\pi^-\pi^+$  final state both contain a  
 3202  $\pi^-$ .

3203 In order to study the  $\pi^-\pi^-\pi^+$  background in the  $K^-\pi^-\pi^+$  sample, we generated a pseudodata  
 3204 sample for the reaction  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$ , which is called  $\pi^-\pi^-\pi^+$  pseudodata sample. In  
 3205 order to follow the same approach as in the  $K^-\pi^-\pi^+$  pseudodata studies in section 5.8 requires  
 3206 a PWD model of this reaction. Fortunately, COMPASS collected the so-far world's largest  
 3207 sample of the reaction  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$  using the dominant  $\pi^-$  component in our beam.  
 3208 Based on this sample, an extensive PWD was performed using the so-far world's largest PWD  
 3209 model in this channel [39]. The results of the COMPASS  $\pi^-\pi^-\pi^+$  analysis were studied in  
 3210 detail and are well understood [38–41, 72, 80, 133]. Based on these results, an improved  
 3211 re-analysis of this reaction based on the 2008 diffraction data set was performed and will be  
 3212 presented in ref. [43].<sup>[cs]</sup> The COMPASS results hence provide a reliable and realistic model  
 3213 for the reaction  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$ . We used the PWD model obtained in the analysis in  
 3214 ref. [43] and summarized in appendix D.4.1 to generate a pseudodata sample for the reaction  
 3215  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$ . We generated 47 405 138 pseudodata events, which corresponds to exactly  
 3216 1/3 of the number of produced events that we expect in the 2008 diffraction data set as predicted  
 3217 by the PWD model.

3218 To determine the amount and the kinematic distribution of the  $\pi^-\pi^-\pi^+$  background in the  
 3219 measured  $K^-\pi^-\pi^+$  sample, we processed the produced  $\pi^-\pi^-\pi^+$  pseudodata events through  
 3220 the COMPASS detector Monte Carlo simulation. Then, we misinterpreted them as  $K^-\pi^-\pi^+$   
 3221 events, i.e. we applied the CEDAR and RICH misidentification probabilities as described in  
 3222 appendices C.2.2 and C.2.3, respectively. Finally, we applied the same event selection criteria  
 3223 to the  $\pi^-\pi^-\pi^+$  pseudodata sample as applied to the measured  $K^-\pi^-\pi^+$  sample (see section 4.1).  
 3224 This procedure yielded the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata sample.

<sup>[cs]</sup> The 2009 diffraction data set was not used in the  $\pi^-\pi^-\pi^+$  analysis when obtaining the model for the  $\pi^-\pi^-\pi^+$  pseudodata, yet.

3225 **5.10.1 The Reconstructed  $\pi^- \pi^- \pi^+$  Pseudodata Sample**

3226 The amount of  $\pi^- \pi^- \pi^+$  background in the measured  $K^- \pi^- \pi^+$  sample can be predicted from  
 3227 the amount of reconstructed  $\pi^- \pi^- \pi^+$  pseudodata events. Analogously to the effective intensity  
 3228 model for the background contributions in equation (5.62), the absolute detector acceptance  
 3229 in the COMPASS  $\pi^- \pi^- \pi^+$  analysis and in this analysis enter the prediction for the amount of  
 3230  $\pi^- \pi^- \pi^+$  background. For the PWD only the modulation of the acceptance in the phase-space  
 3231 variables is important. Imperfections in modeling the absolute acceptance do not bias the results  
 3232 of the PWD.<sup>[ct]</sup> Therefore, the acceptance model was not fine-tuned for the determination the  
 3233 absolute acceptance in either of the two analysis. However, the same approach to determine the  
 3234 experimental acceptance as used in this analysis and described in appendix C.2 was also used  
 3235 in the  $\pi^- \pi^- \pi^+$  analysis in ref. [43], from which we took the model for the  $\pi^- \pi^- \pi^+$  pseudodata  
 3236 sample. Thus, potential systematic effects from imperfect estimates of the absolute acceptances  
 3237 should cancel out to first order [see equation (5.62)]. Hence, we expect the  $\pi^- \pi^- \pi^+$  pseudodata  
 3238 sample to yield a rough but realistic estimate for the predicted amount of  $\pi^- \pi^- \pi^+$  background.

3239 From the 47 405 138 produced  $\pi^- \pi^- \pi^+$  pseudodata events 8934 events were reconstructed as  
 3240  $K^- \pi^- \pi^+$  events. Taking into account that the size of the produced pseudodata sample is only 1/3  
 3241 of the predicted number of produced  $\pi^- \pi^- \pi^+$  events in the measured data, we expect a  $\pi^- \pi^- \pi^+$   
 3242 background of 26 802 events in the measured  $K^- \pi^- \pi^+$  sample of the 2008 diffraction data set.  
 3243 This corresponds to a  $\pi^- \pi^- \pi^+$  contamination of 6.7%. Given the similar acceptance for the  
 3244 2008 and 2009 diffraction data sets, we expect the same  $\pi^- \pi^- \pi^+$  contamination in the combined  
 3245 2008 and 2009  $K^- \pi^- \pi^+$  sample. Compared to other backgrounds, e.g. the background from  
 3246  $K^- + p \rightarrow K^- K^- K^+ + p$  events of about 4%, we expect the  $\pi^- \pi^- \pi^+$  background to be the largest  
 3247 background in the  $K^- \pi^- \pi^+$  sample. A detailed reasoning for the amount of  $\pi^- \pi^- \pi^+$  background  
 3248 is given in appendix D.4.2.

3249 In figure 5.38, we compare the  $\pi^- \pi^- \pi^+$  pseudodata sample reconstructed as  $K^- \pi^- \pi^+$  events (red  
 3250 histograms) to the measured  $K^- \pi^- \pi^+$  sample (blue histograms). The  $\pi^- \pi^- \pi^+$  pseudodata exhibit  
 3251 a broad distribution in  $m_{K\pi\pi}$  shown in figure 5.38a. No clear peaks from  $\pi^- \pi^- \pi^+$  resonances  
 3252 are observed. Thus, the peaks observed in the  $m_{3\pi}$  spectrum in figure 5 of ref. [39] are smeared  
 3253 out by the wrong final-state particle mass assumption and none of the peaks observed in the  
 3254 measured  $m_{K\pi\pi}$  spectrum is caused by the  $\pi^- \pi^- \pi^+$  background.

3255 The  $m_{\pi^- \pi^+}$  spectrum obtained from the reconstructed  $\pi^- \pi^- \pi^+$  pseudodata sample shows similar  
 3256 structures as the one from the  $K^- \pi^- \pi^+$  sample (see figure 5.38b). Both show clear signals from

<sup>[ct]</sup> For example, the energies  $E_{\text{beam}}$ , with which the beam particles in the pseudodata sample were produced, were taken from a sample of measured beam energies in a chosen  $E_{\text{beam}}$  range (see appendix C.2.1). This range is wider than the  $E_{\text{beam}}$  range, in which those pseudodata events were accepted in the  $K^- \pi^- \pi^+$  event selection, as described in section 4.1. The choice of this  $E_{\text{beam}}$  range, in which the pseudodata samples were generated, does not affect the PWD. This is so because only the reconstructed pseudodata events that survived the  $K^- \pi^- \pi^+$  event selection, i.e. that lied within the narrower  $E_{\text{beam}}$  range of the event selection, affect the modulation of the acceptance in the phase-space variables in the acceptance model. However, the choice of this  $E_{\text{beam}}$  range, in which the pseudodata samples were generated, affects the estimate for the absolute acceptance as it affects the fraction of produce pseudodata events that were reconstructed.

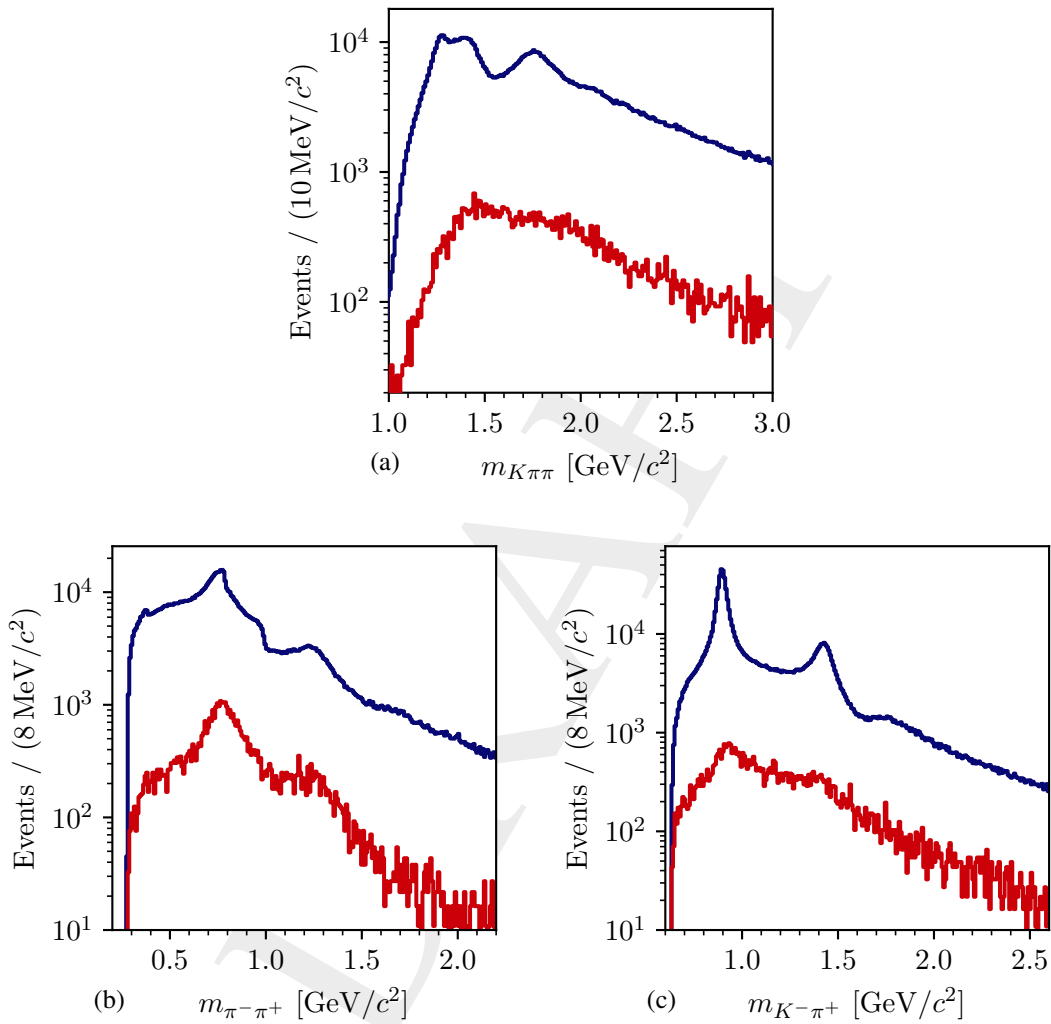


Figure 5.38: Distributions in the invariant masses of (a) the  $K^-\pi^-\pi^+$  system, (b) the  $\pi^-\pi^+$  subsystem, and (c) the  $K^-\pi^+$  subsystem. The red histograms show the  $\pi^-\pi^-\pi^+$  pseudodata sample reconstructed as  $K^-\pi^-\pi^+$  events (see text) and scaled such that the total number of reconstructed  $\pi^-\pi^-\pi^+$  pseudodata events corresponds to the predicted amount of  $\pi^-\pi^-\pi^+$  background in the  $K^-\pi^-\pi^+$  sample. The blue histograms show the measured  $K^-\pi^-\pi^+$  sample (same as figures 4.6a, 4.7a, and 4.7b, respectively).

3257  $\pi^- \pi^+$  resonances such as the  $\rho(770)$  and  $f_2(1270)$ , and a shoulder from the  $f_0(980)$ . This is  
 3258 expected, because both reactions, i.e.  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  and  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , contain  
 3259 the  $\pi^- \pi^+$  subsystem in the final states.

3260 The  $m_{K^- \pi^+}$  spectrum from the reconstructed  $\pi^- \pi^- \pi^+$  pseudodata exhibits a broad distribution  
 3261 shown by the red histogram in figure 5.38c. On top of this distribution we find a peak at about  
 3262  $0.94 \text{ GeV}/c^2$ . This peak corresponds to the  $\rho(770)$  resonance in the  $\pi^- \pi^+$  subsystem of the  
 3263  $\pi^- \pi^- \pi^+$  final state. Compared to the nominal  $\rho(770)$  mass, it is shifted towards higher masses, i.e.  
 3264 when erroneously identifying the  $\pi^-$  as  $K^-$ . Interestingly, this “ $\rho(770)$  peak” is at a similar  $m_{K^- \pi^+}$   
 3265 position as the narrow peak in the measured  $K^- \pi^- \pi^+$  sample, which arises from the  $K^*(892)$   
 3266 resonance in the  $K^- \pi^+$  subsystem. However, the “ $\rho(770)$  peak” is about 4 times broader than the  
 3267  $K^*(892)$  resonance. Furthermore, the  $m_{K^- \pi^+}$  spectrum from the reconstructed  $\pi^- \pi^- \pi^+$  pseudodata  
 3268 sample exhibits a shoulder at about  $1.4 \text{ GeV}/c^2$ , which corresponds to the  $f_2(1270)$  resonance  
 3269 in the  $\pi^- \pi^+$  subsystem. Interestingly, this “ $f_2(1270)$  peak” is at a similar  $m_{K^- \pi^+}$  position as and  
 3270 has an about 1.3 times larger width than the higher-lying peak in the measured  $K^- \pi^- \pi^+$  sample,  
 3271 which partly arises from the  $K_2^*(1430)$  resonance in the  $K^- \pi^+$  subsystem. Despite the similar  
 3272 resonance position, the signals in the measured  $K^- \pi^- \pi^+$  sample and in the reconstructed  $\pi^- \pi^- \pi^+$   
 3273 pseudodata sample arise from different resonances. Hence, they are in detail different and a  
 3274 model for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  may not be able to perfectly describe the  $\pi^- \pi^- \pi^+$   
 3275 background. This is discussed in the following section 5.10.2.

### 3276 5.10.2 Partial-Wave Decomposition of $\pi^- \pi^- \pi^+$ Pseudodata

3277 In order to study the influence of the  $\pi^- \pi^- \pi^+$  background on the PWD of the measured  $K^- \pi^- \pi^+$   
 3278 sample, we performed a PWD of the  $\pi^- \pi^- \pi^+$  pseudodata sample that was reconstructed as  
 3279  $K^- \pi^- \pi^+$  events. In the rest of the text it is called the  $\pi^- \pi^- \pi^+$  background PWD.<sup>[cu]</sup>

3280 To compare the results of the  $\pi^- \pi^- \pi^+$  background PWD to those from the measured  $K^- \pi^- \pi^+$   
 3281 sample, we used the same 238-wave set. In the COMPASS  $\pi^- \pi^- \pi^+$  analysis, the measured  
 3282  $\pi^- \pi^- \pi^+$  sample is described well by a PWD model with a rank = 1 spin-density matrix.<sup>[cv]</sup>  
 3283 However, in the  $\pi^- \pi^- \pi^+$  background PWD performed here, we misinterpreted the pseudodata  
 3284 events as  $K^- \pi^- \pi^+$  events, and we effectively modeled their distribution using partial waves of  
 3285 the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . This means, e.g., that events from different  $m_{3\pi}$  bins, which

<sup>[cu]</sup> The reconstructed  $\pi^- \pi^- \pi^+$  pseudodata sample contains only 8934 events and is thus insufficient to perform a PWD. Since, in the  $K^- \pi^- \pi^+$  event selection, it is mainly the beam-particle identification that suppresses the  $\pi^- \pi^- \pi^+$  events, we omitted the beam-particle identification cut (BPID cut) when selecting the sample that was used for the PWD. The BPID cut affects only the number of accepted events and their distribution in the inclination space of the beam particle (see section 3.2 and figure C.3b). The distribution of the beam particle has a negligible influence on the phase-space distribution of the final-state particles, which was verified. Omitting the BPID cut yielded a reconstructed  $\pi^- \pi^- \pi^+$  pseudodata sample of about  $8.37 \times 10^6$  events, which is well suited to perform a PWD.

<sup>[cv]</sup> The positive-reflectivity waves are modeled by a rank=1 spin-density matrix, the negative-reflectivity waves by a rank=2 spin-density matrix. Also, an incoherent flat wave was added to the model. The latter two account for only 2.2 % and 3.1 % of the total intensity, respectively [39]. Hence, the  $\pi^- \pi^- \pi^+$  background PWD model is dominantly a coherent rank=1 model.

3286 need to be treated incoherently, enter the same  $m_{K\pi\pi}$  bin, which is described by one PWD model.  
 3287 Therefore, the  $\pi^-\pi^-\pi^+$  background PWD requires a model with rank  $>1$ . This was confirmed  
 3288 by tests using a rank=1 PWD model to describe the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata sample,  
 3289 which yielded unsatisfactory results for the  $\pi^-\pi^-\pi^+$  pseudodata sample based on the measured  
 3290  $\pi^-\pi^-\pi^+$  sample as well as for the measured  $K^-\pi^-\pi^+$  sample. For  $\pi^-\pi^-\pi^+$  pseudodata sample for  
 3291 example, the description phase-space distribution of the  $\pi^-\pi^-\pi^+$  pseudodata by the rank=1 PWD  
 3292 model was insufficient. Also, the obtained intensity spectra of the partial waves were strongly  
 3293 fluctuating from  $m_{K\pi\pi}$  bin to  $m_{K\pi\pi}$  bin. For the measured  $K^-\pi^-\pi^+$  sample, taking into account  
 3294 the  $\pi^-\pi^-\pi^+$  background in an RMF to the  $K^-\pi^-\pi^+$  PWD (see chapter 6) using a rank=1 model  
 3295 for the  $\pi^-\pi^-\pi^+$  background PWD, the RMF was not able to describe the partial-waves. Thus,  
 3296 we finally used a rank=2 PWD model in the  $\pi^-\pi^-\pi^+$  background PWD, which turned out to be  
 3297 sufficient to remedy these imperfections as discussed in the following.

3298 Performing a Bootstrapping of the  $\pi^-\pi^-\pi^+$  background PWD was computationally too expen-  
 3299 sive.<sup>[cw]</sup> Thus, we give in the following the maximum-likelihood estimates from the  $\pi^-\pi^-\pi^+$   
 3300 background PWD and we do not give the corresponding uncertainty estimates for the same  
 3301 reason as given in section 5.7.

3302 Figure 5.39 shows the results of the  $\pi^-\pi^-\pi^+$  background PWD (orange data points), i.e. the  
 3303  $\pi^-\pi^-\pi^+$  background predicted in the various partial waves. We find large intensities in partial  
 3304 waves with a  $\rho(770)$  isobar. Figure 5.39a shows exemplarily the intensity spectrum of the  
 3305  $2^+ 1^+ \rho(770) KD$  wave, which is the wave with the largest  $\pi^-\pi^-\pi^+$  background relative the  
 3306 intensity spectrum obtained from the measured  $K^-\pi^-\pi^+$  sample (blue data points). These large  
 3307 backgrounds in waves with a  $\rho(770)$  isobar are expected, as the  $\pi^-\pi^-\pi^+$  pseudodata contain  
 3308 a large contribution from the  $\rho(770)$  isobar in the  $\pi^-\pi^+$  subsystem as shown in figure 5.38b.  
 3309 Interestingly, in the  $2^+ 1^+ \rho(770) KD$  wave the  $\pi^-\pi^-\pi^+$  background PWD yielded a peaking  
 3310 structure at about  $1.5 \text{ GeV}/c^2$ , i.e. at a similar mass as the peak in the measured  $K^-\pi^-\pi^+$  sample,  
 3311 which arises from the  $K_2^*(1430)$  resonance. This similarity of physics and background signals  
 3312 stresses the importance of a proper treatment of the  $\pi^-\pi^-\pi^+$  background contributions in the  
 3313 PWD (see section 5.3) and in the RMF (see chapter 6).

3314 Similarly, the intensity spectra of waves with an  $f_2(1270)$  isobar show small but non-negligible  
 3315 structures in the  $\pi^-\pi^-\pi^+$  background PWD, exemplarily shown for the intensity spectrum of  
 3316 the  $2^- 0^+ f_2(1270) KS$  wave in figure 5.39b. In this wave, the  $\pi^-\pi^-\pi^+$  background peaks at  
 3317  $m_{K\pi\pi} \approx 1.9 \text{ GeV}/c^2$ , similar to the peak observed in the measured  $K^-\pi^-\pi^+$  sample.

3318 The  $\pi^-\pi^-\pi^+$  background PWD exhibits negligible intensity in partial waves with a  $K^*(892)$  isobar  
 3319 exemplarily shown in figure 5.39c. This is expected, because there is no  $K^*(892)$  resonance in  
 3320 the  $\pi^-\pi^-\pi^+$  pseudodata and the structures in the  $m_{K^-\pi^+}$  spectrum of the reconstructed  $\pi^-\pi^-\pi^+$   
 3321 pseudodata sample, especially the peak at about  $0.94 \text{ GeV}/c^2$ , which is caused by the  $\rho(770)$   
 3322 resonance (see figure 5.38c), differ from the shape of the  $K^*(892)$  isobar resonance.

<sup>[cw]</sup> Furthermore, given the much larger size of the  $\pi^-\pi^-\pi^+$  pseudodata sample as compared to the measured  $K^-\pi^-\pi^+$  sample and thus the higher precision, we expect the maximum-likelihood estimates from the  $\pi^-\pi^-\pi^+$  background PWD to be not strongly biased by non-linearities, which are discussed in section 5.4.

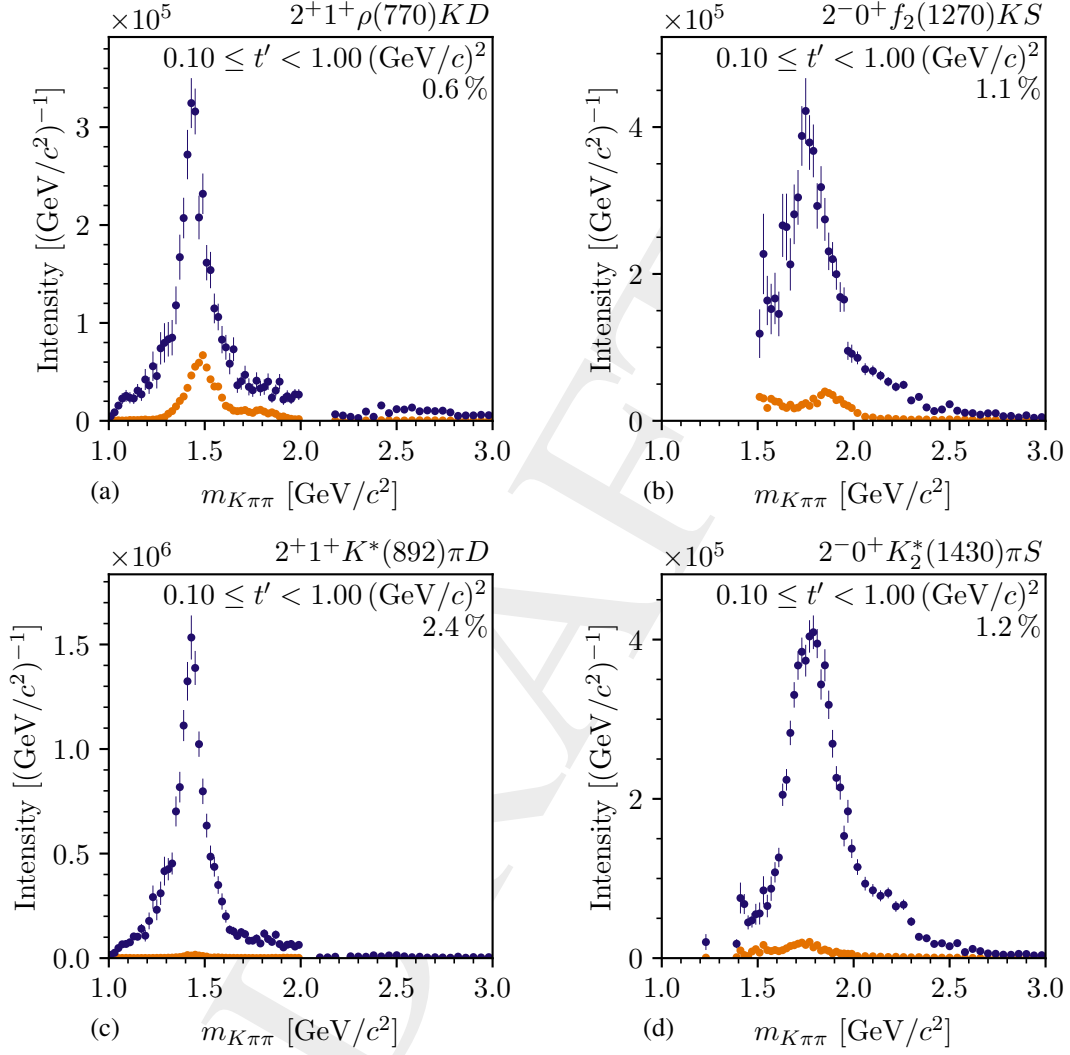


Figure 5.39:  $t'$ -summed intensity spectra of four selected partial waves as obtained from the  $\pi^- \pi^- \pi^+$  background PWD (orange data points). The blue data points show the corresponding results from the PWD of the measured  $K^- \pi^- \pi^+$  sample. The percentages give the contribution of each wave to the total intensity as obtained from the measured  $K^- \pi^- \pi^+$  sample. The results of the  $\pi^- \pi^- \pi^+$  background PWD are scaled such that the total number of reconstructed  $\pi^- \pi^- \pi^+$  pseudodata events corresponds to the predicted amount of  $\pi^- \pi^- \pi^+$  background in the  $K^- \pi^- \pi^+$  sample. We give the maximum-likelihood estimates from the  $\pi^- \pi^- \pi^+$  background PWD. The corresponding uncertainties are not shown (see text).



3323 In contrast to waves with a  $K^*(892)$  isobar, the intensity spectra of waves with  $K_2^*(1430)$  isobar  
 3324 show small but non-negligible structures in the  $\pi^-\pi^-\pi^+$  background PWD (see for example  
 3325 figure 5.39d). Due to the larger width of the  $K_2^*(1430)$  resonance compared to the  $K^*(892)$ , waves  
 3326 with  $K_2^*(1430)$  isobar are used by the PWD more easily to effectively describe the distribution of  
 3327 the  $\pi^-\pi^-\pi^+$  pseudodata. Furthermore, the shoulder at about  $1.4 \text{ GeV}/c^2$  in the  $m_{K^-\pi^+}$  distribution  
 3328 of the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata (see figure 5.38c) is similar to the shape of the  $K_2^*(1430)$   
 3329 isobar. Hence, we expect a non-negligible intensity from the  $\pi^-\pi^-\pi^+$  background PWD in waves  
 3330 with  $K_2^*(1430)$  isobar.

3331 As discussed in section 5.3, we effectively take into account incoherent background processes,  
 3332 such as the  $\pi^-\pi^-\pi^+$  background, in the PWD of the measured  $K^-\pi^-\pi^+$  sample by using a  
 3333 rank=3 PWD model. This requires the phase-space distribution of the background events to be  
 3334 sufficiently well modeled by the  $K^-\pi^-\pi^+$  PWD model, i.e. by the partial waves of the reaction  
 3335  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  that were selected in the 238-wave set. We tested this assumption for  
 3336 the  $\pi^-\pi^-\pi^+$  background by comparing the prediction of the phase-space distribution from the  
 3337  $\pi^-\pi^-\pi^+$  background PWD to the actual distribution of the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata  
 3338 sample as shown in figure 5.40. Hence, we perform a similar comparison as for the measured  
 3339  $K^-\pi^-\pi^+$  sample in section 5.6.

3340 The  $K^-\pi^-\pi^+$  PWD model (orange histogram) describes the  $m_{\pi^-\pi^+}$  distribution of the reconstructed  
 3341  $\pi^-\pi^-\pi^+$  pseudodata sample (blue data points) well as show in figure 5.40a. This is expected,  
 3342 because the  $K^-\pi^-\pi^+$  model contains waves with  $\pi^-\pi^+$  isobars, which were designed to model  
 3343 this distribution. Accordingly, the  $\cos \theta_{\text{GJ}}^{\pi\pi}$  distribution for the decay  $X^- \rightarrow \xi_{\pi^-\pi^+}^0 K^-$  shown in  
 3344 figure 5.40b is also reproduced well by the  $K^-\pi^-\pi^+$  PWD model.

3345 In the low- $m_{K\pi\pi}$  region shown in figure 5.40c, the  $m_{K^-\pi^+}$  distribution of the reconstructed  $\pi^-\pi^-\pi^+$   
 3346 pseudodata sample shows a narrow peak on top of a bump at about  $0.9 \text{ GeV}/c^2$ . This shape arises  
 3347 from a complicated interplay of  $\pi^-\pi^-\pi^+$  events where one of the  $\pi^-$  was erroneously identified  
 3348 as a  $K^-$ . As the waves in the  $K^-\pi^-\pi^+$  PWD model are not explicitly designed to describe this  
 3349 shape, it is effectively described by a combination of various partial waves. The  $K^-\pi^-\pi^+$  model  
 3350 approximates well the  $m_{K^-\pi^+}$  distribution of the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata sample. In the  
 3351 high- $m_{K\pi\pi}$  region, the  $K^-\pi^-\pi^+$  PWD model only roughly reproduces the very broad bump in the  
 3352  $m_{K^-\pi^+}$  distribution of the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata sample as shown in figure 5.40d.

3353 Reviewing our findings presented in this section, the  $K^-\pi^-\pi^+$  partial wave model is able to  
 3354 sufficiently well reproduce the distribution of the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata sample.  
 3355 Thus, our approach to treat the incoherent  $\pi^-\pi^-\pi^+$  background described in section 5.3 is  
 3356 applicable. We expect waves with  $K^*(892)$  isobar to be mainly free of  $\pi^-\pi^-\pi^+$  background,  
 3357 while we expect significant  $\pi^-\pi^-\pi^+$  background in waves with  $\rho(770)$  isobar. In waves with other  
 3358 isobars, such as the  $K_2^*(1430)$  or the  $f_2(1270)$  isobar, we expect modest  $\pi^-\pi^-\pi^+$  background. As  
 3359 the  $\pi^-\pi^-\pi^+$  background is expected to be the dominant background in the  $K^-\pi^-\pi^+$  sample and  
 3360 hence demands the most accurate treatment, we assume that also other incoherent background  
 3361 processes are treated sufficiently well by using a rank=3 PWD model. However, it is important  
 3362 to note that this treatment does not separate physics signals from background at the stage of the  
 3363 PWD. This separation is done at the stage of the resonance-model fits discussed in chapter 6.

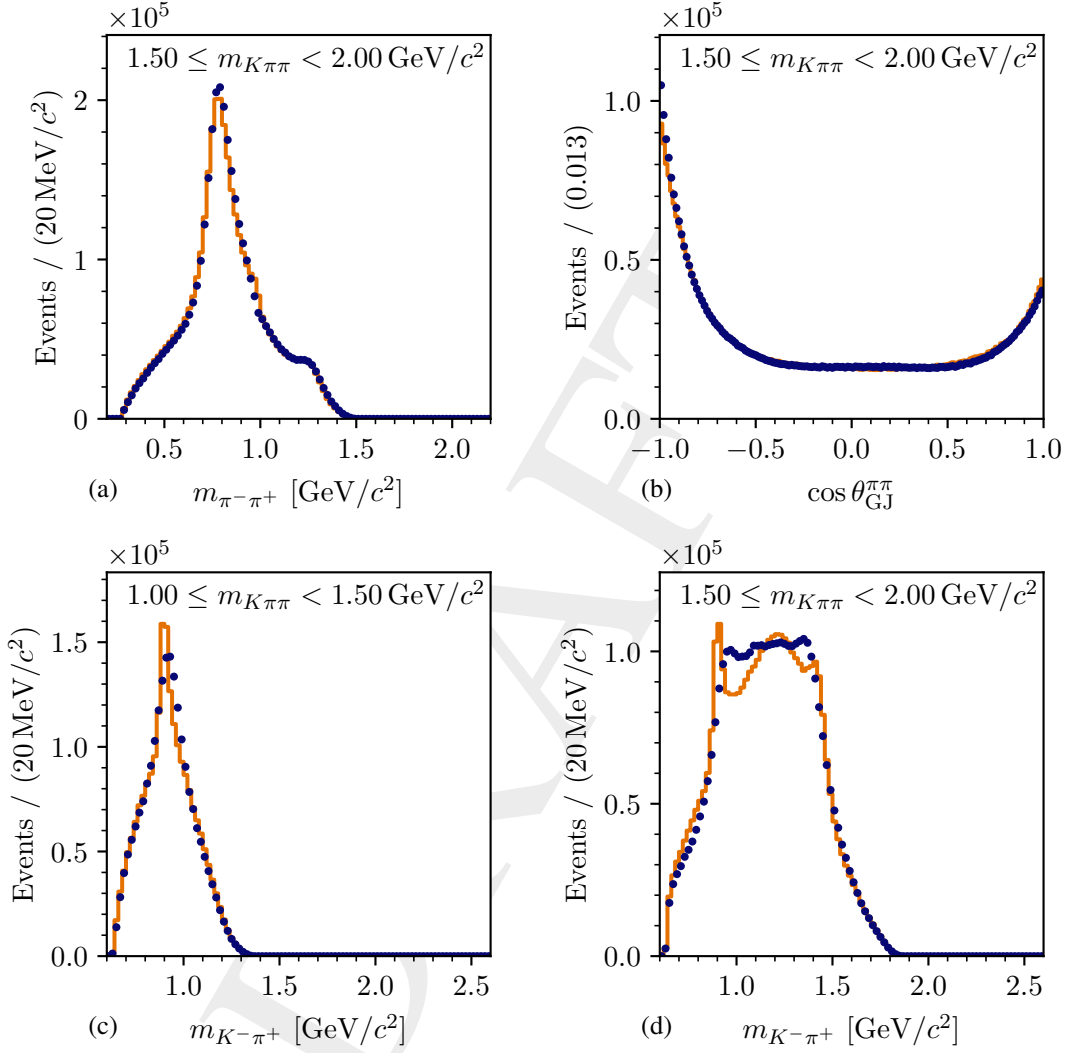


Figure 5.40: Distribution of selected phase-space variables in the mass range  $1.5 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$  ((a), (b), and (d)) and in the mass range  $1.0 \leq m_{K\pi\pi} < 1.5 \text{ GeV}/c^2$  (c), all integrated over the analyzed  $t'$  range. The blue data points show the distribution of the reconstructed  $\pi^-\pi^-\pi^+$  pseudodata sample. The orange histograms show the corresponding predictions from the  $\pi^-\pi^-\pi^+$  background PWD (see appendix C.3 for details on how these histograms were obtained). (a) shows the distribution in  $m_{\pi^-\pi^+}$ . (b) shows the distribution in  $\cos \theta_{GJ}^{\pi\pi}$  of the decay  $X^- \rightarrow \xi_{\pi^-\pi^+}^0 K^-$ . (c) and (d) show the distribution in  $m_{K^-\pi^+}$  in the low- and high- $m_{K\pi\pi}$  region, respectively.

3364

## 6 The Resonance-Model Fit

3365 The so-called resonance-model fit (RMF), which is the second stage of our analysis, aims to  
 3366 identify strange-meson resonances that appear in the various partial waves and to measure their  
 3367 masses and widths. To this end, the  $m_{K\pi\pi}$  dependence of the spin-density matrix elements,  
 3368 which was measured in the PWD, is modeled in the RMF. In order to employ all the available  
 3369 information in a coherent way, all four  $t'$  bins are fit simultaneously in one RMF. While in the  
 3370 PWD, the full  $K^-\pi^-\pi^+$  sample must be modeled, in the RMF we can select a suitable subset of  
 3371 partial waves that we want to study. This is a big advantage of our two-stage analysis approach,  
 3372 as we can select partial waves with clear resonance-like signals, and we can avoid modeling the  
 3373 leakage waves.

3374 We first introduce in section 6.1 the RMF formalism. Then, in section 6.2 we give a first glimpse  
 3375 on the results of the 10-wave RMF, which represents the main results of this analysis. Finally,  
 3376 we discuss in sections 6.3 and 6.4 various systematic and pseudodata studies that we performed  
 3377 in order to scrutinize our results.

### 6.1 Method

#### 6.1.1 Modeling the Spin-Density Matrix

3380 Our  $K^-\pi^-\pi^+$  sample does not only contain events of the signal reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$ ,  
 3381 but has also contributions from background reactions such as  $\pi^-\pi^-\pi^+ + p$ . At the  
 3382 stage of the PWD, we took these background contributions into account in an effective way by  
 3383 formulating a PWD model with a rank=3 spin-density matrix. However, in this approach we did  
 3384 not yet separate the signal from the background contributions. As indicated by equation (5.66),  
 3385 the spin-density matrix that was measured in the PWD is an incoherent sum over the  $K^-\pi^-\pi^+$   
 3386 signal and the various backgrounds. Hence, the measured spin-density matrix  $\rho_{ab}(m_{K\pi\pi}, t')$  is  
 3387 modeled by a sum of spin-density matrices, one for each contribution, i.e.

$$\hat{\rho}_{ab}(m_{K\pi\pi}, t') = \hat{\rho}_{ab}^{K\pi\pi}(m_{K\pi\pi}, t') + \hat{\rho}_{ab}^{3\pi}(m_{K\pi\pi}, t') + \hat{\rho}_{ab}^{\text{eBKG}}(m_{K\pi\pi}, t'). \quad (6.1)$$

3388  $\hat{\rho}_{ab}^{K\pi\pi}(m_{K\pi\pi}, t')$  represents the RMF model for the  $K^-\pi^-\pi^+$  spin-density matrix of the signal  
 3389 reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$ , which is discussed in section 6.1.2.  $\hat{\rho}_{ab}^{3\pi}(m_{K\pi\pi}, t')$  represents the  
 3390 RMF model for the  $\pi^-\pi^-\pi^+$  background, which is explicitly modeled as discussed in section 6.1.3.

3391  $\hat{\rho}_{ab}^{\text{eBKG}}(m_{K\pi\pi}, t')$  represents the effective background component (eBKG), which effectively takes  
 3392 into account all other background contributions. It is explained in section 6.1.4.

### 3393 6.1.2 Modeling the $K^- \pi^- \pi^+$ Signal

3394 We used a naïve model of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , which is based on a sum of  
 3395 Breit-Wigner amplitudes for the resonances. In principle, there are more elaborate models to  
 3396 parameterize resonance amplitudes such as  $K$ -matrix models [23] or  $N$ -over- $D$  models [134].  
 3397 However, they typically require to simultaneously model all decay channels of a studied reso-  
 3398 nance, while we have access to only a limited set of decay channels, i.e. those that finally  
 3399 lead to the  $K^- \pi^- \pi^+$  final state. Also, these more elaborate approaches are theoretically and  
 3400 computationally more demanding, and it turned out that in many cases they yield results similar  
 3401 to those from simpler Breit-Wigner models (compare ref. [41] and ref. [135]). Hence, we used  
 3402 sum-of-Breit-Wigner models in our analysis.

### 3403 Modeling the Transition Amplitudes

3404 Our model  $\hat{\rho}_{ab}^{K\pi\pi}(m_{K\pi\pi}, t')$  for the spin-density matrix of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  is  
 3405 formulated in terms of a model  $\hat{\mathcal{F}}_a^{K\pi\pi}(m_{K\pi\pi}, t')$  for the corresponding transition amplitudes. In this  
 3406 model, multiple resonance components are included for the various strange-meson resonances  
 3407 that appear in the partial waves. In addition, a single so-called non-resonant component is added  
 3408 for each partial wave, which models the coherent non-resonant contributions from processes  
 3409 such as Deck-like reactions discussed in section 2.1.1. The wave components are labeled by  $k$ .

3410 Following equation (5.15), the transition amplitude of component  $k$  in wave  $a$  reads

$$3411 \quad {}^k\hat{\mathcal{F}}_a^{K\pi\pi}(m_{K\pi\pi}, t') = \sqrt{\frac{\mathcal{L}}{(2\pi\mathfrak{I})^2}} \sqrt{m_{K\pi\pi}} \mathcal{P}_{k,a}^{K\pi\pi}(m_{K\pi\pi}, t') \mathcal{D}_k(m_{K\pi\pi}; \zeta_k) \alpha_{k \rightarrow \xi b L} \alpha_\xi \sqrt{\mathfrak{R}_a(m_{K\pi\pi})}, \quad (6.2)$$

3411 where  $\zeta_k$  are the shape parameters of our parameterization  $\mathcal{D}_k(m_{K\pi\pi}; \zeta_k)$  for the dynamic ampli-  
 3412 tude of component  $k$ , e.g. in the case of a resonance components the mass and width of that  
 3413 resonance. The shape parameters are determined in the RMFs.

3414 The production amplitude  $\mathcal{P}_{k,a}^{K\pi\pi}(m_{K\pi\pi}, t')$  can be split into three parts. First, a complex-valued  
 3415 coupling  $\alpha_{K\mathbb{P} \rightarrow k}^{M^e}(t')$ , which represents the strength and phase with which each component  $k$   
 3416 in partial wave  $a$  is produced at the  $K\mathbb{P} \rightarrow k$  vertex (see  $X^-$  production vertex in figure 5.3).  
 3417 Second, a complex-valued coupling  $\alpha_{p\mathbb{P} \rightarrow p}^a(t')$ , which represents the bottom vertex in figure 5.3.  
 3418 Both couplings depend in general on  $t'$ . Third, the production factor  $\mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t')$ . This factor  
 3419 models the scattering process via  $t$ -channel Pomeron exchange, which we assume to dominate at  
 3420 the high center-of-momentum energy at COMPASS. The production factor is the same for all  
 3421 partial waves and for all components. It is given in equation (6.12) below.

3422 With the factorization of the production amplitude discussed above and after re-ordering the  
3423 terms, equation (6.2) reads

$${}^k\hat{\mathcal{F}}_a^{K\pi\pi}(m_{K\pi\pi}, t') = \sqrt{\mathfrak{N}_a(m_{K\pi\pi})m_{K\pi\pi}} \mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t') \sqrt{\frac{\mathcal{L}}{(2\pi\mathfrak{F})^2}} \alpha_{K\mathbb{P}\rightarrow k}^{M^e}(t') \alpha_{p\mathbb{P}\rightarrow p}^a(t') \alpha_{k\rightarrow\xi bL} \alpha_{\xi} \mathcal{D}_k(m_{K\pi\pi}; \zeta_k). \quad (6.3)$$

3424 As only the  $m_{K\pi\pi}$  dependence is explicitly modeled in the RMF, we collect all terms that do not  
3425 depend on  $m_{K\pi\pi}$  in the so-called coupling amplitudes

$${}^k C_a^{K\pi\pi}(t') \equiv \sqrt{\frac{\mathcal{L}}{(2\pi\mathfrak{F})^2}} \alpha_{K\mathbb{P}\rightarrow k}^{M^e}(t') \alpha_{p\mathbb{P}\rightarrow p}^a(t') \alpha_{k\rightarrow\xi bL} \alpha_{\xi}. \quad (6.4)$$

3426 The coupling amplitudes encode the overall strength and phase with which component  $k$  appears  
3427 in partial-wave  $a$  and are in general unknown. The  $t'$  dependence of the coupling amplitudes is  
3428 parameterized by piecewise constant functions in  $t'$ , i.e. there is an independent complex-valued  
3429 parameter for each  $t'$  bin for each coupling amplitude.<sup>[a]</sup> These parameters are determined in the  
3430 RMF. In this way, the  $t'$  dependence of each model component in each partial wave in which it  
3431 appears is determined from the data in a model-independent way.

3432 Finally, our model for the transition amplitude of a single component  $k$  in a wave  $a$  reads

$${}^k\hat{\mathcal{F}}_a^{K\pi\pi}(m_{K\pi\pi}, t') = \sqrt{\mathfrak{N}_a(m_{K\pi\pi})m_{K\pi\pi}} \mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t') {}^k C_a^{K\pi\pi}(t') \mathcal{D}_k(m_{K\pi\pi}; \zeta_k). \quad (6.5)$$

3433 The RMF model for the total transition amplitude of wave  $a$  hence reads

$$\begin{aligned} \hat{\mathcal{F}}_a^{K\pi\pi}(m_{K\pi\pi}, t') &= \sum_{k \in \mathbb{S}_a} {}^k\hat{\mathcal{F}}_a^{K\pi\pi}(m_{K\pi\pi}, t') \\ &= \sqrt{\mathfrak{N}_a(m_{K\pi\pi})m_{K\pi\pi}} \mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t') \sum_{k \in \mathbb{S}_a} {}^k C_a^{K\pi\pi}(t') \mathcal{D}_k(m_{K\pi\pi}; \zeta_k). \end{aligned} \quad (6.6)$$

3434 The sum in equation (6.6) runs over the set  $\mathbb{S}_a$  of all components that we assume to contribute to  
3435 partial wave  $a$ .

### 3436 Modeling the Spin-Density Matrix

3437 In the RMF, the signal reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  is modeled as a fully coherent pro-  
3438 cess. Hence,  $\hat{\rho}_{ab}^{K\pi\pi}(m_{K\pi\pi}, t')$  has rank = 1. It is constructed from the transition amplitudes in  
3439 equation (6.6) in the following way

$$\hat{\rho}_{ab}^{K\pi\pi}(m_{K\pi\pi}, t') = \hat{\mathcal{F}}_a^{K\pi\pi}(m_{K\pi\pi}, t') \left[ \hat{\mathcal{F}}_b^{K\pi\pi}(m_{K\pi\pi}, t') \right]^*. \quad (6.7)$$

<sup>[a]</sup> One coupling amplitude has to be chosen real-valued and positive in order to fix the indeterminable global phase.

### 3440 Parameterization of the Resonance Components

3441 We parameterized the dynamic amplitudes  $\mathcal{D}_k(m_{K\pi\pi}; \zeta_k)$  of resonance appearing in the  $K^-\pi^-\pi^+$   
 3442 system by relativistic Breit-Wigner amplitudes according to equation (5.39). The dynamic width  
 3443 of these Breit-Wigner amplitudes takes into account only the dominant decay channel of the  
 3444 corresponding resonance as listed in tables E.1 and E.5. The shape parameters of the resonance  
 3445 components are the nominal masses and widths of the resonances, i.e.  $\zeta_k = (m_0^k, \Gamma_0^k)$ . In this way,  
 3446 the masses and widths of the strange-meson resonances are measured in the RMF.

### 3447 Parameterization of the Non-Resonant Components

3448 As discussed in section 2.1.1, there are additional processes that also lead to the  $K^-\pi^-\pi^+$  final  
 3449 state, but do not proceed via an intermediate strange-meson resonance in the  $K^-\pi^-\pi^+$  system.  
 3450 Similar to the background contributions, they are effectively decomposed into partial waves in the  
 3451 PWD, and they need to be explicitly treated at the stage of the RMF. In contrast to the background  
 3452 contributions, the non-resonant contributions must be added coherently to the amplitudes for the  
 3453  $K^-\pi^-\pi^+$  resonances.

3454 As there are various non-resonant processes that may contribute and as there are no generally  
 3455 accepted theory models available for them, we parameterized the dynamic amplitudes of the  
 3456 non-resonant components by a phenomenological parameterization with a flexible shape that is  
 3457 adjusted to the data in the RMF. The employed parameterization is inspired by ref. [136] and  
 3458 was used in previous analyses, such as the COMPASS  $\pi^-\pi^-\pi^+$  analysis [40, 41]. It reads

$$\mathcal{D}_k^{\text{NR}}(m_{K\pi\pi}; a_k, c_k) = (m_{K\pi\pi} - m_{\text{thr}})^{a_k} e^{-b(c_k) \tilde{q}_k^2(m_{K\pi\pi})}. \quad (6.8)$$

3459 Here,  $a_k$  and  $c_k$  are the free shape parameters that are determined by the RMF. One should note,  
 3460 that each partial wave has its own non-resonant component with its own set of shape parameters.  
 3461 The pre-factor  $(m_{K\pi\pi} - m_{\text{thr}})^{a_k}$  allows the fit to adjust the low- $m_{K\pi\pi}$  behavior with respect to the  
 3462  $\sqrt{\mathfrak{N}_a(m_{K\pi\pi}) m_{K\pi\pi}} \mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t')$  term in equation (6.6). Here,  $m_{\text{thr}} = m_K + 2m_\pi$  is the kinematic  
 3463 threshold for  $m_{K\pi\pi}$ . The exponential function in equation (6.8) damps the non-resonant amplitude  
 3464 at large masses, i.e. large two-body break-up momenta  $q(m_{K\pi\pi})$  of the isobar-bachelor system, as  
 3465 expected e.g. from models for Deck-like reactions [11, 41, 124].

3466 The slop parameter  $b(c_k)$  of the exponential function in equation (6.8) has to be greater than zero  
 3467 such that the exponential function damps the non-resonant amplitude at large masses. As  $b(c_k)$   
 3468 turned out to be close to zero for the non-resonant component in few partial waves, we limited  
 3469  $b(c_k)$  to be in the range  $b > -1$  (GeV/c)<sup>-2</sup> by using the following parameter mapping of  $b(c_k)$  in  
 3470 terms of  $c_k$ :

$$b(c_k) = -1 \text{ (GeV/c)}^{-2} + 1 \text{ (GeV/c)}^{-2} \cdot \exp[c_k]. \quad (6.9)$$

3471

3472  $q(m_{K\pi\pi}) = q(m_{K\pi\pi}, m_\xi, m_b)$  is the two-body break-up momentum of the isobar-bachelor system  
 3473 using the nominal mass  $m_\xi$  of the isobar resonance and the mass  $m_b$  of the bachelor particle.  
 3474 According to equation (5.41), it is not defined for  $m_{K\pi\pi} < m_\xi + m_b$ . However, there can be events  
 3475 below this limit due to the finite width of the isobar resonance and equation (6.8) still needs  
 3476 to be valid in these cases. Therefore, in equation (6.8), an extension of the two-body break-up  
 3477 momentum is used, which takes into account the finite width of the isobar and is thus valid also  
 3478 below this limit. It is given by

$$\tilde{q}_k(m_{K\pi\pi}) = q(m_{\text{norm}}, m_\xi, m_b) \frac{m_{K\pi\pi} \mathfrak{N}_{a_k}(m_{K\pi\pi})}{m_{\text{norm}} \mathfrak{N}_{a_k}^{m_{\text{norm}}}(m_{K\pi\pi})}, \quad (6.10)$$

3479 where  $a_k$  is the partial wave that belongs to the non-resonant component  $k$ . This approximation  
 3480 is motivated by the facts that  $\mathfrak{N}_a(m_{K\pi\pi})$  can be interpreted as the phase-space volume occupied  
 3481 by wave  $a$  and that the two-body phase space of the isobar-bachelor system is proportional  
 3482 to  $q(m_{K\pi\pi})/m_{K\pi\pi}$ . By equalizing  $\mathfrak{N}_a(m_{K\pi\pi})$  to the quasi-two-body phase space and requiring  
 3483  $\tilde{q}_k(m_{\text{norm}}) = q(m_{\text{norm}})$  at  $m_{\text{norm}} = 3 \text{ GeV}/c^2$  one obtains equation (6.10), which is valid over the  
 3484 full analyzed  $m_{K\pi\pi}$  range.

3485 For most of the studied partial waves, a simplified version of equation (6.8) with  $a_k = 0$  and  
 3486  $b(c_k) = b_k$ , i.e.

$$\mathcal{D}_k^{\text{NR}}(m_{K\pi\pi}; b_k) = e^{-b_k \tilde{q}_k^2(m_{K\pi\pi})}, \quad (6.11)$$

3487 turned out to be sufficient to describe the non-resonant components.

### 3488 Parameterization of the Production Factor

3489 For the production factor, the same parameterization as in the COMPASS  $\pi^- \pi^- \pi^+$  analysis [41,  
 3490 72] is used. It is based on a phenomenological Regge approach to describe central-production  
 3491 reactions by double-Pomeron exchange [69], analogously to those shown in figure 2.3a. It  
 3492 reads<sup>[b]</sup>

$$|\mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t')|^2 = \left( \frac{s}{m_{K\pi\pi}^2} \right)^{2\alpha_{\mathbb{P}}(t')-1}. \quad (6.12)$$

3493 Here,  $s$  is the overall center-of-momentum energy of the  $K^- p$  system, which is fixed by the beam  
 3494 momentum. For the Regge trajectory of the Pomeron,<sup>[c]</sup>

$$\alpha_{\mathbb{P}}(t') = \alpha_0 - \alpha' t', \quad (6.13)$$

3495 we used  $\alpha_0 = 1.2$  as measured in ref. [137] and  $\alpha' = 0.26 (\text{GeV}/c)^{-2}$  as measured in ref. [138].

<sup>[b]</sup> For each of the four  $t'$  bins,  $\alpha_{\mathbb{P}}(t')$  is evaluated at the bin center.

<sup>[c]</sup> Here, we use  $\alpha(t) = \alpha_0 + \alpha' t \approx \alpha_0 - \alpha' t'$ , because  $t' \approx -t$  as  $|t|_{\text{min}}$  is negligibly small in our kinematic range.

3496 **Branching Amplitudes**

3497 The  $t'$  dependence of the coupling amplitudes  ${}^k C_a^{K\pi\pi}(t')$  defined in equation (6.4) only depends  
 3498 on the production of the resonance, not on its decay. The same resonance may appear in different  
 3499 partial waves with the same  $J^P M^E$  quantum numbers, but with different decay modes. The  
 3500 coupling amplitudes that correspond to the different decay modes are hence expected to be propor-  
 3501 tional to each other. The complex-valued proportionality constant is called branching amplitude.  
 3502 For a given component  $k$ , this constraint is implemented in the RMF by replacing the coupling  
 3503 amplitudes  ${}^k C_b^{K\pi\pi}$  of all partial waves  $b$  that have the same  $J^P M^E$  quantum numbers, except for  
 3504 one selected wave  $a$ , by the coupling amplitudes  ${}^k C_a^{K\pi\pi}$  of wave  $a$  and one branching amplitude  
 3505  ${}^k \mathcal{B}_a^{K\pi\pi}$  for each partial wave  $b$ , which is independent of  $t'$ , i.e.

$${}^k C_b^{K\pi\pi}(t') = {}^k \mathcal{B}_a^{K\pi\pi} {}^k C_a^{K\pi\pi}(t'). \quad (6.14)$$

3506 This drastically reduces the number of coupling amplitudes, which are free parameters in the  
 3507 RMF, and thereby improves the fit stability.

3508 **6.1.3 Modeling the  $\pi^- \pi^- \pi^+$  Background**

3509 We modeled the  $\pi^- \pi^- \pi^+$  background by the results of the PWD of the  $\pi^- \pi^- \pi^+$  pseudodata sample  
 3510 that was obtained from the  $\pi^- \pi^- \pi^+$  COMPASS analysis as discussed in section 5.10.2. This  
 3511 means that the background is modeled based on data that where obtained in the same data taking  
 3512 campaigns at the same experiment as our  $K^- \pi^- \pi^+$  sample. The  $\pi^- \pi^- \pi^+$  background component  
 3513 in equation (6.1) is parameterized by

$$\hat{\rho}_{ab}^{\pi\pi\pi}(m_{K\pi\pi}, t') = |C^{\pi\pi\pi}|^2 \rho_{ab}^{\pi\pi\pi}(m_{K\pi\pi}, t'). \quad (6.15)$$

3514 Here,  $\rho_{ab}^{\pi\pi\pi}(m_{K\pi\pi}, t')$  is the spin-density matrix of  $K^- \pi^- \pi^+$  partial waves as obtained from the PWD  
 3515 of the  $\pi^- \pi^- \pi^+$  pseudodata sample using the  $K^- \pi^- \pi^+$  238-wave set, and the  $\pi^- \pi^- \pi^+$  pseudodata  
 3516 sample is based on the  $\pi^- \pi^- \pi^+$  sample measured at COMPASS. It is important to note that  
 3517  $\rho_{ab}^{\pi\pi\pi}(m_{K\pi\pi}, t')$  is fully determined by the pseudodata sample, i.e. it has no free parameters. This  
 3518 means that at the stage of the RMF, a fixed parameterization for the  $\pi^- \pi^- \pi^+$  background in our  
 3519  $K^- \pi^- \pi^+$  sample is used. The absolute amount of  $\pi^- \pi^- \pi^+$  background in our sample is given by  
 3520 the free parameter  $|C^{\pi\pi\pi}|^2$ . This means  $|C^{\pi\pi\pi}|^2$  is determined from the measured  $K^- \pi^- \pi^+$  sample,  
 3521 while  $\rho_{ab}^{\pi\pi\pi}(m_{K\pi\pi}, t')$  is completely determined by the measured  $\pi^- \pi^- \pi^+$  sample.

3522 **6.1.4 Modeling the Effective Background**

3523 Other incoherent background processes, such as  $K^- + p \rightarrow K^- K^- K^+ + p$ , also contribute to the  
 3524  $K^- \pi^- \pi^+$  sample. As there are no explicit models available for these processes, we parameterized  
 3525 them in an effective way by using the same approach as used for the non-resonant components.



3526 Following equation (6.5), the RMF model for the effective background components reads<sup>[d]</sup>

$$\hat{\mathcal{F}}_a^{\text{eBKG}}(m_{K\pi\pi}, t') = \sqrt{\mathfrak{N}_a(m_{K\pi\pi})m_{K\pi\pi}} \mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t') C_a^{\text{eBKG}}(t') \mathcal{D}_{k_a}^{\text{eBKG}}(m_{K\pi\pi}; a_{k_a}, c_{k_a}). \quad (6.16)$$

3527 For the dynamic amplitudes of the effective background components, the same parameterizations  
3528 as for the non-resonant components are used, but with independent shape parameters. For most  
3529 of the partial waves, we used the simplified parameterization [same as equation (6.11)]:

$$\mathcal{D}_k^{\text{eBKG}}(m_{K\pi\pi}; b_k) = e^{-b_k \tilde{q}_k^2(m_{K\pi\pi})}. \quad (6.17)$$

3530 For some partial waves we used the full parameterization [same as equation (6.8)]:

$$\mathcal{D}_k^{\text{eBKG}}(m_{K\pi\pi}; a_k, c_k) = (m_{K\pi\pi} - m_{\text{thr}})^{a_k} e^{-b(c_k) \tilde{q}_k^2(m_{K\pi\pi})}. \quad (6.18)$$

### 3531 6.1.5 $\chi^2$ Formalism

3532 In order to estimate the free parameters of the RMF model, we performed a  $\chi^2$  fit. In order  
3533 to measure the deviation between the RMF Model  $\hat{\rho}_{ab}(m_{K\pi\pi}, t')$  and the measured spin-density  
3534 matrix elements  $\rho_{ab}(m_{K\pi\pi}, t')$ , the real-valued spin-density matrix,<sup>[e]</sup>

$$\Lambda_{ab}(m_{K\pi\pi}, t') = \begin{cases} \Re(\rho_{ab}(m_{K\pi\pi}, t')) & , \text{ if } a \leq b \\ \Im(\rho_{ba}(m_{K\pi\pi}, t')) & , \text{ if } a > b \end{cases}, \quad (6.19)$$

3535 is constructed. The diagonal elements of  $\Lambda_{ab}(m_{K\pi\pi}, t')$  are the partial-wave intensities. The  
3536 upper-right triangular part of  $\Lambda_{ab}(m_{K\pi\pi}, t')$  contains the real parts of the spin-density matrix  
3537 elements, whereas the lower-left triangular part of  $\Lambda_{ab}(m_{K\pi\pi}, t')$  contains the imaginary parts of  
3538 the spin-density matrix elements. As the spin-density matrix is Hermitian,  $\Lambda_{ab}(m_{K\pi\pi}, t')$  contains  
3539 the full information of  $\rho_{ab}(m_{K\pi\pi}, t')$ . The vector  $\vec{\lambda}(m_{K\pi\pi}, t')$  is the vectorization of  $\Lambda_{ab}(m_{K\pi\pi}, t')$ ,  
3540 whose elements read

$$\lambda_i(m_{K\pi\pi}, t') = \Lambda_{ab}(m_{K\pi\pi}, t'), \quad \text{where } i = a \cdot n_{\text{waves}} + b \quad (6.20)$$

3541 and where  $n_{\text{waves}}$  is the number of waves in the spin-density matrix.

3542 Analogously, the equivalent quantities of the RMF model read

$$\hat{\Lambda}_{ab}(m_{K\pi\pi}, t') = \begin{cases} \Re(\hat{\rho}_{ab}(m_{K\pi\pi}, t')) & , \text{ if } a \leq b \\ \Im(\hat{\rho}_{ba}(m_{K\pi\pi}, t')) & , \text{ if } a > b \end{cases}, \quad (6.21)$$

<sup>[d]</sup> As the transition amplitude for the effective background of each wave contains only one component, the coupling amplitude  $C_a^{\text{eBKG}}(t')$  has no additional component label and the component label  $k_a$  of the dynamic amplitude is fixed by the wave label  $a$ .

<sup>[e]</sup> Here and in equations (6.20) to (6.22) we use the wave labels  $a$  and  $b$  as indices that run from 1 to  $n_{\text{waves}}$ , where  $n_{\text{waves}}$  is the number of partial waves in the spin-density matrix.

3543 and

$$\hat{\lambda}_i(m_{K\pi\pi}, t') = \hat{\Lambda}_{ab}(m_{K\pi\pi}, t'), \quad \text{where } i = a \cdot n_{\text{waves}} + b. \quad (6.22)$$

3544 Using the data and model vectors given in equations (6.20) and (6.22), respectively, the  $\chi^2$   
3545 function that is minimized in the RMF reads

$$\chi_{\text{RMF}}^2 = \sum_{t', m_{K\pi\pi}} \sum_{i,j=1}^{n_{\text{waves}}} \Delta\lambda_i(m_{K\pi\pi}, t') \text{Prec} \left[ \lambda_i(m_{K\pi\pi}, t'), \lambda_j(m_{K\pi\pi}, t') \right] \Delta\lambda_j(m_{K\pi\pi}, t'). \quad (6.23)$$

3546 The residuals  $\Delta\lambda_i$ , which represent the difference between measured spin-density matrix elements  
3547 and the RMF model, are given by

$$\Delta\lambda_i(m_{K\pi\pi}, t') = \lambda_i(m_{K\pi\pi}, t') - \hat{\lambda}_i(m_{K\pi\pi}, t'). \quad (6.24)$$

3548 The outer sum in equation (6.23) runs over all  $(m_{K\pi\pi}, t')$  cells, which are independent.

3549 The precision matrix  $\text{Prec}[\lambda_i, \lambda_j]$  is the inverse of the covariance matrix  $\text{Cov}[\lambda_i, \lambda_j]$  of the  
3550 measured spin-density matrix elements  $\lambda_i$ .  $\text{Cov}[\lambda_i, \lambda_j]$  is determined by our Bootstrapping  
3551 approach of the PWD that is discussed in section 5.4.

3552 The maximal possible rank of  $\text{Cov}[\lambda_i, \lambda_j]$  is  $n_{\text{waves}}^2$  with  $n_{\text{waves}}$  being the number of considered  
3553 partial waves, because there are  $n_{\text{waves}}^2$  real-valued spin-density matrix elements. However, we  
3554 limited the rank  $r$  of the spin-density matrix to be  $r = 3$  when formulating the PWD model (see  
3555 sections 5.1.2 and 5.3.1). Consequently, the number of free parameters of the spin-density matrix  
3556 is given by

$$n_{\text{para}}^{\rho} = r(2n_{\text{waves}} - r). \quad (6.25)$$

3557 This means that the  $n_{\text{waves}}^2$  real-valued spin-density matrix elements are build up from  $n_{\text{para}}^{\rho}$   
3558 free parameters. In our case,  $n_{\text{para}}^{\rho}$  is much smaller than  $n_{\text{waves}}^2$ . Hence, there are functional  
3559 dependencies among the spin-density matrix elements. As a consequence,  $^{\text{MLE}}\text{Cov}[\lambda_i, \lambda_j]$  as  
3560 obtained from the covariance matrix of the maximum-likelihood estimates of the transition  
3561 amplitudes via linear error propagation, is singular and cannot be directly inverted.

3562 However, we determined  $\text{Cov}[\lambda_i, \lambda_j]$  using the Bootstrapping approach, which does not determine  
3563 the covariance matrix at a fixed point in the  $\vec{\lambda}$  space, but determines the covariance matrix  
3564 from the spread in the distribution of  $\vec{\lambda}$ . This distribution also includes non-linear effects  
3565 from the calculation of the spin-density matrix elements [see equations (5.67) and (5.68)].  
3566 Hence, the functional dependencies among the spin-density matrix elements are not exactly  
3567 implemented in  $\text{Cov}[\lambda_i, \lambda_j]$  from Bootstrapping, so that  $\text{Cov}[\lambda_i, \lambda_j]$  is not exactly singular  
3568 anymore. In fact, it has full rank and can be inverted. In order to make the inversion procedure  
3569 of  $\text{Prec}[\lambda_i, \lambda_j]$  used in equation (6.23) numerically more stable<sup>[f]</sup> and to implement the mass  
3570 ranges as described below, we employed the Moore-Penrose pseudo-inverse [139–142]<sup>[g]</sup> when

<sup>[f]</sup> Although,  $\text{Cov}[\lambda_i, \lambda_j]$  is not exactly singular anymore, some eigenvalues of  $\text{Cov}[\lambda_i, \lambda_j]$  are still numerically close to zero. This leads to numerical instabilities when using the conventional matrix inverse.

<sup>[g]</sup> See equations (27) and (28) on page 207 of ref. [139].

3571 calculating  $\text{Prec}[\lambda_i, \lambda_j]$ .<sup>[h]</sup> A systematic study investigating effects from the rank of  $\text{Cov}[\lambda_i, \lambda_j]$   
 3572 can be found in section 6.3.2.

3573 Some  $m_{K\pi\pi}$  ranges of partial waves that are studied in the RMF are excluded from  $\chi^2_{\text{RMF}}$ . An  
 3574 elegant way of implementing these mass ranges in the RMF is to take advantage of the pseudo  
 3575 inverse that is used to calculate  $\text{Prec}[\lambda_i, \lambda_j]$ . To this end, for each  $(m_{K\pi\pi}, l')$  cell the elements  
 3576 of  $\text{Cov}[\lambda_i, \lambda_j]$  that belong to waves outside their mass ranges are set to zero before calculating  
 3577  $\text{Prec}[\lambda_i, \lambda_j]$ .

### 3578 6.1.6 Fit Procedure

3579 In an RMF, the  $\chi^2$  function in equation (6.23) is minimized with respect to the free parameters  
 3580 of the RMF model, which are shape parameters, e.g. the masses and widths of the resonance  
 3581 components, and the coupling and branching amplitudes.<sup>[i]</sup> In general, the  $\chi^2$  function is multi-  
 3582 modal in the parameter space. In order to map out the parameter space, to avoid bias induced  
 3583 by the choice of the start-parameter values, and to reliably find the parameter values that yield  
 3584 the minimal  $\chi^2$  value, multiple minimizations are performed for the same RMF model using  
 3585 different start-parameter values.

3586 While we have some prior knowledge about the shape parameters, e.g. from previous measure-  
 3587 ments of the studied resonances, we have only poor prior knowledge about the coupling and  
 3588 branching amplitudes. For the shape parameters of the resonance components, the non-resonant  
 3589 components, and the effective background components, the start-parameter values are randomly  
 3590 drawn from uniform distributions with ranges that we chose individually for each component  
 3591 based on prior knowledge. These start-parameter ranges are listed and discussed in section 6.2  
 3592 and appendices E.1.1 and E.2. For the real and imaginary parts of the coupling amplitudes  
 3593 and the branching amplitudes, the start-parameter values are randomly drawn from a uniform  
 3594 distribution in the wide range  $(-1, 1)$ .<sup>[j]</sup>

3595 Optimizing all parameters at once frequently leads to artificial solutions far away from the physics  
 3596 parameters, because some parameters of the RMF model are highly correlated.<sup>[k]</sup> Therefore,  
 3597 the fit procedure is performed in two steps. In the first step, the parameters for the coupling

<sup>[h]</sup> In order to calculate the Moore-Penrose pseudo-inverse a singular-value decomposition is used, where numerically small singular values  $s_j$  are set to zero in the inverse, i.e. a singular value is set to zero if  $s_j < \max_k[s_k] \cdot 10^{-14}$ . Here,  $j$  and  $k$  label the various singular values determined in the singular-value decomposition.

<sup>[i]</sup> We used the `iminuit` package [143] for minimization, which is a Python module that implements the MINUIT minimizer.

<sup>[j]</sup> In the “sitter” fitting software (see table H.1), the coupling and branching amplitudes defined in equations (6.4) and (6.14) to (6.16) are normalized by introducing normalization constants, such that the magnitudes of the real and imaginary parts of the coupling amplitudes are of the order of 1, i.e. of the same order as the shape parameters. This was mandatory to improve the stability of the MINUIT minimization.

<sup>[k]</sup> We performed studies where the optimization was performed by freeing all parameter simultaneously in a single step. This approach yielded the same best  $\chi^2$  value as the two-step approach. However, it required much more minimization attempts with different start-parameter values as the best solution was found less frequently. See section 6.2.2 for a discussion on the stability of the RMF.

and branching amplitudes are optimized, while keeping the shape parameters fixed to their start-parameter values, which are based on prior knowledge. In the second step, the results from the first step are used as start-parameters values and also the shape parameters are freed such that all parameters are optimized simultaneously.

In summary, the RMF formalism described in this section 6.1 allowed us to identify strange-meson resonances and to measure their masses and widths. In contrast to the PWD, the resonance, non-resonant, and background contributions are explicitly modeled in the RMF. This allowed us to separate the resonance signals from the non-resonant and background contributions.

## 6.2 The 10-Wave RMF

### 6.2.1 The 10-Wave RMF Model

In order to study resonances appearing in the  $K^-\pi^-\pi^+$  final state and to measure their masses and widths, we used the formalism developed in section 6.1 to fit RMF models to the results of the PWD of the measured  $K^-\pi^-\pi^+$  sample. We selected ten partial waves with  $J^P = 1^+, 2^+, 2^-,$  and  $4^+$  to be included into the RMF. We chose waves that show interesting signals, e.g. from excited states such as the  $K_2(2250)$  that needs further clarification. We also chose waves that show clear signals from well-known resonances such as the  $K_2^*(1430)$ . These clear signals can be reliably modeled and act as reference amplitudes for weaker signals to interfere with, which makes the fit more robust. In addition, comparing our measurements of the resonance parameters of these well-known states to previous ones allows us to identify potential bias in the analysis. The so-called 10-wave RMF is defined in the remaining of this section. Its results are discussed in sections 6.2.2 and 7.1 to 7.4. When developing the so-called 10-wave RMF model employed in the 10-wave RMF, we started with RMFs of individual waves, and then successively added partial waves and model components, and tuned the parameters of the model. In total, we performed more than 200 individual RMFs during this procedure. We studied further partial waves from other  $J^P$  sectors using the 10-wave RMF model as a starting point for extended RMFs. These studies are discussed in sections 7.5 to 7.8.

Table 6.1 lists the waves included in the 10-wave RMF. In the following, we give a short reasoning for how we constructed this model. A detailed discussion about the signals in the individual waves can be found in chapter 7. The  $2^+$  and  $4^+$  waves exhibit resonance-like signals of the corresponding ground-state resonances (see figures 5.19d and 5.20b). We modeled them accordingly by including the  $K_2^*(1430)$  and  $K_4^*(2045)$  resonance components. Apart from these dominant signals, the waves exhibit no further resonance-like structures. The  $1^+$  and  $2^-$  waves exhibit dominant signals in the  $m_{K\pi\pi}$  region of the known ground-state resonances; which are the  $K_1(1270)$  and  $K_1(1400)$  resonances, and the  $K_2(1780)$  and  $K_2(1820)$  resonances, respectively (see figures 5.19f and 5.19a). Hence, we added the corresponding resonance components to our model. In addition, some  $1^+$  and  $2^-$  waves exhibit high-mass tails, which may arise from excited states. We modeled them by including resonance components for the  $K_1'$  and  $K_2(2250)$  states. As

Table 6.1: List of partial waves and model components included in the 10-wave RMF. The second column lists the resonance components included in  $\mathbb{S}_a$  in equation (6.6). They are specified in table E.1. The third column lists the parameterization used for the dynamic amplitudes of the non-resonant components (NR). The fourth column lists the model used for the  $\pi^- \pi^- \pi^+$  background components. The fifth column lists the parameterizations used for the dynamic amplitudes of the effective background components (eBKG) in equation (6.16).<sup>[1]</sup> The last two columns list the  $m_{K\pi\pi}$  range in which data from this partial wave are considered in the RMF. A detailed discussion of the individual components is given in appendix E.1.1.

Partial Wave	Resonances	NR	$\pi^- \pi^- \pi^+$	eBKG	$m_{K\pi\pi}$ Range GeV/ $c^2$
$1^+ 0^+ \rho(770) K S$	$\{K_1(1270), K_1(1400)\}$	(6.11)	(6.15)	(6.17)	1.10 2.50
$1^+ 1^+ \rho(770) K S$		(6.11)	(6.15)	(6.17)	1.10 2.50
$2^+ 1^+ K^*(892) \pi D$	$\{K_2^*(1430)\}$	(6.11)	(6.15)	(6.17)	1.20 1.70
$2^+ 1^+ \rho(770) K D$		(6.11)	(6.15)	(6.17)	1.30 1.70
$2^- 0^+ K^*(892) \pi F$	$\{K_2(1770), K_2(1820)\}$	(6.11)	(6.15)	(6.17)	1.60 2.00
$2^- 0^+ K_2^*(1430) \pi S$		(6.8)	(6.15)	(6.18)	1.50 2.80
$2^- 0^+ \rho(770) K F$		(6.11)	(6.15)	(6.17)	1.60 2.00
$2^- 0^+ f_2(1270) K S$		(6.11)	(6.15)	(6.17)	1.60 2.80
$4^+ 1^+ K^*(892) \pi G$	$\{K_4^*(2045)\}$	(6.11)	(6.15)	(E.1)	1.80 2.50
$4^+ 1^+ \rho(770) K G$		(6.11)	(6.15)	(6.17)	1.80 2.50

3635 our estimate for the mass of the  $K_1'$  component is significantly higher than the nominal mass of  
3636 the  $K_1(1650)$  state, which is listed by the PDG, we call this component  $K_1'$  instead of  $K_1(1650)$   
3637 in our model (see discussion in section 7.1.1).

3638 We chose the  $m_{K\pi\pi}$  range in which we considered data points of the spin-density matrix elements  
3639 that correspond to a wave individually for each wave. The selected  $m_{K\pi\pi}$  ranges cover the  
3640 resonances we want to study and a sufficiently large region around these resonances that allows us  
3641 to reliably determine not only the parameters of the resonances but also those of the non-resonant  
3642 and background components. With the given model we were not able to describe the region  
3643  $m_{K\pi\pi} \geq 2 \text{ GeV}/c^2$  of the  $2^- 0^+ K^*(892) \pi F$  and  $2^- 0^+ \rho(770) K F$  waves (see section 7.4). Thus,  
3644 we excluded this mass region from the RMF for these two waves. Also, we excluded the region  
3645  $m_{K-\pi^+} \geq 1.7 \text{ GeV}/c^2$  from the RMF for the two  $2^+$  waves, because both waves exhibit no  
3646 resonance-like signal in this mass region.

3647 We use the same set of resonance components for partial waves with the same  $J^P$  quantum  
3648 numbers. Except for the  $1^+$  waves, all waves with the same  $J^P$  have also the same  $M^E$ . Hence,  
3649 we required that a resonance component has the same  $t'$  dependence in all partial waves in which  
3650 it is included by applying equation (6.14). This leaves us with one set of  $t'$ -dependent coupling  
3651 amplitudes for each resonance component and one  $t'$ -independent branching amplitude for each  
3652 additional wave in which this resonance component appears. As the two included  $1^+$  waves have  
3653 different  $M^E$ , we do not expect the  $t'$  dependence of resonances appearing in both waves to be the

3654 same. Thus, we did not apply equation (6.14) for the  $K_1(1270)$  and  $K'_1$  resonance components.  
 3655 As discussed in section 7.1, the  $K_1(1400)$  is only a weak signal in the included  $1^+$  waves. In  
 3656 order to reduce the number of free parameters and thereby stabilize the fit, we applied a modified  
 3657 version of equation (6.14), where the expected change of the  $t'$  shape due to the different spin  
 3658 projections, which will be given in equation (6.29), is taken into account, i.e. we applied

$$K_1(1400)C_{1^+ 1^+ \rho(770)KS}^{K\pi\pi}(t') = \sqrt{t'} \cdot {}_{1^+ 1^+ \rho(770)KS}^{K_1(1400)}\mathcal{B}_{1^+ 0^+ \rho(770)KS}^{K\pi\pi} \cdot {}_{1^+ 0^+ \rho(770)KS}^{K_1(1400)}C_{1^+ 0^+ \rho(770)KS}^{K\pi\pi}(t'). \quad (6.26)$$

3659 For all eight resonance components we used a relativistic Breit-Wigner amplitude given in  
 3660 section 5.1.4 with a dynamic width that takes into account a single decay channel. In order to  
 3661 measure the Breit-Wigner mass  $m_0$  and width  $\Gamma_0$ , we optimized the corresponding fit parameters  
 3662 in the RMF (see section 6.1.6 for details on the fitting procedure). We chose the parameter  
 3663 limits for the  $m_0$  and  $\Gamma_0$  parameters to be as little restrictive as possible in order to not bias our  
 3664 results. Furthermore, we selected the start-parameter ranges for  $m_0$  and  $\Gamma_0$  such that their cover a  
 3665 reasonable range including previous measurements [91] plus a safety margin. The resonance  
 3666 components, their parameter limits, and the start-parameter ranges are listed in table E.1. In  
 3667 appendix E.1.1 we discuss their choice in more detail. As the  $K_1(1400)$  is only a weak signal  
 3668 in the two considered  $1^+$  waves, we could not reliably determine its mass and width in the  
 3669 10-wave RMF. Thus, we fixed the mass and width parameters of the  $K_1(1400)$  component to the  
 3670 corresponding PDG average values [91] as listed in table E.1.

3671 Using the simplified shape for the non-resonant and effective background components given in  
 3672 equations (6.11) and (6.17) turned out to be sufficient in most of the 10 waves (see table 6.1). Only  
 3673 for the  $2^- 0^+ K_2^*(1430)\pi S$  and  $4^+ 1^+ K^*(892)\pi G$ <sup>[1]</sup> waves, which exhibit larger non-resonant  
 3674 and background contributions, we used the extended non-resonant and effective background  
 3675 shapes in equations (6.8) and (6.18). We chose the parameter limits of the non-resonant and  
 3676 effective background components in all 10 waves to be much larger than expected, i.e. larger than  
 3677 observed in the first RMFs and larger than the typical values observed in the COMPASS  $\pi^-\pi^-\pi^+$   
 3678 analysis [41] where a similar non-resonant parameterization was used. Similarly, we chose the  
 3679 start-parameter ranges to cover typical values for the non-resonant and effective background  
 3680 parameters. The final choice of the parameter limits and start-parameter ranges is listed in  
 3681 appendix E.1.1.

3682 Finally, we modeled the  $\pi^-\pi^-\pi^+$  background using the results of the  $\pi^-\pi^-\pi^+$  partial-wave  
 3683 decomposition as discussed in section 6.1.3. This model has only one free fit parameter, which is  
 3684 the overall amount of  $\pi^-\pi^-\pi^+$  background in the  $K^-\pi^-\pi^+$  sample. We estimated this parameter  
 3685 in the RMF.

<sup>[1]</sup> For the effective background component in the  $4^+ 1^+ K^*(892)\pi G$  wave we used a modified version of equation (6.18) as discussed in appendix E.1.1.

3686 In total, the 10-wave RMF model has 291 free fit parameters: 7  $m_0$  and 7  $\Gamma_0$  parameters of  
 3687 7 resonance components,<sup>[m]</sup> 8 shape parameters of the non-resonant components,<sup>[n]</sup> 12 shape  
 3688 parameters of the effective background components, and 257 parameters for the coupling and  
 3689 branching amplitudes. These 291 free parameters are constrained by 7816 data points, i.e. the  
 3690 real and imaginary parts of the spin-density matrix elements obtained from the PWD of the  
 3691  $K^- \pi^- \pi^+$  sample.

## 3692 6.2.2 A First Glimpse on the Results of the 10-Wave RMF

3693 We fitted the 10-wave RMF model defined in section 6.2.1 to the PWD results of the  $K^- \pi^- \pi^+$   
 3694 sample presented in section 5.5. In order to explore the parameter space of the RMF sufficiently  
 3695 well we performed a large number of 2000 fit attempts with random start-parameter values.  
 3696 Figure 6.1a shows the  $\chi^2$  distribution obtained from these 2000 attempts. The best fit result  
 3697 yielded a  $\chi^2$  value of 6215.61, i.e. this is the smallest  $\chi^2$  value found in all attempts. Taking into  
 3698 account the number of degrees of freedom, this corresponds to a reduced  $\chi^2$  of  $\chi^2_{\text{red}} = 0.826$ .  
 3699 The interpretation of this value is discussed further in section 6.3.1. In total, 121 of the 2000 fit  
 3700 attempts found this best result,<sup>[o]</sup> which represents the final result of this RMF, i.e. which yielded  
 3701 the final parameter estimates. There are further results that were found frequently. However, they  
 3702 all have a  $\chi^2$  value that is at least 12 units larger, i.e. significantly worse, than the best fit result.  
 3703 Hence, they are not of interest here. Finally, there are rarely found fit results with  $\chi^2 < \chi^2_{\text{best}} + 12$   
 3704 as shown in figure 6.1b. These rare fit results have resonance parameters that agree with those  
 3705 from the best fit result. Thus, they are also not of further interest. The large number of fit attempts  
 3706 that found the best fit result, the consistency of the parameter values for fit results with similar  
 3707  $\chi^2$ , and the significantly larger  $\chi^2$  of other fit results demonstrates that we reliably found the  
 3708 minimal  $\chi^2$ , i.e. the set of parameters that describes the data best.

3709 Figure 6.2 shows for illustration purposes the real and imaginary parts of the spin-density matrix  
 3710 elements of the 10 waves included in the 10-wave RMF in the lowest  $t'$  bin. The data points  
 3711 represent the spin-density matrix elements obtained from the PWD of the measured  $K^- \pi^- \pi^+$   
 3712 sample. We refer to the corresponding intensities as measured intensities and to the off-diagonal  
 3713 spin-density matrix elements as measured spin-density matrix elements in the following. The  
 3714 1954 data points from the first  $t'$  bin shown in blue are those that entered the RMF. In total, we  
 3715 included all four spin-density matrices from the four analyzed  $t'$  bins simultaneously in one RMF.  
 3716 This results in a total amount for 7816 data points that entered the RMF. All four spin-density  
 3717 matrices are shown in appendix E.1.2. These data points were calculated from the transition  
 3718 amplitudes, i.e. from a smaller number of fit parameters compared to the number of real and  
 3719 imaginary parts of the spin-density matrix elements. Hence, spin-density matrix elements from

<sup>[m]</sup> The mass and width of the  $K_1(1400)$  component were fixed.

<sup>[n]</sup> The shape parameters of the non-resonant terms in the  $2^+$  waves and in the  $2^- 0^+$   $K^*(892) \pi F$  wave were fixed (see appendix E.1.1).

<sup>[o]</sup> We consider two fit results to be the same if their  $\chi^2$  values differ by less than  $10^{-2}$  units, if for each parameter the difference of the estimates is less than 10 % of the corresponding uncertainty from the best fit result, and if each for each parameter the difference of the uncertainty estimates is less than 50 % of the uncertainty estimate from the best result. The latter criterion was chosen to identify unrealistic uncertainty estimates appearing in unstable fits.

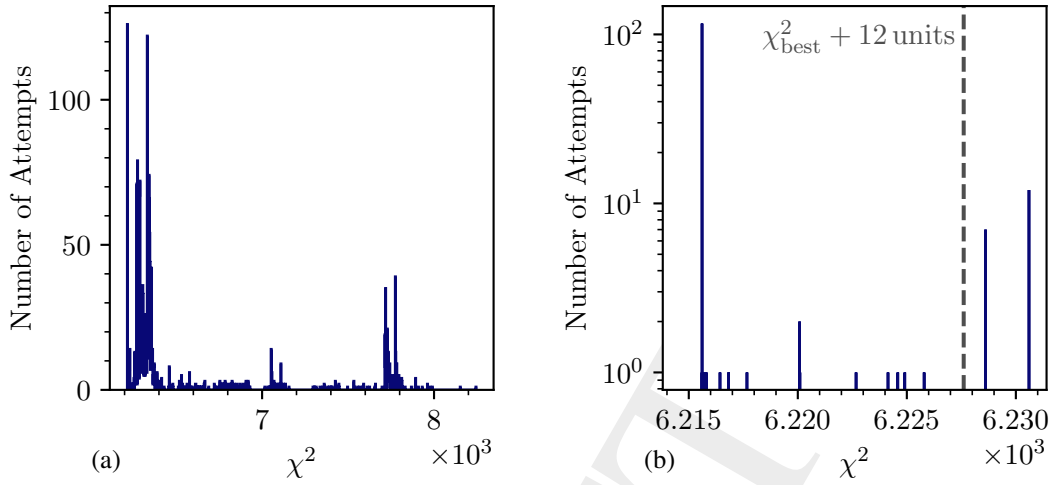


Figure 6.1:  $\chi^2$  distribution obtained from the 2000 attempts of the 10-wave RMF. (a) shows the full  $\chi^2$  range of all 2000 attempts. (b) shows in log-scale only those attempts that yielded a  $\chi^2$  that is at most 15 units worse than the smallest found  $\chi^2$ . The dashed dark-gray vertical line indicates  $\chi^2 = \chi_{\text{best}}^2 + 12$  units.

3720 the same  $(m_{K\pi\pi}, t')$  cell are strongly correlated. Spin-density matrix elements from different  
 3721  $(m_{K\pi\pi}, t')$  cells are independent. The red curves in figure 6.2 represent the result of the 10-wave  
 3722 RMF. We discuss in the following the fit quality. Detailed discussions and interpretations of the  
 3723 results for the individual waves are given in chapter 7.

3724 Overall, the RMF is able to reproduce the measured intensities and the off-diagonal spin-density  
 3725 matrix elements sufficiently well. Figure 6.3a shows exemplarily the  $t'$ -summed intensity  
 3726 spectrum of the  $1^+ 0^+ \rho(770) K S$  wave. The total RMF model (red curve) reproduces well  
 3727 the features of the measured intensity spectrum (blue data points). As expected, the peak  
 3728 at about  $1.3 \text{ GeV}/c^2$  is dominantly described by the  $K_1(1270)$  component of the RMF (blue  
 3729 curve). We find small contributions to the total model intensity from the non-resonant component  
 3730 (green curve), the  $\pi^- \pi^- \pi^+$  background component (orange curve), and the effective background  
 3731 component (brown curve). The RMF underestimates the measured intensity in the low-mass tail  
 3732 of the peak, especially in the extrapolation below the fitted  $m_{K\pi\pi}$  region shown by the gray data  
 3733 points and lighter curves. We expect artifacts in form of these low-mass enhancements in our  
 3734 analysis (see section 5.5). Thus, we excluded this low-mass region from the  $m_{K\pi\pi}$  fit range.

3735 Similarly, the peak at about  $1.4 \text{ GeV}/c^2$  in the  $2^+ 1^+ \rho(770) K D$  wave shown in figure 6.3b is  
 3736 reproduced well by the RMF, while it underestimates the measured intensity in the tails of the  
 3737 peak. We find a large contribution of the  $\pi^- \pi^- \pi^+$  background component (orange curve) to this  
 3738 wave, while the total RMF model curve seems to be completely saturated by the  $K_2^*$  component.  
 3739 The reason is, that the  $K_2^*$  component destructively interferes with the non-resonant component  
 3740 in this wave (green curve) such that the intensity  $\hat{\rho}_{aa}^{K\pi\pi}(m_{K\pi\pi}, t')$  of the RMF model for the  $K^- \pi^- \pi^+$   
 3741 spin-density matrix is smaller than the measured intensity. Adding the  $\pi^- \pi^- \pi^+$  background  
 3742 component, the total RMF model reproduced well the peak region.



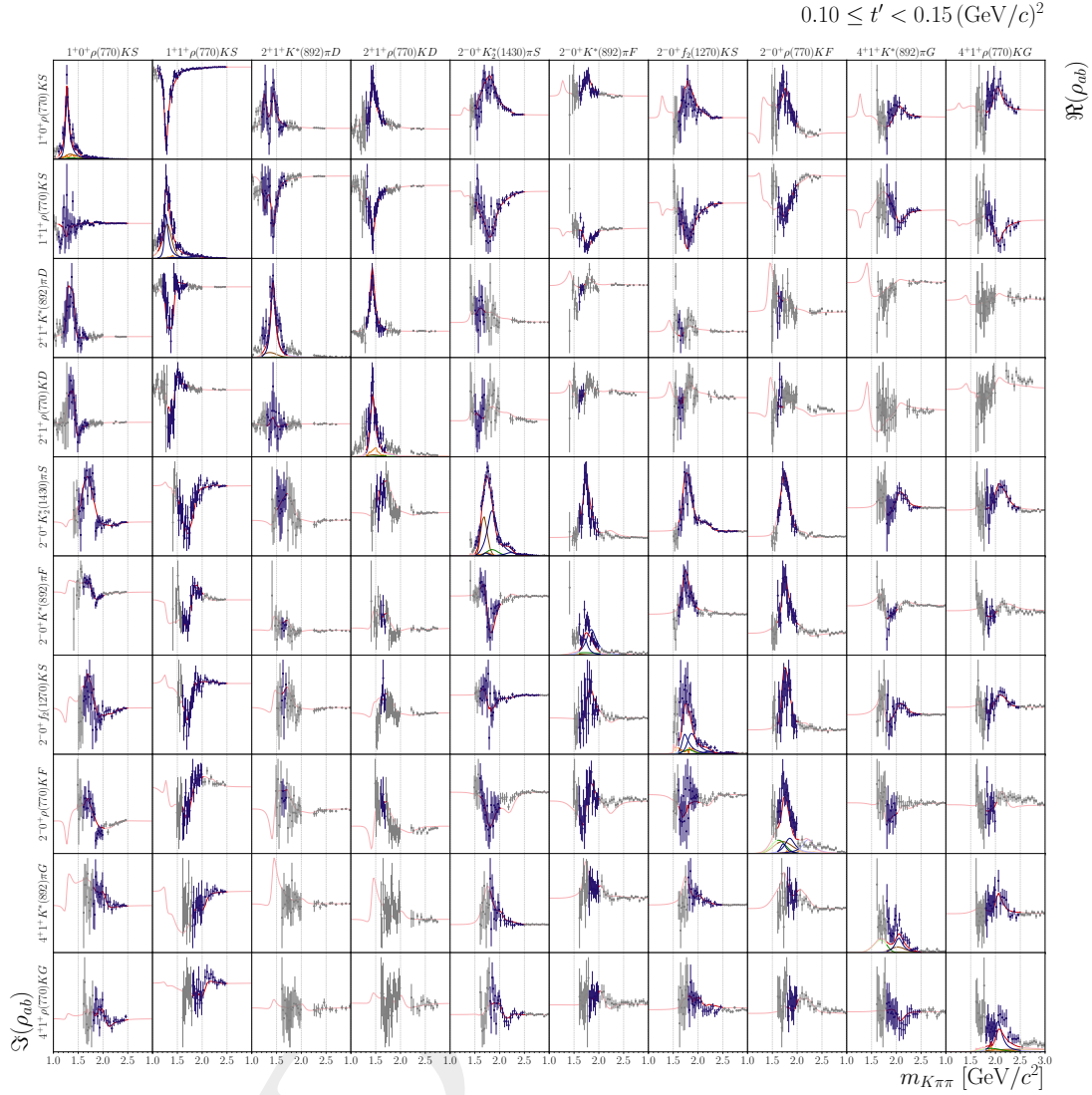


Figure 6.2: Real and imaginary parts of the spin-density matrix elements, i.e.  $\Lambda_{ab}(m_{K\pi\pi}, t')$  in equation (6.19), as a function of  $m_{K\pi\pi}$  in the lowest of the four  $t'$  bins for the 10 partial waves that were included in the 10-wave RMF. The figures on the diagonal show the intensity spectra. The upper-right and lower-left off-diagonal figures show the real and imaginary parts of the off-diagonal elements of the spin-density matrix, respectively. The blue data points represent the measured spin-density matrix elements. The curves represent the result of the 10-wave RMF to these data points. The red curves represent the total RMF model. The blue curves represent the individual resonance components, the green curves the non-resonant components, the orange curves the  $\pi^- \pi^- \pi^+$  background components, and the brown curves the effective background components. The extrapolations beyond the  $m_{K\pi\pi}$  fit ranges are shown in lighter colors. The corresponding data points are shown in gray. The ranges of the vertical axes are different for each subplot. They are adjusted to the data shown in each subplot. Hence, we do not show tick marks for the vertical axes.

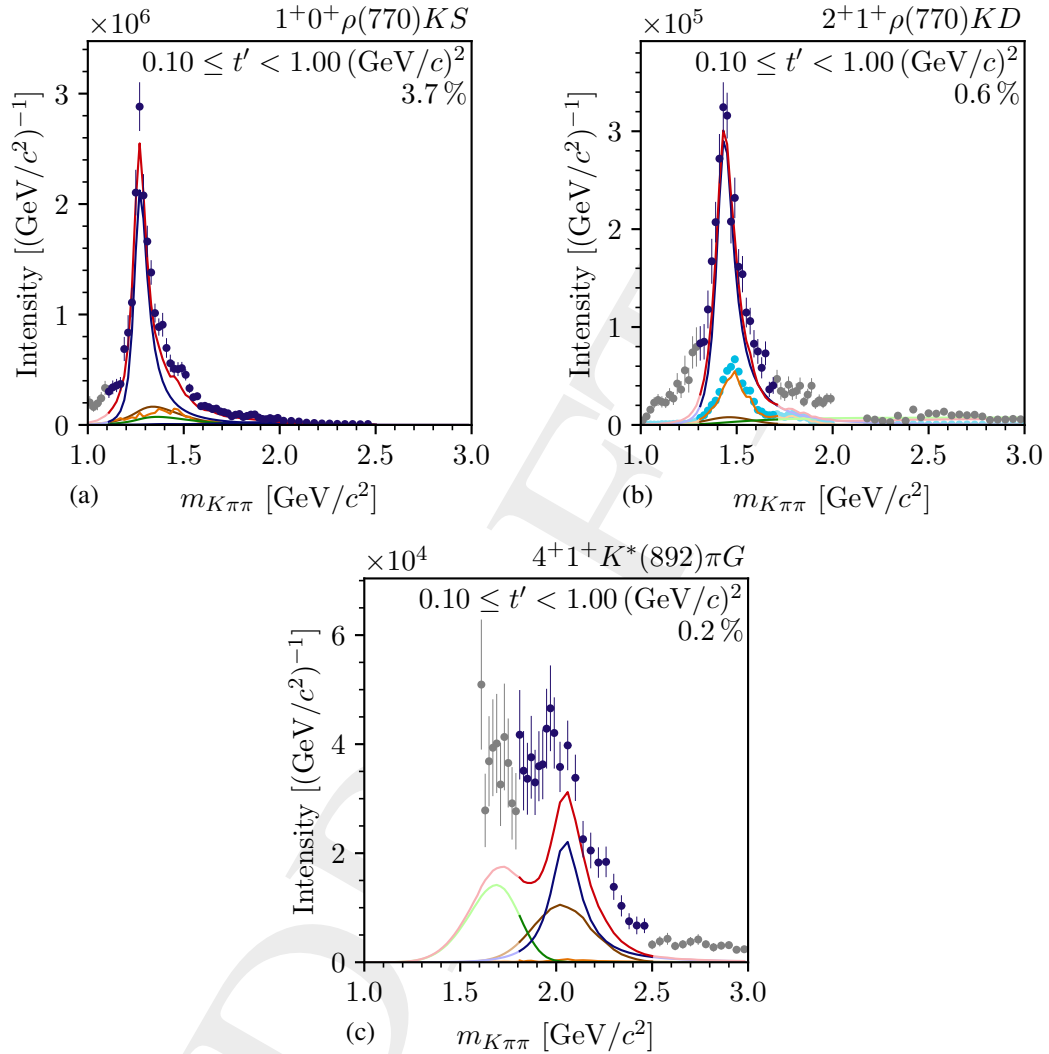


Figure 6.3: 10-wave RMF result for the  $t'$ -summed intensity spectra of three selected partial waves. The blue data points represent the measured spin-density matrix elements. The curves represent the result of the 10-wave RMF. The red curves represent the total RMF model. The blue curves represent the individual resonance components, the green curves the non-resonant components, the orange curves the  $\pi^-\pi^-\pi^+$  background components, and the brown curves the effective background components. The extrapolations beyond the  $m_{K\pi\pi}$  fit ranges are shown in lighter colors. The corresponding data points are shown in gray. The cyan data points in (b) show the result of the  $\pi^-\pi^-\pi^+$  background PWD scaled such that the total number of reconstructed  $\pi^-\pi^-\pi^+$  pseudodata events corresponds to the predicted amount of  $\pi^-\pi^-\pi^+$  background in the  $K^-\pi^-\pi^+$  sample (same as orange data points in figure 5.39a).

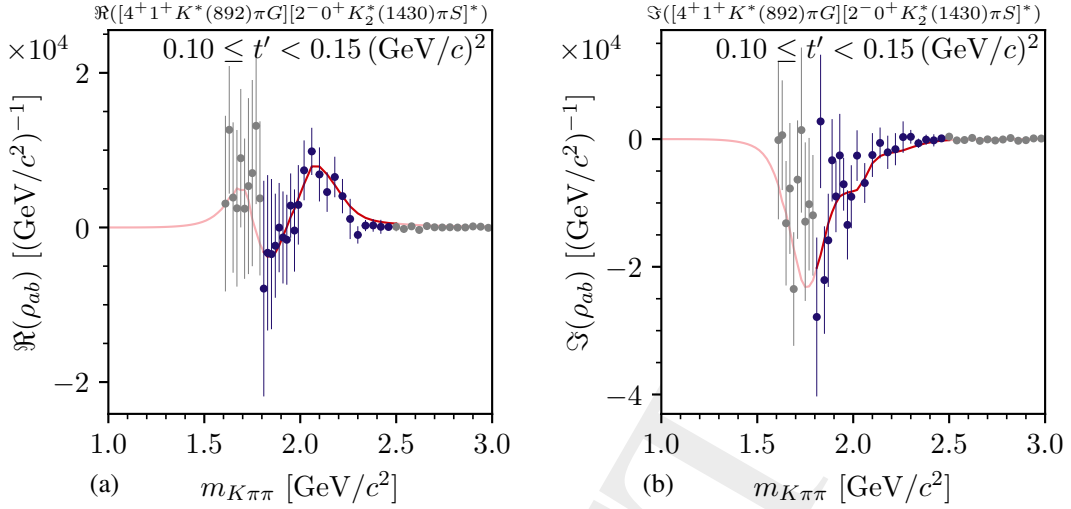


Figure 6.4: Same as figure 6.3, but for (a) the real part and (b) the imaginary part of the off-diagonal spin-density matrix element of the  $4^+ 1^+ K^*(892)\pi G$  and  $2^- 0^+ K_2^*(1430)\pi S$  waves in the lowest  $t'$  bin.

3743 The shape of the  $\pi^- \pi^- \pi^+$  background component is the same as the shape from the  $\pi^- \pi^- \pi^+$   
 3744 background PWD by construction (see section 6.1.3), while the amount of  $\pi^- \pi^- \pi^+$  background  
 3745 is a free parameter in the RMF. Remarkably, the amount of  $\pi^- \pi^- \pi^+$  background as estimated  
 3746 by the RMF based on the measured  $K^- \pi^- \pi^+$  sample agrees well with the expected amount of  
 3747  $\pi^- \pi^- \pi^+$  background (cf. orange curve and cyan data points in figure 6.3b, respectively). The  
 3748 estimate of the  $\pi^- \pi^- \pi^+$  background from the RMF was obtained from the measured  $K^- \pi^- \pi^+$   
 3749 sample. The expected amount of  $\pi^- \pi^- \pi^+$  background is based on the  $\pi^- \pi^- \pi^+$  pseudodata, which  
 3750 were obtained from the measured  $\pi^- \pi^- \pi^+$  sample, i.e. from an independent data sample. This  
 3751 good agreement strongly supports our approach to effectively model the incoherent background  
 3752 contributions by a rank=3 spin-density matrix in the PWD and explicitly model them at the level  
 3753 of the RMF. As the strength parameter of the  $\pi^- \pi^- \pi^+$  background component is independent of  
 3754 the partial wave by construction, we find the same good agreement in all 10 partial waves.

3755 We observe discrepancies between the RMF curve and the measured intensity spectra of the  $4^+$   
 3756 waves, exemplarily shown for the  $t'$ -summed intensity spectrum of the  $4^+ 1^+ K^*(892)\pi G$  wave in  
 3757 figure 6.3c. While the RMF roughly reproduces the shape of the spectrum, it underestimates the  
 3758 overall intensity by about 20%. However, the RMF reproduces well the measured off-diagonal  
 3759 spin-density matrix elements of the  $4^+ 1^+ K^*(892)\pi G$  wave with respect to all other partial  
 3760 waves. Figure 6.4 exemplarily shows the real and imaginary parts of one of these off-diagonal  
 3761 elements. Especially noteworthy is that the magnitudes of the measured off-diagonal elements  
 3762 are not underestimated, which would naively be expected from the discrepancy observed in the  
 3763 intensity spectrum. This suggests that there are contributions to the measured intensity spectrum  
 3764 of this wave that do not enter the off-diagonal spin-density matrix elements and that are not  
 3765 reproduced by the RMF.

3766 The spin-density matrix element for a given  $(m_{K\pi\pi}, t')$  cell is the sum over all physics processes  
 3767  $p$  that contribute to wave  $a$  or  $b$ :<sup>[p]</sup>

$$\rho_{ab} = \sum_p \mathcal{T}_a^p [\mathcal{T}_b^p]^*. \quad (6.27)$$

3768 Assume, a process  $p_1$  contributes only to wave  $a$  but not to wave  $b$ , i.e.  $\mathcal{T}_b^{p_1} = 0$ . This process  
 3769 affects the intensity of wave  $a$ , because  $\mathcal{T}_a^{p_1} [\mathcal{T}_a^{p_1}]^*$  appears in equation (6.27) for  $a = b$ . However,  
 3770  $p_1$  does not affect the off-diagonal spin-density matrix element of waves  $a$  and  $b$ , because  
 3771  $\mathcal{T}_a^{p_1} [\mathcal{T}_b^{p_1}]^*$  appears in equation (6.27) for  $a \neq b$  and  $\mathcal{T}_b^{p_1} = 0$ . Hence, the off-diagonal spin-  
 3772 density matrix elements are less affected by processes that dominantly contribute to only a subset  
 3773 of waves.

3774 We expect the process under study in this work, i.e.  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , to contribute to all  
 3775 partial waves as the wave set was designed for this process. However, background processes  
 3776 may significantly contribute to only a subset of partial waves. For example, we know from the  
 3777  $\pi^- \pi^- \pi^+$  background PWD that this background does practically not contribute to waves with  
 3778  $K^*(892)$  isobar (see section 5.10.2). Therefore, we expect not only the intensities of waves  
 3779 with  $K^*(892)$  isobar to be practically free of  $\pi^- \pi^- \pi^+$  background, but also the off-diagonal  
 3780 spin-density matrix elements of all waves with respect to waves with  $K^*(892)$  isobar. Thus,  
 3781 in general the intensities may be most affected by backgrounds. In addition, the model for  
 3782 the effective background components is only an approximation, which may be imperfect (see  
 3783 section 6.1.4). This may explain the discrepancy between the RMF curve and the measured  
 3784 intensity spectra of the  $4^+$  waves, while the off-diagonal elements of those waves are reproduced  
 3785 well. Furthermore, one should note that 6504 of the 7816 data points that entered the RMF  
 3786 represent off-diagonal spin-density matrix elements, while only 1312 represent intensities.<sup>[q]</sup>  
 3787 Hence, the off-diagonal elements influence the results of the RMF more strongly such that  
 3788 imperfections in the description of the intensities may not strongly pull the results.

3789 We performed the PWD independently in four bins in  $t'$ . This allowed us to determine not  
 3790 only the  $m_{K\pi\pi}$  dependence, but also the  $t'$  dependence of the spin-density matrix elements. We  
 3791 employed this  $t'$  resolved information in the RMF, where we separate resonances from non-  
 3792 resonant and background contributions. Hence, we studied the  $t'$  dependence of the amplitudes of  
 3793 the individual model components. However, given the low number of  $t'$  bins, we could determine  
 3794 only the coarse features of their  $t'$  dependence. Due to the normalization of the measured spin-  
 3795 density matrix elements,  $|\hat{\mathcal{T}}_a^z(m_{K\pi\pi}, t')|^2$  from equation (6.5) represents the predicted number of  
 3796 produced events in each  $(m_{K\pi\pi}, t')$  cell for a single wave  $a$  and the coherent sector  $z$  and if there  
 3797 would be only component  $k$  in wave  $a$ . The corresponding intensity as a function of  $t'$ , i.e. the

<sup>[p]</sup> As discussed in section 5.1, we cannot disentangle the transition amplitudes  $\mathcal{T}_a^p$  of the physics processes. The transition amplitudes  $\mathcal{T}_a^z$  that appear in the PWD model are only an effective parameterization of the spin-density matrix.

<sup>[q]</sup> The number of off-diagonal elements and intensities must be calculated for each  $(m_{K\pi\pi}, t')$  cell individually and summed up. This is because not all the 10 waves were considered in the RMF in all  $(m_{K\pi\pi}, t')$  cells (see table 6.1). The number of considered waves ranges from one to eight. There are no  $(m_{K\pi\pi}, t')$  cells where all the 10 waves are considered, because the  $2^+$  and  $4^+$  waves have non-overlapping fit ranges. On average, about five waves are considered in each  $(m_{K\pi\pi}, t')$  cell.

3798 number density in  $t'$  summed over the analyzed  $m_{K\pi\pi}$  region, reads

$$3800 \quad {}^k\mathfrak{S}_a(t') = \frac{1}{\Delta t'_{\text{bin}}} \sum_{m_{K\pi\pi}} \left| {}^k\hat{\mathcal{T}}_a(m_{K\pi\pi}, t') \right|^2, \quad (6.28)$$

3799 where  $\Delta t'_{\text{bin}}$  is the width of the considered  $t'$  bin. As each model component appears only in  
 3800 one coherent sector, we dropped the sector label. In general, the  $t'$  dependence of the intensity  
 3801 of a model component may be different in different partial waves. However, for most of these  
 3802 resonance components we applied equation (6.14). Hence, the  $t'$  dependence of the intensities  
 3803 of a such component in the various waves is the same by construction and only the total  
 3804 intensities differ by mainly  $|{}_b^k\mathcal{B}_a^z|^2$ .<sup>[r]</sup> As  ${}^k\mathfrak{S}_a(t')$  depends in a complicated, non-linear way on the  
 3805 fit parameters, determining its uncertainties requires elaborate and computationally expensive  
 3806 Monte Carlo uncertainty propagation. As we discuss  ${}^k\mathfrak{S}_a(t')$  only on a quantitative level in this  
 3807 work, we show the central values without uncertainties in the following.

3808 Figure 6.5 shows the  $t'$ -dependence of the intensity of the  $K_1(1270)$  component in the  $1^+ 0^+$   
 3809  $\rho(770) K S$  wave, i.e. the so-called  $t'$  spectrum. It exhibits an approximately exponentially falling  
 3810 shape. This is expected for resonances in waves with  $M = 0$  from Regge theory, assuming  
 3811 single Pomeron exchange in the scattering process [46]. For partial waves with  $M \neq 0$ , the  
 3812 exponentially falling shape is modified by an additional factor  $(t')^{|M|}$  such that the expected shape  
 3813 for the  $t'$  spectra reads<sup>[s]</sup>

$$3814 \quad {}^k\hat{\mathfrak{S}}_a(t') = {}^k\mathfrak{A}_a \cdot (t')^{|M|} \cdot e^{-{}^k\mathfrak{b}_a t'}. \quad (6.29)$$

3814 Here,  ${}^k\mathfrak{A}_a$  is the parameter for magnitude of  ${}^k\hat{\mathfrak{S}}_a(t')$  and  ${}^k\mathfrak{b}_a$  the slope of the exponential function.  
 3815 Figure 6.6 illustrates the effect of the additional factor  $(t')^{|M|}$  on the  $t'$  spectra for a wave with  
 3816  $M = 0$  and a wave with  $M = 1$ , where both  $t'$  spectra have a similar slope and magnitude in the  
 3817 high- $t'$  region.

3818 Finally, the quantities we are mainly interested in are the resonance parameters, i.e. the masses  
 3819 and widths of the appearing strange-meson resonances. Table 6.2 lists our estimates for  $m_0$  and  $\Gamma_0$   
 3820 of the seven resonance components that were freely fitted in the 10-wave RMF. These values are  
 3821 discussed in the corresponding sections of chapter 7. We give the  $\chi^2$  estimates for the statistical  
 3822 uncertainties of the resonance parameters (symmetric uncertainties in table 6.2).<sup>[t]</sup> Realistic  
 3823 estimates for systematic uncertainties of the resonance parameters require a comprehensive set

<sup>[r]</sup> Due to the different wave-normalization integrals in equation (6.5) for different partial waves, the total value and the convolution of the production factor with the other functions in equation (6.5) is different for different partial waves. As the production factor depends on  $t'$ , the  $t'$  dependence of a component in various waves is slightly different, even if equation (6.14) is applied. However, this effect is small.

<sup>[s]</sup> For  $M \neq 0$ , the intensity is suppressed when the  $X^-$  goes in forward direction in the reaction  $K^- + p \rightarrow X^- + p$ . This suppression is purely of kinematic origin and is given by the forward-limit of the Wigner  $D$ -functions, which yields the  $(t')^{|M|}$  factor in the intensity [46, 72].

<sup>[t]</sup> We determined the  $\chi^2$  estimates for the uncertainties from the inverse of the Hessian matrix in the minimum of the  $\chi^2$  function in equation (6.23) (see equation (40.24) in ref. [9]). In principle, those uncertainty estimates may be improved using the same Bootstrapping approach as discussed in section 5.4 for the PWD. However, this requires a very robust RMF model. Bootstrapping of the RMF was beyond the scope of this work. As the systematic effects on the resonance parameters are typically larger than the statistical uncertainties, we expect the  $\chi^2$  estimates for the statistical uncertainties to be sufficiently accurate.

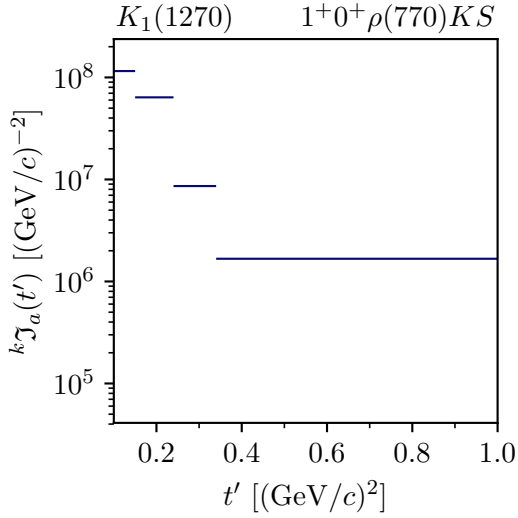


Figure 6.5: The  $t'$  spectrum of the  $K_1(1270)$  component in the  $1^+0^+\rho(770)KS$  wave as obtained from the 10-wave RMF. The horizontal blue bars represent the intensity in each  $t'$  bin according to equation (6.28).

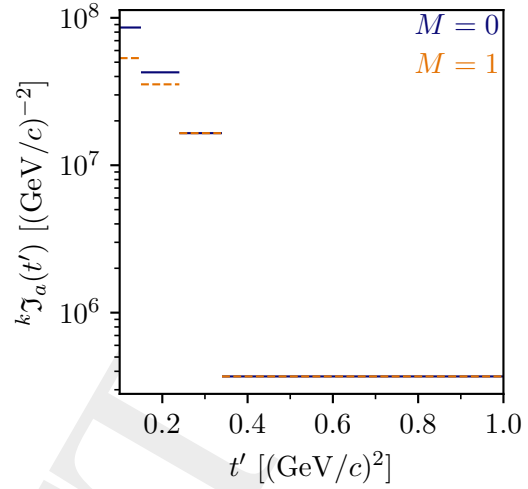



Figure 6.6: Two exemplary  $t'$  spectra following the theory model in equation (6.29) for  $M = 0$  in blue and  $M = 1$  in orange. We chose  ${}^k b_{M=0} = 10 (\text{GeV}/c)^{-2}$  for the spectrum in blue, and we chose  ${}^k b_{M=1} = 12.2 (\text{GeV}/c)^{-2}$  and  ${}^k \mathfrak{I}_{M=1} = 6.53 {}^k \mathfrak{I}_{M=0}$  for the spectrum in orange such that both spectra agree in the two highest  $t'$  bins.

3824 of studies of all relevant systematic effects that may bias the results of the RMF as has been  
 3825 done for the COMPASS  $\pi^-\pi^-\pi^+$  analysis in ref. [40]. We present in sections 5.7 and 6.3 several  
 3826 systematic studies of the PWD and the RMF, respectively. However, a complete set of studies  
 3827 was beyond the scope of this work. Hence, our estimates for the asymmetric uncertainties in  
 3828 table 6.2 should be considered as are lower limits on the actual systematic uncertainties. Based  
 3829 on the studies presented in section 6.3 the systematic effects are at least as large as the statistical  
 3830 uncertainties. The parameter estimates for the shape parameters of the non-resonant and effective  
 3831 background components are listed in tables E.2 and E.3, respectively.


### 3832 6.3 Systematic Studies

3833 In addition to the various systematic effects discussed in section 5.7, also the formalism of the  
 3834 RMF and the employed model may introduce systematic effects. During the development of the  
 3835 10-wave RMF, we already performed many studies with different RMF models, which gave us a  
 3836 first impression on systematic effects. Once we finished the 10-wave RMF, we performed six  
 3837 dedicated systematic studies described in the following sections 6.3.1 to 6.3.3 and labeled by


Table 6.2: Resonance parameters as obtained from the 10-wave RMF. The first quoted uncertainties are statistical, the second systematic uncertainties. The quoted systematic uncertainties determined from a limited set of performed systematic studies represent only a lower limit on the actual systematic uncertainties (see section 6.3). The parameters of the  $K_1(1400)$  component were fixed to the corresponding PDG average values. The values and uncertainties are rounded to the same precision according to the PDG rounding [9]. The number of significant digits is given by the total uncertainty. For the total uncertainty, we quadratically add the statistical uncertainty to the upper and lower systematic uncertainties. For comparison, the PDG averages from ref. [9] are listed. The PDG lists more than one average value for the  $K_2^*(1430)$  resonance. We list here the PDG average values for the charged  $K_2^*(1430)$  from measurements of only the  $K\pi$  final state.

		(a) $K_1$ -like resonances			
Discussed in section		$K_1(1270)$ 7.1	$K_1'$ 7.1		
	$m_0$ [MeV/ $c^2$ ]	$1267.7 \pm 1.9$	$^{+1.6}_{-4.5}$	$1940 \pm 10$	$^{+90}_{-70}$
	$\Gamma_0$ [MeV/ $c^2$ ]	$83 \pm 4$	$^{+15}_{-4}$	$462 \pm 22$	$^{+27}_{-119}$
PDG	$m_0$ [MeV/ $c^2$ ]	$1253 \pm 7$		$1672 \pm 50$	
	$\Gamma_0$ [MeV/ $c^2$ ]	$90 \pm 20$		$158 \pm 50$	

		(b) $K_2$ -like resonances					
Discussed in section		$K_2(1770)$ 7.4	$K_2(1820)$ 7.4	$K_2(2250)$ 7.4			
	$m_0$ [MeV/ $c^2$ ]	$1715 \pm 4$	$^{+1}_{-6}$	$1848 \pm 5$	$^{+6}_{-20}$	$2230 \pm 11$	$^{+7}_{-61}$
	$\Gamma_0$ [MeV/ $c^2$ ]	$139 \pm 7$	$^{+14}_{-7}$	$250 \pm 10$	$^{+17}_{-23}$	$266 \pm 29$	$^{+225}_{-16}$
PDG	$m_0$ [MeV/ $c^2$ ]	$1773 \pm 8$		$1819 \pm 12$		$2247 \pm 17$	
	$\Gamma_0$ [MeV/ $c^2$ ]	$186 \pm 14$		$264 \pm 34$		$180 \pm 30$	

		(c) $K_J^*$ -like resonances			
Discussed in section		$K_2^*(1430)$ 7.2	$K_4^*(2045)$ 7.3		
	$m_0$ [MeV/ $c^2$ ]	$1430.1 \pm 1.5$	$^{+1.3}_{-2.0}$	$2059 \pm 6$	$^{+9}_{-1}$
	$\Gamma_0$ [MeV/ $c^2$ ]	$109 \pm 3$	$^{+6}_{-2}$	$188 \pm 11$	$^{+27}_{-18}$
PDG	$m_0$ [MeV/ $c^2$ ]	$1427.3 \pm 1.5$		$2048$	$^{+8}_{-9}$
	$\Gamma_0$ [MeV/ $c^2$ ]	$100.0 \pm 2.1$		$199$	$^{+27}_{-19}$

3838 **A** to **F** to investigate systematic effects.<sup>[u]</sup> We selected studies to investigate the potentially largest  
 3839 systematic effects on the RMF. Performing a complete set of systematic studies was beyond the  
 3840 scope of this analysis. We studied whether the assumptions and approximations that entered the  
 3841  $\chi^2$  function in equation (6.23), which is minimized in the RMFs, may introduce systematic effects.  
 3842 Such effects are discussed in sections 6.3.1 and 6.3.2. We also studied potential systematic effects  
 3843 introduced by the  $K_1(1400)$  and  $K_2(1820)$  components that are discussed in section 6.3.3. In the  
 3844 same section also the influence of our choice for the rank of the  $K^-\pi^-\pi^+$  spin-density matrix is  
 3845 discussed. The resonance parameters obtained in the six systematic studies are listed in table 6.4.  
 3846 Findings that are specific to individual waves are discussed in chapter 7 and only general findings  
 3847 are discussed in the following subsections.

### 3848 6.3.1 Effects from Using Bootstrapping vs. Maximum-Likelihood Estimates

3849 As discussed in sections 5.4.2 and 6.1.5, we not only used the Bootstrapping estimates for the  
 3850 covariance matrix of the measured spin-density matrix elements, but also for the measured values  
 3851 of the spin-density matrix elements, i.e. the central values of the data points that entered the  
 3852 RMF. To study the effect of this approach, we performed an RMF in study **A** where we used the  
 3853 maximum-likelihood estimates<sup>[v]</sup> as data points, i.e. we used  $\lambda_i(m_{K\pi\pi}, t') = \lambda_i^{\text{MLE}}(m_{K\pi\pi}, t')$  in  
 3854 equation (6.23). For the covariance matrix of the spin-density matrix elements, we still used the  
 3855 Bootstrapping estimates as done in the main analysis.

3856 Compared to the main analysis, study **A** yielded slightly different resonance parameters. These  
 3857 differences have a similar size as other systematic effects (see table 6.4). Hence, we consider the  
 3858 results of this study to be consistent with the results of the main analysis within the expected  
 3859 uncertainties.

3860 The main analysis, which used the Bootstrapping means as data points, yielded and  $\chi_{\text{red}}^2$  value of  
 3861 0.826. This  $\chi_{\text{red}}^2$  value corresponds to an unexpectedly large  $p$ -value of practically one. Such a  
 3862 low  $\chi_{\text{red}}^2$  may arise for two reasons. First, the RMF has too much freedom and overfits the data.  
 3863 However, this would disagree with the statistically large deviations between some measured  
 3864 spin-density matrix elements and the corresponding RMF result in the main analysis. Such  
 3865 deviations are discussed for example for the intensity spectrum of the  $4^+ 1^+ K^*(892)\pi G$  wave in  
 3866 section 6.2.2. Hence, we expect the  $\chi_{\text{red}}^2$  value to be even larger than one. i.e.  $\chi_{\text{red}}^2 \gtrsim 1.0$ . Second,  
 3867 the uncertainty estimates of the measured spin-density matrix elements are too large.

<sup>[u]</sup> Except for the changes explicitly mentioned in the systematic studies discussed in the following; the RMF model, the  $\chi^2$  definition, and the fitting procedure remain the same as in the main analysis discussed in sections 6.1 and 6.2. To reduce the computational costs of the systematic studies, we performed about 200 fit attempts with random start-parameter values for each study. This turned out to be sufficient to reliably find the best result, i.e. to find the result with the lowest  $\chi^2$  value in more than 10 of the 200 fit attempts.

<sup>[v]</sup> As defined in section 5.4, the maximum-likelihood estimates are the results of the maximum-likelihood fit of equation (5.38) to the measured  $K^-\pi^-\pi^+$  sample.



Table 6.4: Resonance parameters of the eight resonance components included in the 10-wave RMF as obtained in the main analysis (Main) and in the systematic studies **A** to **F**. The last column shows the largest positive and negative deviation from the values obtained in the main analysis that were observed across all systematic studies. As the set of systematic studies is not complete, these deviations give only a lower limit for the full systematic uncertainties. Parameters of resonance components that were not included in the model in a study are indicated by “—”. The estimates for the mass and width of the  $K_2(1770)$  from study **E** (shown in gray) are not included in the corresponding deviations (see text). The resonance parameters of the  $K_1(1400)$  component that are marked by (\*) were fixed to the corresponding PDG average values. We do not give statistical uncertainties here. The values are rounded according to the corresponding statistical uncertainty from the main analysis following the PDG rounding rules [9].

Resonance	Parameter	Main	A	B	C	D	E	F	Extremes
$K_1(1270)$	$m_0$ [MeV/ $c^2$ ]	1267.7	1264.6	1269.2	1265.2	1264.0	1266.5	1263.2	+1.6 -4.5
	$\Gamma_0$ [MeV/ $c^2$ ]	83	79	98	83	82	82	86	+15 -4
$K_1(1400)$	$m_0$ [MeV/ $c^2$ ]	(*)1403	(*)1403	(*)1403	1514	—	(*)1403	(*)1403	+111 -0
	$\Gamma_0$ [MeV/ $c^2$ ]	(*)174	(*)174	(*)174	178	—	(*)174	(*)174	+4 -4
$K'_1$	$m_0$ [MeV/ $c^2$ ]	1938	1978	1929	1907	1930	2031	1866	+93 -71
	$\Gamma_0$ [MeV/ $c^2$ ]	462	457	489	455	428	448	343	+27 -119
$K^*_2(1430)$	$m_0$ [MeV/ $c^2$ ]	1430.1	1431.4	1428.0	1430.7	1430.0	1429.9	1430.0	+1.3 -2.0
	$\Gamma_0$ [MeV/ $c^2$ ]	108.9	107.3	113.3	109.9	114.5	110.4	112.5	+5.7 -1.6
$K_2(1770)$	$m_0$ [MeV/ $c^2$ ]	1714.6	1716.0	1714.8	1715.4	1715.8	1740.1	1708.7	+25.5 -6.0
	$\Gamma_0$ [MeV/ $c^2$ ]	139	151	146	131	144	210	153	+71 -7
$K_2(1820)$	$m_0$ [MeV/ $c^2$ ]	1848	1854	1840	1842	1849	—	1827	+6 -20
	$\Gamma_0$ [MeV/ $c^2$ ]	250	267	262	236	237	—	227	+17 -23
$K_2(2250)$	$m_0$ [MeV/ $c^2$ ]	2230	2237	2222	2232	2222	2170	2232	+7 -61
	$\Gamma_0$ [MeV/ $c^2$ ]	266	283	303	250	298	491	274	+225 -16
$K^*_4(2045)$	$m_0$ [MeV/ $c^2$ ]	2059	2062	2067	2058	2060	2068	2060	+9 -1
	$\Gamma_0$ [MeV/ $c^2$ ]	188	177	189	195	185	170	214	+27 -18

3868 Study A, which used the maximum-likelihood estimates as data points, yielded an increased  
 3869  $\chi_{\text{red}}^2$  value of 1.071, which is in agreement with our expectation of  $\chi_{\text{red}}^2 \gtrsim 1.0$ .<sup>[w]</sup> This  $\chi_{\text{red}}^2$  value  
 3870 corresponds to a low  $p$ -value of about  $10^{-5}$ .

3871 The uncertainties of the spin-density matrix elements from Bootstrapping were determined  
 3872 from the distribution of the maximum-likelihood estimates that were obtained from each of  
 3873 the Bootstrapping samples. Hence, the uncertainties estimate the uncertainty of the maximum-  
 3874 likelihood estimates. Using in study A the maximum-likelihood estimates as data points yielded  
 3875 an  $\chi_{\text{red}}^2$  value in the expected range. Thus, we conclude that the Bootstrapping yielded realistic  
 3876 estimates for the uncertainties of the maximum-likelihood estimates. However, using these  
 3877 uncertainty estimates in the main analysis together with the Bootstrapping means as data points  
 3878 yielded an unexpectedly small  $\chi_{\text{red}}^2$ . This indicates that the uncertainty estimates for the maximum-  
 3879 likelihood estimates overestimate the uncertainties of the Bootstrapping means. This can be  
 3880 directly observed in some spin-density matrix elements. For example; in figure 6.4 the scatter of  
 3881 the data points, which are the Bootstrapping means, is smaller than expected from the shown  
 3882 uncertainties.<sup>[x]</sup>

3883 A possible explanation for the larger uncertainties, i.e. larger spread, of the maximum-likelihood  
 3884 estimates compared to the Bootstrapping means is the leakage effect discussed in section 5.9.  
 3885 It leads not only to large artifacts in the leakage waves. As it is approximately an ambiguity  
 3886 in the partial-wave model, whose magnitude is given by the specifics of the data sample, e.g.  
 3887 by fluctuation, the leakage effect may also introduce an additional spread in the distributions  
 3888 of the spin-density matrix elements from the different Bootstrapping samples, thereby yielding  
 3889 larger the uncertainty estimates. Even non-leakage waves may be influenced by this spread to a  
 3890 small degree. Also, the maximum-likelihood estimates from the measured  $K^-\pi^-\pi^+$  sample are  
 3891 affected by the leakage effect, i.e. by one realization of this ambiguity with a certain magnitude  
 3892 given by the specifics of the measured  $K^-\pi^-\pi^+$  sample. Thus, we expect the uncertainties from  
 3893 Bootstrapping to yield a realistic estimate for the actual uncertainties of the maximum-likelihood  
 3894 estimates by including the leakage effect. In contrast, when calculating the Bootstrapping means,  
 3895 the additional spread introduced by the leakage effect may average out to some extent, because  
 3896 we average over different data samples, which potentially have a different magnitude of the  
 3897 leakage effect. Thus, the Bootstrapping means should be less biased by the spread introduced by  
 3898 the leakage effect and should have smaller uncertainties.<sup>[y]</sup> This would be consistent with the  
 3899 observation that our estimates of the uncertainties overestimate the actual uncertainties of the  
 3900 Bootstrapping means.

3901 We used the Bootstrapping means in the main analysis as data points in order to potentially  
 3902 reduce the bias, e.g. from the leakage effect, on the measured spin-density matrix elements. We

<sup>[w]</sup> We used the same 10-wave RMF model for the main analysis and for study A. Similar to the main analysis, the RMF could not describe some measured spin-density matrix elements.

<sup>[x]</sup> One should note that considering individual spin-density matrix elements gives an incomplete picture as the spin-density matrix elements from the same  $(m_{K\pi\pi}, t')$  cell are strongly correlated.

<sup>[y]</sup> While calculating the Bootstrapping means may reduce the spread introduced by the leakage effect, it cannot purge the leakage effect. This means in particular that we still expect the leakage waves to be biased by the leakage effect.

3903 did this at the expense of using potentially overestimated uncertainties.<sup>[z]</sup> This also means, that  
 3904 the  $\chi^2$  value of the RMF in equation (6.23) is systematically too small. However, it is still a valid  
 3905 measure for the deviation of the RMF from the measured spin-density matrix elements and can  
 3906 thus be used to estimate the parameter values of the RMF model. Only its interpretation in terms  
 3907 of a  $\chi^2$  distributed test statistic is limited. For example, this means that  $\chi_{\text{red}}^2$  values from fits with  
 3908 different numbers of degrees of freedom are hard to compare.

### 3909 6.3.2 Effects from the Eigenvalue Spectrum of the Precision Matrix

3910 As discussed in section 6.1.5, for a single PWD fit the rank of the covariance matrix of the  
 3911 real-valued elements of the spin-density matrix is the number of free parameters  $n_{\text{para}}^\rho$  of that  
 3912 spin-density matrix. However, we estimated the covariance matrix of the spin-density matrix  
 3913 elements from Bootstrapping, i.e. from the distribution of 2000 independent PWD fits. The rank  
 3914 of this covariance matrix does not correspond to  $n_{\text{para}}^\rho$  of a rank=3 spin-density matrix. In fact,  
 3915 the covariance matrix has full rank. Hence, also the precision matrix, which is the inverse of  
 3916 the covariance matrix, that appears in the  $\chi^2$  formulation of the RMF in equation (6.23) has full  
 3917 rank. To test for potential systematic effects from the higher rank of the precision matrix, we  
 3918 performed an RMF in study **B** where we constructed a precision matrix with rank  $n_{\text{para}}^\rho$ . To this  
 3919 end, we considered only the  $n_{\text{para}}^\rho$  largest eigenvalues of the covariance matrix when constructing  
 3920 the precision matrix in each  $(m_{K\pi\pi}, t')$  cell, i.e.

$$\text{Prec}'[\lambda_i, \lambda_j] = \sum_{h=1}^{n_{\text{para}}^\rho} \frac{1}{e^h} v_i^h [v_j^h]^* . \quad (6.30)$$

3921 Here,  $e^h$  is the  $h$ 'th largest eigenvalue of the covariance matrix of the spin-density matrix  
 3922 elements and  $v_i^h$  is the  $i$ 'th entry of the corresponding eigenvector. The precision matrix as  
 3923 given in equation (6.30) is similar to the Moore-Penrose pseudo-inverse as used in the main  
 3924 analysis. However, here we did not only set the inverse of zero eigenvalues to zero, but we  
 3925 also set the inverse of all but the  $n_{\text{para}}^\rho$  largest eigenvalues to zero, and we used the eigenvalue  
 3926 decomposition<sup>[aa]</sup> instead of the singular-value decomposition.

3927 This means that there are some directions in the  $\vec{\lambda}(m_{K\pi\pi}, t')$  space in which deviations between  
 3928 the measured spin-density matrix elements and the RMF are not considered in  $\chi_{\text{RMF}}^2$ . These  
 3929 directions are given by the eigenvectors belonging to eigenvalues whose inverse is set to zero  
 3930 according to equation (6.30). In principle, the elements of a rank=3 spin-density matrix are  
 3931 already constrained in these directions by the limited rank. However, the Bootstrapping means  
 3932 of the spin-density matrix elements, which are used as data points in the RMF, do not exactly  
 3933 fulfill this constraints due to the averaging in the mean calculation. Also, the RMF model  
 3934 for the spin-density matrix in equation (6.1) has rank=[ 4], which is larger than the rank of  
 3935 the measured spin-density matrix, and hence is less constrained. Thus, neglecting in  $\chi_{\text{RMF}}^2$  all

<sup>[z]</sup> Explicitly determining Bootstrapping estimates for the uncertainties of the Bootstrapping means would be computationally prohibitively expensive (see section 5.4.2).

<sup>[aa]</sup> See equation (8) on page 43 and equation (19) on page 156 of ref. [139].

directions belonging to eigenvalues whose inverse is set to zero according to equation (6.30) removes constraints from the RMF and is hence not exactly correct. Furthermore, we determined these directions only with a finite precision given by the precision with which we measured the covariance matrix of the spin-density matrix elements in the Bootstrapping. Hence, study **B** is an extreme test for effects from the eigenvalue spectrum of the precision matrix.

Using the precision matrix given in equation (6.30) in the RMF in study **B** yielded  $\chi_{\text{red}}^2 = 0.899$ , which is slightly worse than  $\chi_{\text{red}}^2 = 0.826$  from the main analysis.<sup>[ab]</sup> A reason for this may be, that the eigenvectors of the  $n_{\text{para}}^{\rho}$  largest eigenvalues only approximately span the space of the degrees of freedom of a rank=3 spin-density matrix. This is mainly because of two effects: (i) the finite precision of the eigenvectors given by the finite precision, with which the covariance matrix was determined from the finite set of Bootstrapping samples; (ii) the non-linear effects in the calculation of the spin-density matrix elements, which are discussed in section 5.4. For some resonance parameters, the parameter estimates from study **B** define the extreme deviations with respect to the estimates from the main analysis. Hence, systematic effects from the eigenvalue spectrum of the precision matrix are part of our systematic uncertainties. However, in general the systematic effects observed in study **B**, which can be considered as an extreme test for the effects from the eigenvalue spectrum of the precision matrix, are of similar size as other systematic effects (see table 6.4). Therefore, we expect no artifacts from the eigenvalue spectrum of the precision matrix on the results of the RMF.

### 6.3.3 Effects from the Formulation of the $K^{-}\pi^{-}\pi^{+}$ RMF Model

#### Effects from the $K_1(1400)$ Component

As the  $K_1(1400)$  is only a weak signal in the  $1^{+}$  waves included in the 10-wave RMF, we fixed its resonance parameters to the corresponding PDG average values in the main analysis. Although the  $K_1(1400)$  is one of the best known strange mesons, previous measurements of its resonance parameters exhibit a considerable spread (see section 7.1). To test whether the PDG average values for the  $K_1(1400)$  are consistent with our data, we performed an RMF in study **C** where we left the mass and width parameters of the  $K_1(1400)$  component as free fit parameters.

To study the influence of the  $K_1(1400)$  component on the measurement of the other resonance parameters, we performed an RMF in study **D** where we omitted the  $K_1(1400)$  component from the RMF model, i.e. where we modeled the  $1^{+}$  waves by only two resonances.<sup>[ac]</sup> The results of these studies are discussed in section 7.1.

<sup>[ab]</sup> Using equation (6.30) reduces the number of degrees of freedom in the RMF; because by setting the inverse of certain eigenvalues to zero, we ignore certain direction in the  $\vec{\lambda}$  space. This means we effectively remove some data from the  $\chi^2$  term. The number of degrees of freedom in the RMF **B** is the sum over the rank of  $\text{Prec}'[\lambda_i, \lambda_j]$  from all  $(m_{K\pi\pi}, t')$  cells minus the number of free parameters in the fit.

<sup>[ac]</sup> The model for the  $1^{+}$  waves still included the non-resonant components, the  $\pi^{-}\pi^{-}\pi^{+}$  background components, and the effective background components as in the 10-wave RMF model in table 6.1.

### 3967 Effects from the $K_2(1820)$ Component

3968 As discussed in section 7.4, many previous measurements of the  $K_2$  resonances considered  
 3969 only one  $K_2$  state in the region  $1.7 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$ , while we included the  $K_2(1780)$   
 3970 and  $K_2(1820)$  components in the 10-wave RMF. To obtain resonance parameter estimates that  
 3971 are directly comparable with these previous measurements, we performed an RMF in study *E*  
 3972 where we omitted the  $K_2(1820)$  component, i.e. where we modeled the low- $m_{K\pi\pi}$  region of the  
 3973  $2^-$  waves by only the  $K_2(1780)$  component.<sup>[ad]</sup> As the model without the  $K_2(1820)$  component  
 3974 represents a fundamentally different interpretation of the  $2^-$  waves for  $m_{K\pi\pi} \lesssim 2 \text{ GeV}/c^2$ , we  
 3975 did not consider the results of this study in our estimates for the systematic uncertainties of the  
 3976 resonance parameters of the  $K_2(1770)$  in table 6.2. The results of this study are discussed in  
 3977 section 7.4.

### 3978 Effects from the Chosen Rank of the Model for the $K^- \pi^- \pi^+$ Spin-Density Matrix

3979 When constructing the RMF model for the  $K^- \pi^- \pi^+$  spin-density matrix in section 6.1.2, we  
 3980 assumed that the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  is dominated by Pomeron exchange. Accordingly,  
 3981 we modeled the  $K^- \pi^- \pi^+$  spin-density matrix  $\hat{\rho}_{ab}^{K\pi\pi}$  in equation (6.7) as a rank=1 matrix. To  
 3982 study this choice we performed an RMF in study *F* where we constructed a rank=2 spin-density  
 3983 matrix,

$$\rho_{ab}^{K\pi\pi}(m_{K\pi\pi}, t') = \sum_{z=1}^2 \mathcal{T}_a^{K\pi\pi,z}(m_{K\pi\pi}, t') \left[ \mathcal{T}_b^{K\pi\pi,z}(m_{K\pi\pi}, t') \right]^*, \quad (6.31)$$

3984 to model the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . Therefore, we defined two sets of transition  
 3985 amplitudes analogously to equation (6.6),

$$\hat{\mathcal{F}}_a^{K\pi\pi,z}(m_{K\pi\pi}, t') = \sqrt{\mathfrak{N}_a(m_{K\pi\pi}) m_{K\pi\pi}} \mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t') \sum_{k \in \mathbb{S}_a} {}^k C_a^{K\pi\pi,z}(t') \mathcal{D}_k(m_{K\pi\pi}; \zeta_k) \quad (6.32)$$

3986 one for each of the two coherent sectors  $z$ , including the same resonance components with the  
 3987 same mass and width parameters in both sectors, but with independent coupling amplitudes  
 3988  ${}^k C_a^{K\pi\pi,z}(t')$ .<sup>[ae]</sup> The non-resonant components were included only in the first set of transition  
 3989 amplitudes with  $z = 1$ . In this study *F*, we significantly increased the number of free fit  
 3990 parameters from 291 parameters in the main analysis to 391 parameters.

3991 The reduced  $\chi^2$  decreased in this study from  $\chi_{\text{red}}^2 = 0.826$  as obtained in the main analysis to  
 3992  $\chi_{\text{red}}^2 = 0.738$ . This means that the measured spin-density matrix elements are better described  
 3993 by the RMF model using a  $K^- \pi^- \pi^+$  spin-density matrix of rank=2. However, as discussed in

<sup>[ad]</sup> The model for the  $2^-$  waves still included the  $K_2(2250)$  component for the high- $m_{K\pi\pi}$  region and the non-resonant components, the  $\pi^- \pi^- \pi^+$  background components, and the effective background components as in the 10-wave RMF model in table 6.1.

<sup>[ae]</sup> As in the main analysis, we also enforced the  $t'$  dependence of a resonance component that appears in multiple waves with the same  $J^P M^s$  to be the same by applying equation (6.14). We introduced an independent set of branching amplitudes  ${}^k \mathcal{B}_a^{K\pi\pi,2}$  for the additional set of transition amplitudes.

section 6.3.1, the  $\chi^2$  defined in equation (6.23) can be interpreted in terms of a  $\chi^2$  distribution only to a limited extent. Furthermore, the shape parameters  $b_k$  of the effective background components of the  $2^- 0^+ K^*(892) \pi F$  and  $4^+ 1^+ \rho(770) K G$  waves end up at the lower parameter-limit of  $-0.1 (\text{GeV}/c)^{-2}$ . This indicates that for these waves the result of this study is biased towards an unphysical solution.<sup>[af]</sup> For some resonance parameters, e.g. for the mass and width of the  $K'_1$ , this study yielded the largest deviation from the results of the main analysis. These deviations are discussed in chapter 7.

## 6.4 Pseudodata Studies using the $K^- \pi^- \pi^+$ RMF Model

In this section, we discuss input-output studies based on pseudodata samples to investigate the consistency of the full analysis chain up to the measurement of resonance parameters in the RMF, similar to section 5.8, where we used pseudodata samples to investigate effects on the results of the PWD. To this end, we generated pseudodata samples based on the results of the 10-wave RMF. Hence, we know a priori which resonances appear in the pseudodata with which strength and, most notably, which resonance parameters they have. As we explicitly modeled the background contributions and hence separated the backgrounds from the signals in the RMF, we also control the background contributions in these pseudodata samples. This is in contrast to the  $K^- \pi^- \pi^+$  PWD pseudodata studies presented in section 5.8 and allows us to test for systematic effects from our treatment of background contributions (see sections 5.3, 6.1.3, and 6.1.4).

First, we generated a pseudodata sample of  $50 \times 10^6$  events, whose distribution is given only by the resonances and the non-resonant contributions. To this end, we took from the result the 10-wave RMF discussed in section 6.2.2 only the  $K^- \pi^- \pi^+$  signal part given by the  $K^- \pi^- \pi^+$  spin-density matrix in equation (6.7).<sup>[ag]</sup> We used the 10-wave RMF result of  $\hat{\rho}_{ab}^{K\pi\pi}(m_{K\pi\pi}, t')$  as input to a PWD model as defined in equation (5.19). Using this PWD model, we produced a pseudodata sample applying the same approach as in section 5.8. We call this sample the 10-wave pseudodata sample. It is distributed according to the resonant and non-resonant components of the 10 waves included in the 10-wave RMF. The contributions from the other 228 waves of the 238-wave set are zero. Hence, the 10-wave pseudodata sample does not follow the same distribution as the full  $K^- \pi^- \pi^+$  sample. Still, this pseudodata sample allow us to study the consistency of the measurement of resonances parameters. Finally, only both sets of pseudodata studies, those based in the  $K^- \pi^- \pi^+$  RMF model discussed here and those based on the 238-wave PWD discussed in section 5.8, yield a complete picture of our analysis.

We applied the complete analysis chain presented in this work to the produced 10-wave pseudodata sample. This means, we processed it through the COMPASS detector Monte Carlo simulation (see appendix C.2) and we applied the same event selection criteria as applied to the

<sup>[af]</sup> The lower parameter limit of  $-0.1 (\text{GeV}/c)^{-2}$  was chosen such that fit results with this parameter value are not completely unphysical and can still be interpreted in terms of physics signals to some extent. However, we consider such results to be not sufficient for the main analysis.

<sup>[ag]</sup> Technically we achieved this by setting  $C^{\pi\pi\pi}(t') = 0$  in equation (6.15) and  ${}^k C_a^{\text{BKG}}(t') = 0$  in equation (6.16).

4028 measured  $K^- \pi^- \pi^+$  sample (see section 4.1). Then, we performed a PWD of the reconstructed  
 4029 pseudodata sample using the rank=3 model of the 238-wave set.<sup>[ah]</sup> In contrast to all previous  
 4030 pseudodata and systematic studies, we performed here a Bootstrapping of the PWD as discussed  
 4031 for the main analysis in section 5.4. This allows us to study the consistency of our Bootstrapping  
 4032 approach. Finally, we performed a fit of the 10-wave RMF model defined in section 6.2.1 to the  
 4033 results from the Bootstrapping of the PWD.

4034 The 10-wave pseudodata sample described above is free of background as we used only the  
 4035  $K^- \pi^- \pi^+$  RMF model part of the 10-wave RMF to generate it. In order to study effects from inco-  
 4036 herent background processes, we admixed events from the reconstructed  $\pi^- \pi^- \pi^+$  pseudodata sam-  
 4037 ple (see section 5.10) to the reconstructed 10-wave pseudodata sample on an event-by-event basis.  
 4038 Hence, the combined 10-wave pseudodata sample with admixed  $\pi^- \pi^- \pi^+$  background mimics  
 4039 the situation in the measured  $K^- \pi^- \pi^+$  sample as realistically as possible. We chose the amount of  
 4040 admixed  $\pi^- \pi^- \pi^+$  events such that it corresponds to the amount of  $\pi^- \pi^- \pi^+$  background in the mea-  
 4041 sured  $K^- \pi^- \pi^+$  sample as predicted by the  $\pi^- \pi^- \pi^+$  pseudodata.<sup>[ai]</sup> Analogously to the 10-wave  
 4042 pseudodata sample without admixed  $\pi^- \pi^- \pi^+$  background, we performed a PWD with Bootstrap-  
 4043 ping,<sup>[aj]</sup> and we performed an RMF to the results of this PWD. As the  $\pi^- \pi^- \pi^+$  background is  
 4044 the only background in the 10-wave pseudodata sample with admixed  $\pi^- \pi^- \pi^+$  background, we  
 4045 expect the effective background components as obtained from this RMF to be small. Furthermore,  
 4046 we performed an additional RMF omitting the effective background components from the model.  
 4047

4048 Table 6.5 lists the resonance-parameter estimates from the RMFs to the 10-wave pseudodata  
 4049 sample with and without admixed  $\pi^- \pi^- \pi^+$  background. For some resonance parameter, e.g.  
 4050 the  $m_0$  parameter of the  $K_1(1270)$  component, the estimates deviate from the reference value,  
 4051 i.e. the result of the 10-wave RMF from the measured  $K^- \pi^- \pi^+$  sample, by more than their  
 4052 statistical uncertainty. However, all deviations are smaller than the systematic effects discussed  
 4053 in section 6.3, except for the  $m_0$  parameter of the  $K_2(2250)$  component, whose deviation is,  
 4054 however, still of similar size as the systematic effects.<sup>[ak]</sup> This means that the bias on our  
 4055 resonance-parameter estimates as determined in this pseudodata study is small. This also  
 4056 indicates that our first estimates for systematic uncertainties have a realistic size (see section 6.3).  
 4057

<sup>[ah]</sup> We used the correct acceptance model in the PWD fits, in contrast to the previous studies where we used the detuned acceptance model as discussed e.g. in section 5.8.2.

<sup>[ai]</sup> As the 10-wave RMF model represents only part of the  $K^- \pi^- \pi^+$  sample, while the  $\pi^- \pi^- \pi^+$  background distributes to all 238  $K^- \pi^- \pi^+$  partial waves, the fraction of  $\pi^- \pi^- \pi^+$  background events in the 10-wave pseudodata sample with admixed  $\pi^- \pi^- \pi^+$  background is not 6.7% as predicted for the total measured  $K^- \pi^- \pi^+$  sample (see section 5.10.1). The reconstructed 10-wave pseudodata sample with admixed  $\pi^- \pi^- \pi^+$  background contains about 28%  $\pi^- \pi^- \pi^+$  background events.

<sup>[aj]</sup> As the  $\pi^- \pi^- \pi^+$  background distributes to all 238  $K^- \pi^- \pi^+$  partial waves, we used a rank=3 model of the 238-wave set as in the main analysis. Therefore, we expect the same projections of the  $\pi^- \pi^- \pi^+$  background into the individual partial waves as predicted by the  $\pi^- \pi^- \pi^+$  background PWD.

<sup>[ak]</sup> The largest positive deviation for the  $m_0$  parameter of the  $K_2(2250)$  component observed in the systematic studies is 7 MeV/ $c^2$ , i.e. smaller than the deviation of 26 MeV/ $c^2$  found in the pseudodata studies. However, the largest negative deviation observed in the systematic studies is -61 MeV/ $c^2$ , i.e. larger in magnitude than the deviation found here.

Table 6.5: Resonance parameters of seven resonance components obtained from fits of the 10-wave RMF model to the 10-wave pseudodata sample with and without admixed  $\pi^-\pi^-\pi^+$  background. For the pseudodata sample with admixed  $\pi^-\pi^-\pi^+$  background, we performed two RMFs, one with the full 10-wave RMF model and one omitting the effective background (eBKG) components from the 10-wave RMF model. The ‘‘Reference’’ column lists the resonance parameters used to generate these pseudodata samples, which are the resonance parameters obtained in the 10-wave RMF to the measured  $K^-\pi^-\pi^+$  sample (see table 6.2). The last column shows the largest positive and negative deviation from the reference values observed in all three studies. We do not list the resonance parameters of the  $K_1(1400)$  component as they were fixed in all three studies. We do not give uncertainties. The values are rounded according to the corresponding statistical uncertainty from the main analysis following the PDG rounding rules [9].

		Reference	10-wave pseudodata			Extremes
$\pi^-\pi^-\pi^+$ admixed			✓	✓	✗	
eBKG component			✓	✗	✓	
$K_1(1270)$	$m_0$ [MeV/ $c^2$ ]	1267.7	1267.4	1264.1	1263.5	+ 0.0 - 4.2
	$\Gamma_0$ [MeV/ $c^2$ ]	83	88	88	88	+ 5 - 0
$K'_1$	$m_0$ [MeV/ $c^2$ ]	1938	1940	1945	1944	+ 7 - 0
	$\Gamma_0$ [MeV/ $c^2$ ]	462	433	453	454	+ 0 -29
$K_2^*(1430)$	$m_0$ [MeV/ $c^2$ ]	1430.1	1431.4	1431.9	1431.8	+ 1.8 - 0.0
	$\Gamma_0$ [MeV/ $c^2$ ]	108.9	111.4	110.2	111.6	+ 2.7 - 0.0
$K_2(1770)$	$m_0$ [MeV/ $c^2$ ]	1714.6	1714.5	1713.3	1713.5	+ 0.0 - 1.3
	$\Gamma_0$ [MeV/ $c^2$ ]	139	144	143	142	+ 5 - 0
$K_2(1820)$	$m_0$ [MeV/ $c^2$ ]	1848	1853	1850	1849	+ 5 - 0
	$\Gamma_0$ [MeV/ $c^2$ ]	250	249	247	245	+ 0 - 5
$K_2(2250)$	$m_0$ [MeV/ $c^2$ ]	2230	2240	2256	2253	+26 - 0
	$\Gamma_0$ [MeV/ $c^2$ ]	266	267	248	255	+ 1 -17
$K_4^*(2048)$	$m_0$ [MeV/ $c^2$ ]	2059	2057	2058	2060	+ 1 - 2
	$\Gamma_0$ [MeV/ $c^2$ ]	188	179	196	200	+13 - 8



4058 Figure 6.7 shows the results of the RMF to the 10-wave pseudodata sample with admixed  $\pi^- \pi^- \pi^+$   
 4059 background as solid curves exemplarily for the  $t'$ -summed intensity spectrum of the  $2^+ 1^+$   
 4060  $\rho(770) K D$  wave. The result for the  $K_2^*(1430)$  component (solid blue curve) agrees well with  
 4061 the  $K_2^*(1430)$  component in the reference (dash-dotted blue curve), i.e. with the result of the  
 4062 10-wave RMF from the measured  $K^- \pi^- \pi^+$  sample. We find similar agreement for all resonance  
 4063 components included in the 10-wave RMF. This means that we were able to reproduce not only  
 4064 the resonance parameters but also the coupling and branching amplitudes of the resonances  
 4065 components in this pseudodata study. Also, the shape of the non-resonant component obtained  
 4066 from the pseudodata sample (solid green curve) agrees well with the reference (dash-dotted  
 4067 green curve). The RMF slightly overestimates the amount of the non-resonant contribution in  
 4068 this wave. This overestimation is small compared to typical systematic effects on the yield of  
 4069 the model components. We find similar agreement for the non-resonant components also in  
 4070 the nine other partial waves. Hence, we conclude that we are able to consistently extract also  
 4071 the non-resonant contributions and separate them from resonance signals in the RMFs. The  
 4072 non-resonant contributions are typically harder to determine, because they have less distinctive  
 4073 features compared to resonances, e.g. we assume that their amplitudes have a constant phase  
 4074 independent of  $m_{K\pi\pi}$ . Thus, a consistent separation of resonant and non-resonant contributions is  
 4075 a strong indication for the reliability and robustness of our results.

4076 The  $\pi^- \pi^- \pi^+$  background component as obtained from the RMF to the pseudodata (solid orange  
 4077 curve) underestimates the actual amount of  $\pi^- \pi^- \pi^+$  background, shown by cyan data points,  
 4078 by about a factor of 0.4.<sup>[all]</sup> We also find a significant contribution of the effective background  
 4079 component (solid brown curve), while there is no such background contribution in the pseudodata.  
 4080 We observe a similar behavior also in other waves. Hence, the RMF describes the  $\pi^- \pi^- \pi^+$   
 4081 background by a combination of the  $\pi^- \pi^- \pi^+$  and the effective background components. To  
 4082 further study this behavior, we performed an RMF where we omitted the effective background  
 4083 components from the model. Figure 6.8a shows the result of this study. Again, the resonant and  
 4084 non-resonant components agree well with the reference (cf. solid and dash-dotted curves). The  
 4085  $\pi^- \pi^- \pi^+$  component is larger compared to the previous RMF, because it is the only incoherent  
 4086 component in the model that can be used to account for the  $\pi^- \pi^- \pi^+$  background. However, the  
 4087  $\pi^- \pi^- \pi^+$  component still underestimates the amount of  $\pi^- \pi^- \pi^+$  background by about a factor of  
 4088 0.5. In a further study, we admixed three times more  $\pi^- \pi^- \pi^+$  background events to the 10-wave  
 4089 pseudodata sample. This yielded an underestimation of the  $\pi^- \pi^- \pi^+$  background by about the  
 4090 same factor. Hence, we conclude that the RMF systematically underestimates the amount of  
 4091  $\pi^- \pi^- \pi^+$  background by about a factor of 0.5 in the pseudodata studies.

4092 Also, the 10-wave RMF to the measured  $K^- \pi^- \pi^+$  sample yielded an amount of  $\pi^- \pi^- \pi^+$  back-  
 4093 ground that is smaller than predicted by the  $\pi^- \pi^- \pi^+$  pseudodata sample (see figure 6.3b). How-  
 4094 ever, it is smaller by a factor of only about 0.8. A possible explanation is that the amount of  
 4095  $\pi^- \pi^- \pi^+$  background predicted by the  $\pi^- \pi^- \pi^+$  pseudodata sample is too small, assuming that the  
 4096 RMF underestimated the amount of  $\pi^- \pi^- \pi^+$  background in the measured  $K^- \pi^- \pi^+$  sample by the  
 4097 same factor as in the pseudodata studies. This explanation may be the case, because the prediction

<sup>[all]</sup> The shape of the  $\pi^- \pi^- \pi^+$  component and of the  $\pi^- \pi^- \pi^+$  background PWD are the same by construction (see section 6.1.3).

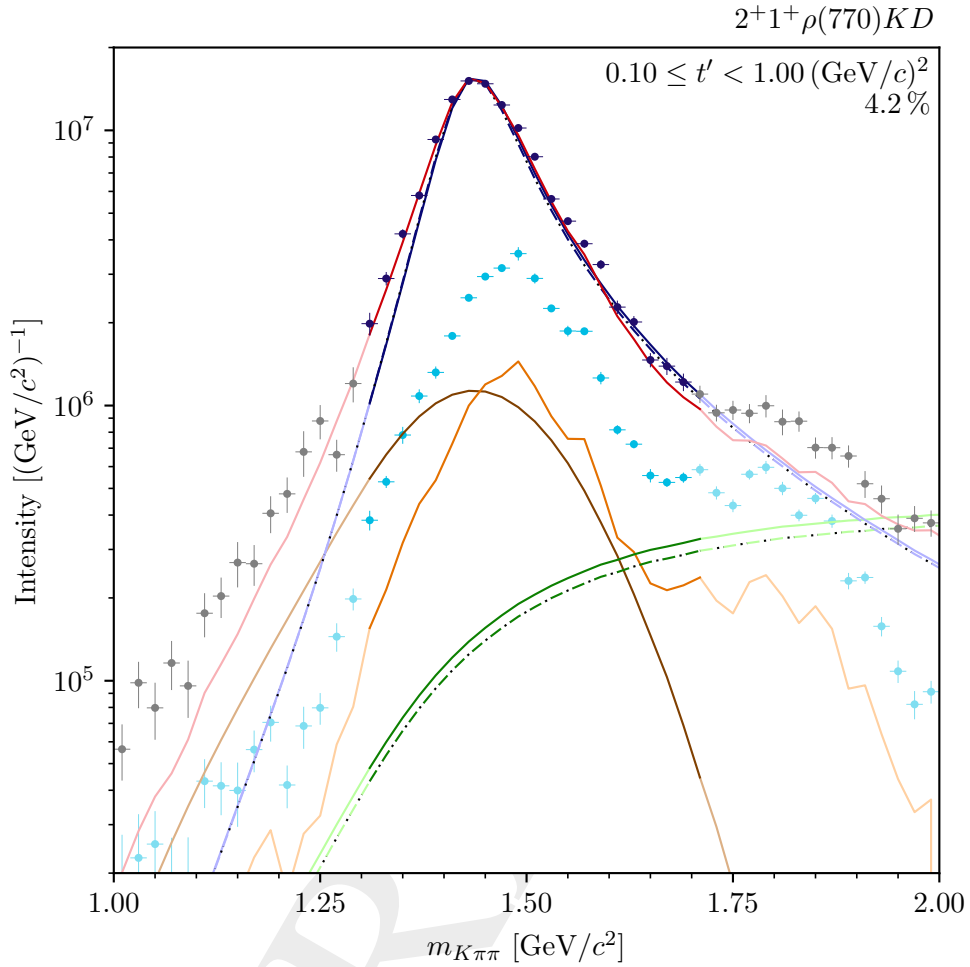


Figure 6.7: Results from fitting the 10-wave RMF model to the PWD of the 10-wave pseudodata sample with admixed  $\pi^-\pi^-\pi^+$  background (solid curves) for the  $t'$ -summed intensity spectrum of the  $2^+ 1^+ \rho(770) K D$  wave. The blue data points represent the PWD of the 10-wave pseudodata sample with admixed  $\pi^-\pi^-\pi^+$  background. The dash-dotted curves represent the model reference, i.e. the results of the 10-wave RMF to the measured data (same as solid curves in section 6.2.2), scaled according to the number of produced pseudodata events. The cyan data points show the results of the  $\pi^-\pi^-\pi^+$  background PWD, scaled such that it corresponds to the amount of  $\pi^-\pi^-\pi^+$  background in the pseudodata sample. The effective background component was not included in the pseudodata model. Also, the  $\pi^-\pi^-\pi^+$  component was not included in the pseudodata model, but  $\pi^-\pi^-\pi^+$  events from the  $\pi^-\pi^-\pi^+$  pseudodata sample were admixed to the 10-wave pseudodata sample. Hence, we do not show the background component, the  $\pi^-\pi^-\pi^+$  component, and the total model curve for the model reference. The red curve represents the total RMF model. The blue curves represent the resonance component. The green curves represent the non-resonant component. The orange curve represents the  $\pi^-\pi^-\pi^+$  background component. The brown curve represents the effective background component. The extrapolation to the  $m_{K\pi\pi}$  region that was not included in the RMF is shown in brightened colors. The corresponding data points are shown in gray. Only the range  $1.0 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$  is shown. The percentage gives the relative intensity of this wave in the PWD of the pseudodata sample.

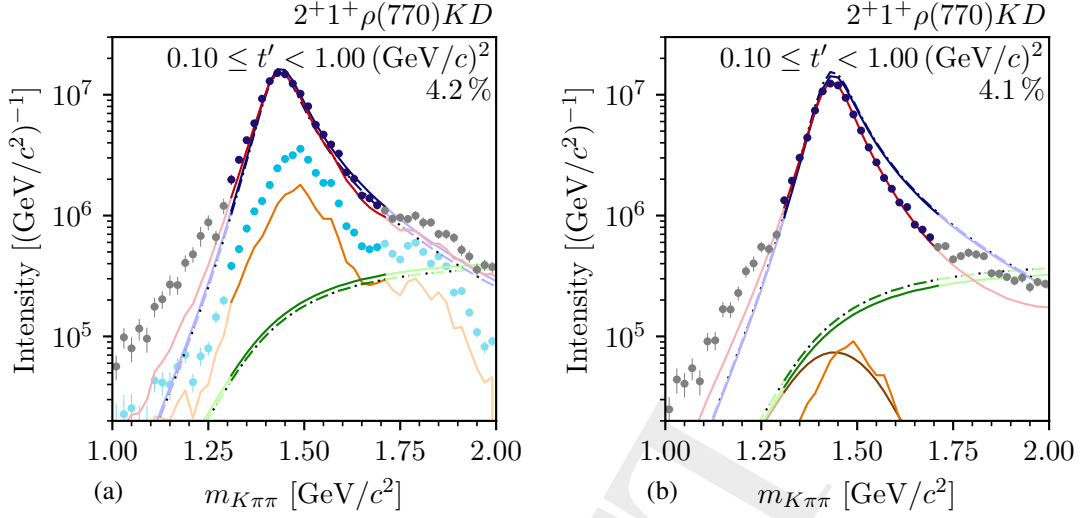


Figure 6.8: Same as figure 6.7, but (a) for the RMF omitting the effective background components in the model, and (b) for the RMF to the 10-wave pseudodata sample without admixed  $\pi^- \pi^- \pi^+$  background.

4098 by the  $\pi^- \pi^- \pi^+$  pseudodata sample is only a rough estimate, because the absolute acceptance  
 4099 is not accurately known as discussed in section 5.10.1.<sup>[am]</sup> Another possible explanation is  
 4100 based on the fact that the 10-wave pseudodata sample represents only a part of the measured  
 4101  $K^- \pi^- \pi^+$  sample. Whether the  $\pi^- \pi^- \pi^+$  background is admixed to the full  $K^- \pi^- \pi^+$  sample as  
 4102 in the measured data, or only to the 10-wave pseudodata sample may affect the result of the  
 4103 PWD of the  $\pi^- \pi^- \pi^+$  background. This is because the background contributions are treated only  
 4104 effectively in the PWD (see section 5.3), and imperfections in this description of the  $\pi^- \pi^- \pi^+$   
 4105 background may have different implications depending on the other contributions in the data sam-  
 4106 ple. We also observe that the fit uses a combination of the  $\pi^- \pi^- \pi^+$  and the effective background  
 4107 components to describe the actual  $\pi^- \pi^- \pi^+$  background when including the effective background  
 4108 component in the RMF model. This indicates that the exact shape of the  $\pi^- \pi^- \pi^+$  background  
 4109 in the partial waves slightly differs from the  $\pi^- \pi^- \pi^+$  background PWD.<sup>[an]</sup> Hence, the bias on  
 4110 the RMF estimate of the amount of  $\pi^- \pi^- \pi^+$  background may be larger in the pseudodata studies  
 4111 than in the 10-wave RMF to the measured  $K^- \pi^- \pi^+$  sample. In the worst case, we expect that the  
 4112 RMF underestimates the actual amount of  $\pi^- \pi^- \pi^+$  background in the measured  $K^- \pi^- \pi^+$  sample  
 4113 by at most a factor of 0.5.

4114 To further study the separation between signal and background components in the RMF and  
 4115 to test whether the  $\pi^- \pi^- \pi^+$  and effective background components can be partly misused by  
 4116 the RMF to account for other effects in the data, we performed an RMF that included both  
 4117 background components to the 10-wave pseudodata sample without admixed  $\pi^- \pi^- \pi^+$  background.  
 4118 Figure 6.8b shows the result of this study exemplarily for the intensity spectrum of the  $2^+ 1^+$

<sup>[am]</sup> In contrast to the measured  $K^- \pi^- \pi^+$  sample, we know the amount of  $\pi^- \pi^- \pi^+$  background in the pseudodata sample exactly.

<sup>[an]</sup> This difference must be small, because the RMF results for the resonance and non-resonant components are consistent with the reference.

4119  $\rho(770) K D$  wave. As in the previous studies, the results for the resonant and non-resonant  
 4120 components (solid blue and green curves) agree with the corresponding references (dash-dotted  
 4121 curves). The  $\pi^- \pi^- \pi^+$  and effective background components (solid orange and brown curves)  
 4122 practically do not contribute to the total model intensity.<sup>[ao]</sup> This is expected, because the  
 4123 analyzed pseudodata sample does not contain background events. Hence, we conclude that the  
 4124 RMF does not misuse the  $\pi^- \pi^- \pi^+$  and effective background components to describe other effects  
 4125 in the data. This is a strong indication that the RMF is able to reliably separate resonance and  
 4126 non-resonant contributions from background.

4127 The pseudodata studies presented in this section allowed us to test our full analysis chain: starting  
 4128 with the event selection, over the Bootstrapping of the PWD, up to the RMF. Reviewing our  
 4129 findings, the extraction of the resonance parameters, which is the main goal of this analysis,  
 4130 is consistent within the systematic effects discussed in section 6.3 in all performed studies. It  
 4131 is not strongly affected by the estimate for the  $\pi^- \pi^- \pi^+$  background. Hence, we conclude that  
 4132 our treatment of the  $\pi^- \pi^- \pi^+$  background works sufficiently well. As the  $\pi^- \pi^- \pi^+$  background  
 4133 is the largest background contribution to the  $K^- \pi^- \pi^+$  sample and as we treat other background  
 4134 contributions similarly (see sections 5.3 and 6.1.4), we expect that the RMF is able to separate  
 4135 resonance and non-resonant contributions from background contributions sufficiently well. As  
 4136 the results from the pseudodata studies for also the non-resonant components agree with the  
 4137 reference, we conclude that the RMF is able to separate well resonances from non-resonant  
 4138 contributions. We hence conclude from our pseudodata studies that our analysis scheme is able  
 4139 to reliably measure the resonance parameters of strange mesons decaying to the  $K^- \pi^- \pi^+$  final  
 4140 state.

<sup>[ao]</sup> Also, the magnitude of the non-resonant component is small for  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$ . However, the non-resonant component is coherently added to the resonance component (see section 6.1.2), while the  $\pi^- \pi^- \pi^+$  and effective background components are added incoherently. Hence, even the small non-resonant component can significantly contribute to the total model intensity via its interference terms with the large resonance components. These contributions of the non-resonant components can be seen by the difference between the total model (red curve) and the resonance components (blue curves).

## 4141 7 Results for Selected Partial Waves

4142 In the previous chapters, we have discussed the main stages of our analysis starting from the  
4143 measurement of the data sets (see chapter 2), over the selection of  $K^-\pi^-\pi^+$  event candidates  
4144 (see chapters 3 and 4), and over the partial-wave decomposition using the 238-wave set (see  
4145 chapter 5), up to the resonance-model fit of 10 selected partial waves (see chapter 6). We  
4146 performed extensive systematic and pseudodata studies (see sections 5.7, 5.8, 5.10, 6.3, and 6.4)  
4147 to verify the robustness and reliability of our analysis results. All of this allows us to finally  
4148 interpret the results in terms of physics signals, i.e. strange-meson resonances appearing in the  
4149  $K^-\pi^-\pi^+$  final state, to measure their masses and widths, and to compare our results to previous  
4150 measurements.

4151 In sections 7.1 to 7.4, we discuss the results for partial waves with  $J^P = 1^+, 2^+, 4^+$ , and  $2^-$ ;  
4152 i.e. with  $J^P$  quantum numbers of the waves included in the well-studied 10-wave RMF. If not  
4153 explicitly stated differently, we show data from the first  $t'$  bin or show  $t'$ -summed distributions to  
4154 exemplarily represent our results. Our estimates for the masses and widths of these resonances  
4155 are summarized in table 6.2. In table 6.2 and in the following, the first quoted uncertainties are  
4156 statistical, the second systematic uncertainties. The quoted systematic uncertainties determined  
4157 from a limited set of performed systematic studies represent only a lower limit on the actual  
4158 systematic uncertainties (see section 6.3). In sections 7.5 to 7.8, we discuss the results for further  
4159 partial waves with  $J^P = 3^-, 0^-, 3^+$ , and  $4^-$ . In order to study a possible resonance content of  
4160 these waves, we performed extended RMFs, where we added selected waves from these  $J^P$   
4161 sectors to the 10-wave RMF model. However, these extended RMFs are not as well studied as  
4162 the 10-wave RMF. Hence, their results must be interpreted as a first attempt to also study signals  
4163 in these waves, and we only quote rough values for our estimates on the corresponding resonance  
4164 parameters rounded to a precision of  $10 \text{ MeV}/c^2$  without giving the uncertainties. The technical  
4165 details of the extended RMFs are summarized in appendix E.2. In section 7.9, we discuss further  
4166 interesting results from the PWD.

### 4167 7.1 $J^P = 1^+$ Partial Waves

4168 The blue data points in figure 7.1a show the measured intensity spectrum of the  $1^+ 0^+ \rho(770) K S$   
4169 wave in the lowest  $t'$  bin as obtained from the 238-wave PWD. The spectrum exhibits a clear peak  
4170 at about  $1.3 \text{ GeV}/c^2$ . The RMF describes this peak using dominantly the  $K_1(1270)$  component  
4171 (blue curve) with a mass of  $(1267.7 \pm 1.9_{-4.5}^{+1.6}) \text{ MeV}/c^2$  and a width of  $(83 \pm 4_{-4}^{+15}) \text{ MeV}/c^2$ . The

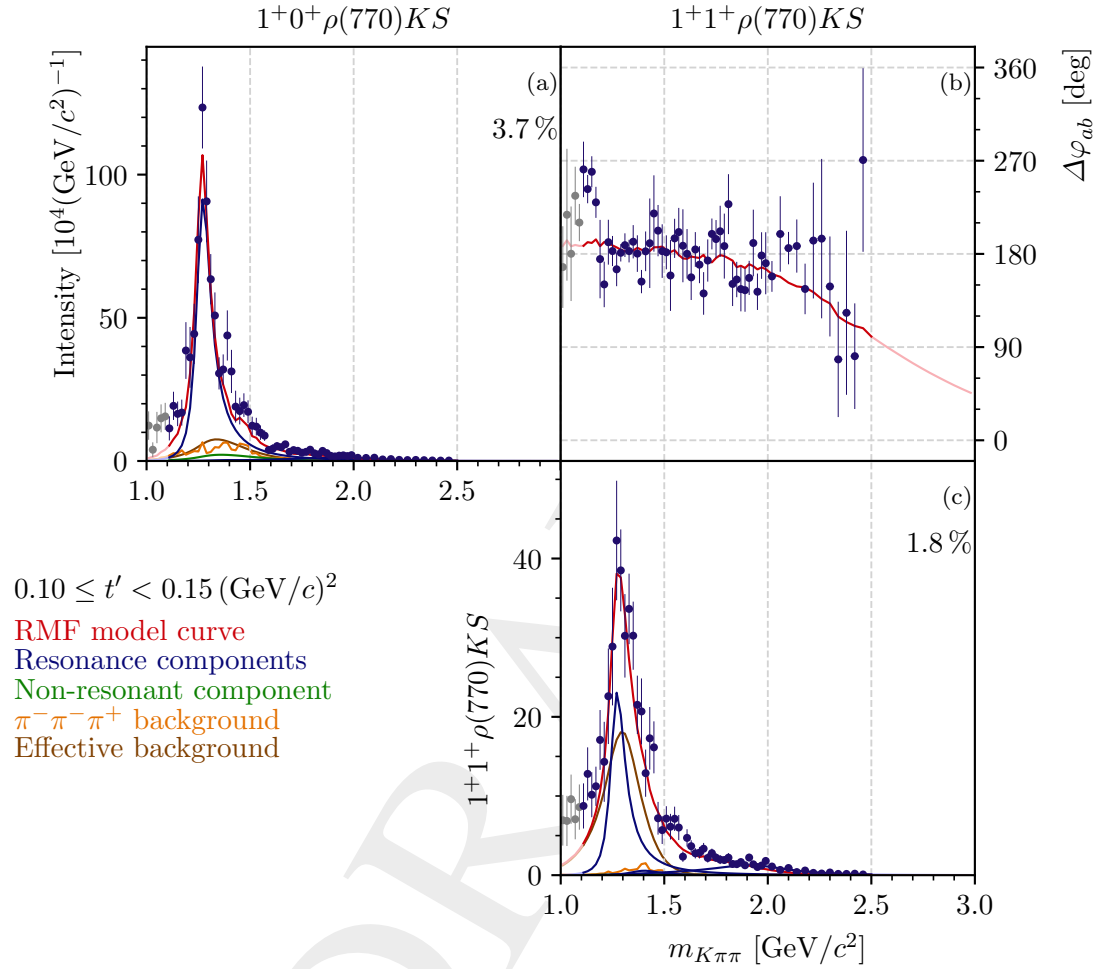


Figure 7.1: Representation of the Spin-density matrix in the lowest  $t'$  bin of the two waves with  $J^P = 1^+$  that were included in the 10-wave RMF. The figures on the diagonal show the intensity spectra. The off-diagonal figure shows the relative phase as defined in equation (5.74).<sup>[c]</sup> It represents the off-diagonal element of the spin-density matrix, i.e. the interference term between the two waves. The blue data points represent the measured spin-density matrix elements. The curves represent the result of the 10-wave RMF. The red curves represent the total RMF model. The blue curves represent the individual resonance components, the green curves the non-resonant components, the orange curves the  $\pi^-\pi^-\pi^+$  background components, and the brown curves the effective background components. The extrapolations beyond the  $m_{K\pi\pi}$  fit ranges are shown in lighter colors. The corresponding data points are shown in gray. The percentages given in the graphics showing intensity spectra give the relative intensity as defined in equation (5.76).

4172 RMF yielded only a small intensity for the  $K_1(1400)$  component, with a peak reaching about  $10^4$   
 4173 produced events per  $\text{GeV}/c^2$  as shown in figure 7.2a. Leaving the resonance parameters of the  
 4174  $K_1(1400)$  component free in the RMF as done in systematic study **C** or removing the  $K_1(1400)$   
 4175 component from the RMF model as done in systematic study **D** has only small effects on the other  
 4176 resonance parameters (see table 6.4).<sup>[a]</sup> All of these effects are similar in size or smaller than  
 4177 other systematic effects. Hence, using fixed resonance parameters for the  $K_1(1400)$  component  
 4178 does not significantly bias the results of our analysis.

4179 The intensity spectrum of the  $1^+ 0^+ \rho(770) K S$  wave exhibits a shoulder at about  $1.5 \text{ GeV}/c^2$ ,  
 4180 which is clearly seen in the  $t'$ -summed intensity spectrum in figure 7.2a. This shoulder is too  
 4181 high in  $m_{K\pi\pi}$  in order to arise from the  $K_1(1400)$  resonance. Also, the RMF does not use the  $K'_1$   
 4182 component (see table 6.1) to describe it. Even in an additional study where we added another  
 4183 resonance component to the RMF model that was dedicated to describe the  $1.5 \text{ GeV}/c^2$  shoulder,  
 4184 it was not described by any resonance component. Hence, this shoulder is not consistent with  
 4185 a Breit-Wigner resonance. Also, we observe no phase motion that would be consistent with  
 4186 a resonance at  $1.5 \text{ GeV}/c^2$ . Overall, the non-resonant (green curve), the  $\pi^-\pi^-\pi^+$  background  
 4187 (orange curve), and the effective background components contribute only little to the total RMF  
 4188 model intensity (red curve). The intensity spectrum of the  $1^+ 0^+ \rho(770) K S$  wave exhibits a  
 4189 small, broader shoulder at  $m_{K\pi\pi} \approx 1.9 \text{ GeV}/c^2$  as shown in figure 7.2a. The RMF describes this  
 4190 shoulder by a dominant contribution of the  $K'_1$  component with a mass of  $(1940 \pm 10^{+90}_{-70}) \text{ MeV}/c^2$   
 4191 and a width of  $(462 \pm 22^{+27}_{-119}) \text{ MeV}/c^2$ .

4192 We also included the  $1^+ 1^+ \rho(770) K S$  wave in the 10-wave RMF, i.e. a wave with the same  
 4193 quantum numbers and decay mode, except for the spin-projection which is  $M = 1$ . The  $M = 1$   
 4194 wave has about half the intensity of the  $M = 0$  wave. Figure 7.1c shows the intensity spectrum  
 4195 of this wave in the lowest  $t'$  bin. It exhibits the same narrow peak as the intensity spectrum  
 4196 of the  $M = 0$  wave. As for the  $M = 0$  wave, the peak in the  $M = 1$  wave is described  
 4197 by a large contribution of the  $K_1(1270)$  component.<sup>[b]</sup> Figure 7.1b shows the relative phase  
 4198 between the  $1^+ 0^+ \rho(770) K S$  wave and the  $1^+ 1^+ \rho(770) K S$  wave.<sup>[c]</sup> It is practically constant  
 4199 for  $m_{K\pi\pi} \gtrsim 1.2 \text{ GeV}/c^2$  with a phase difference of about  $180^\circ$ . Interpreting this relative phase as  
 4200 the phase difference between the corresponding transition amplitudes of the coherent process  
 4201  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  [see equation (5.75)], this means that the amplitudes of both waves have  
 4202 the same phase motion, but opposite sign. It is expected that the amplitudes of both waves have  
 4203 the same phase motion as both waves are dominated by the same  $K_1(1270)$  resonance. Below  
 4204  $1.2 \text{ GeV}/c^2$  the relative phase is larger than  $180^\circ$ . This may be caused by the enhanced low-mass  
 4205 tail in both waves, which we assume to be analysis artifacts. Compared to the  $1^+ 0^+ \rho(770) K S$   
 4206 wave, the  $1^+ 1^+ \rho(770) K S$  wave exhibits a more pronounced high-mass tail, which is described  
 4207 in the RMF mainly by the  $K'_1$  component.

<sup>[a]</sup> In study **C**, the largest effect is that the  $K'_1$  becomes about  $30 \text{ MeV}/c^2$  lighter. In study **D**, the largest effects are that the  $K_1(1270)$  becomes about  $4 \text{ MeV}/c^2$  lighter and the  $K_2^*(1430)$  becomes about  $6 \text{ MeV}/c^2$  broader.

<sup>[b]</sup> We use the same  $K_1(1270)$  component in the  $M = 0$  and  $M = 1$  waves with the same mass and width parameters.

<sup>[c]</sup> In contrast to other figures of relative phases, which show the phase in the range  $-180 \leq \Delta\varphi_{ab}(m_{K\pi\pi}, t') < 180^\circ$ , we chose in figure 7.1b the range  $0 \leq \Delta\varphi_{ab}(m_{K\pi\pi}, t') < 360^\circ$  in order to better visualize the phase offset between the two  $1^+$  waves.

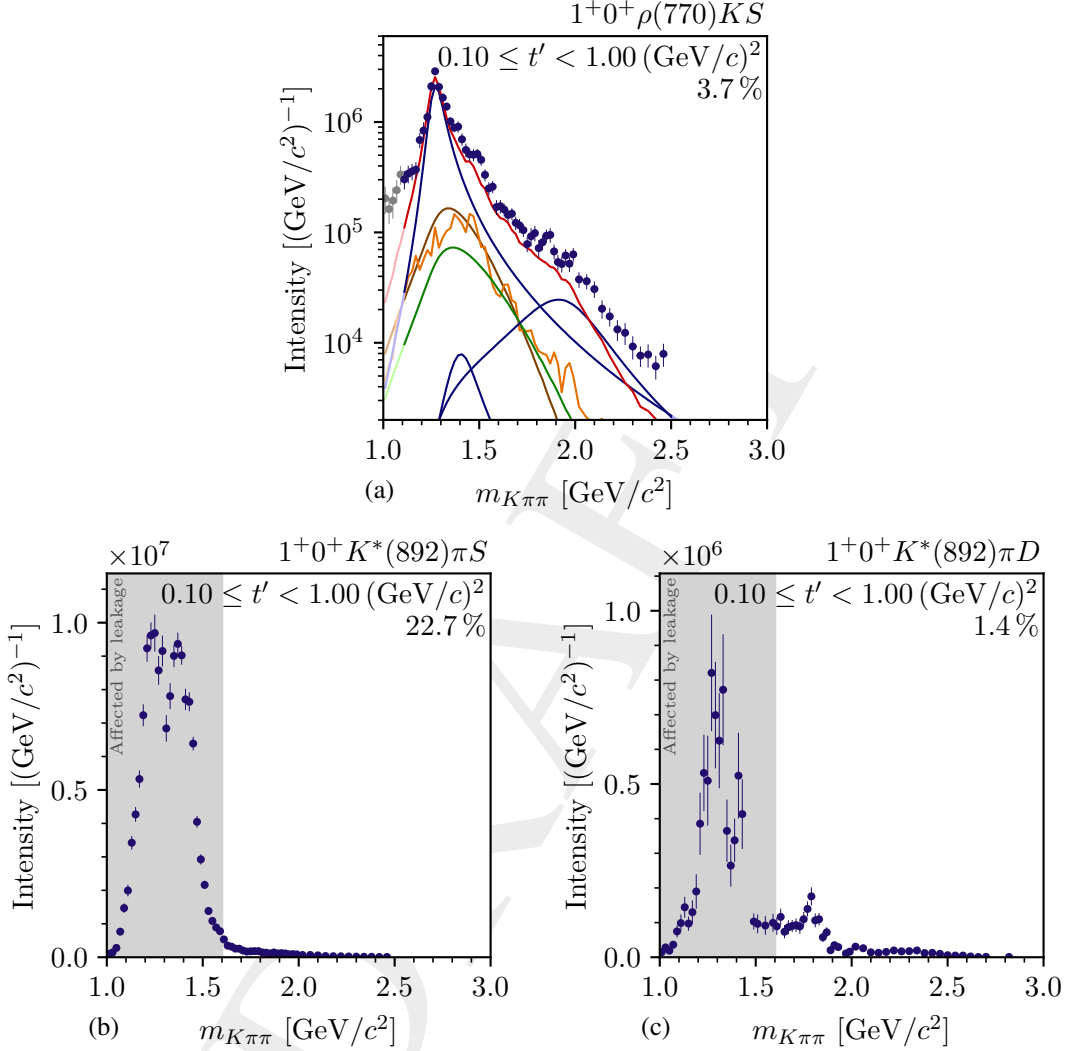


Figure 7.2:  $t'$ -summed intensity spectra of (a) the  $1^+0^+ \rho(770)KS$  wave in log-scale, (b) the  $1^+0^+ K^*(892)\pi S$  wave, and (c) the  $1^+0^+ K^*(892)\pi D$  wave. The blue data points represent the measured intensities. The gray shaded area indicates the  $m_{K\pi\pi}$  range affected by the leakage effect (see section 5.9). The percentages give the relative intensity as defined in equation (5.76). The curves in (a) represent the result of the 10-wave RMF. The red curve represents the total RMF model. The blue curves represent the individual resonance components, the green curve the non-resonant component, the orange curve the  $\pi^-\pi^-\pi^+$  background component, and the brown curve the effective background component. The extrapolations beyond the  $m_{K\pi\pi}$  fit ranges are shown in lighter colors. The corresponding data points are shown in gray.



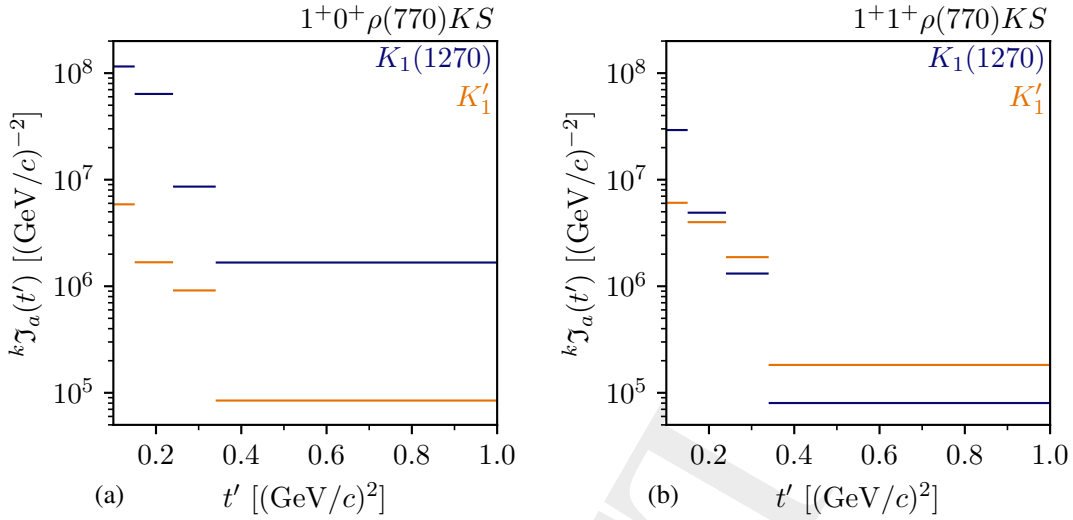


Figure 7.3:  $t'$  spectra of the  $K_1(1270)$  (blue bars) and the  $K_1'$  (orange bars) components (a) in the  $1^+ 0^+ \rho(770) K S$  wave and (b) in the  $1^+ 1^+ \rho(770) K S$  wave as obtained from the 10-wave RMF. The horizontal bars represent the intensity in each  $t'$  bin according to equation (6.28). The blue bars in (a) are the same as in figure 6.5.

4208 The RMF yields a large effective background component (brown curve) for the  $1^+ 1^+ \rho(770) K S$   
 4209 wave that peaks at a slightly higher mass than the  $K_1(1270)$  component. In general, we do not  
 4210 expect such large and peaking background contributions. In a study, where we excluded such a  
 4211 peaking shape for the effective background component by using a more restrictive the parameter  
 4212 limit of the corresponding shape parameter yielded a parameter value at the more restrictive  
 4213 parameter limit. Hence, there is no fit solution without such a peaking effective background  
 4214 component. Furthermore, in this study the RMF was not able to describe the intensity spectrum  
 4215 of the  $1^+ 1^+ \rho(770) K S$  wave sufficiently well. We studied this peaking effective background  
 4216 component also using the 10-wave pseudodata that do not contain background contributions (see  
 4217 section 6.4).<sup>[d]</sup> Thus, the effective background component in RMFs to this pseudodata sample is  
 4218 expected to be small. Indeed, we find practically zero contribution from the effective background  
 4219 component to the  $1^+ 1^+ \rho(770) K S$  wave in all pseudodata studies. In particular, the RMFs did  
 4220 not yield any peaking effective background. Hence, we conclude that the peaking effective  
 4221 background component that we observe in the measured data is driven by the data and not by the  
 4222 construction of the RMF model. Therefore, it is needed in the RMF in order to describe the data.  
 4223 However, the fact that we need such unexpected component in order to describe the data points  
 4224 towards the limitations of the Breit-Wigner RMF model employed in our analysis.

4225 Figure 7.3 shows the  $t'$  spectra as defined in equation (6.28) for the  $K_1(1270)$  and  $K_1'$  components  
 4226 in the two  $1^+$  waves. In the  $1^+ 0^+ \rho(770) K S$  wave, both components show an approximately  
 4227 an exponential  $t'$  dependence, as expected. The  $t'$ -dependencies of the resonance components  
 4228 are independent in the  $1^+ 0^+ \rho(770) K S$  and  $1^+ 1^+ \rho(770) K S$  waves. The  $K_1'$  component in the

<sup>[d]</sup> In some studies, we admixed  $\pi^- \pi^+ \pi^+$  background events to the 10-wave pseudodata sample. However, these contributions should be accounted for by the  $\pi^- \pi^+ \pi^+$  background component in the RMF.

4229  $1^+ 1^+ \rho(770) K S$  wave (orange bars in figure 7.3b) shows an approximately exponential  $t'$  shape,  
 4230 which flattens towards  $t' = 0.1 \text{ (GeV}/c)^2$  as mainly seen in the lowest  $t'$  bin. This flattening  
 4231 is expected for an  $M = 1$  wave due to the additional  $(t')^{|M|}$  factor as given in equation (6.29).  
 4232 However, the  $K_1(1270)$  component in the  $M = 1$  wave exhibits no flattening for the approximately  
 4233 exponential  $t'$  shape. In particular, in the lowest  $t'$  bin, the intensity of the  $K_1(1270)$  component is  
 4234 much larger than expected. A reason for this may be that the RMF cannot reliably assign intensity  
 4235 to the  $K_1(1270)$  component due to its interplay with the peaking effective background component  
 4236 in this  $t'$  bin. In summary, our observation that the  $t'$  dependencies of the resonance components,  
 4237 except for the  $K_1(1270)$  component in the lowest  $t'$  bin of the  $M = 1$  wave, follow the expected  
 4238 shape is another indication for a reliable extraction of the  $K_1(1270)$  and  $K'_1$  contribution to the  
 4239 data in the RMF.

4240 We observe structures also in other waves with  $J^P = 1^+$  that were not included in the 10-wave  
 4241 RMF, for example, in the  $1^+ 0^+ K^*(892) \pi S$  wave, which is the largest wave in our wave set.<sup>[e]</sup>  
 4242 Its intensity spectrum is shown in figure 7.2b. It exhibits a clear double-peak in the  $m_{K\pi\pi}$  region  
 4243 of the  $K_1(1270)$  and  $K_1(1400)$  resonances, as expected. We observed this double peak already  
 4244 in the measured  $m_{K\pi\pi}$  spectrum shown in figure 4.6a. However, the  $1^+ 0^+ K^*(892) \pi S$  wave is  
 4245 strongly affected by the leakage effect for  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$ . This prevents us from interpreting  
 4246 the observed structures on a quantitative level.

4247 Figure 7.2c shows the intensity spectrum of the  $1^+ 0^+ K^*(892) \pi D$  wave. The low- $m_{K\pi\pi}$  region  
 4248 of also this wave is affected by the leakage effect. It exhibits a broad enhancement at about  
 4249  $1.3 \text{ GeV}/c^2$  that is very jumpy and that is strongly biased by the leakage effect. Also, we observe  
 4250 a peak at about  $1.8 \text{ GeV}/c^2$  that may arise from the  $K'_1$  resonance. As this wave is also affected  
 4251 by the leakage effect, we did not include it in the RMF.

### 4252 7.1.1 Discussion

4253 The PDG [9] lists three strange mesons with  $1^+$  quantum numbers; i.e. the well-established  
 4254  $K_1(1270)$  and  $K_1(1400)$ ,<sup>[f]</sup> and an excited  $K_1(1650)$  that was just recently marked as an established  
 4255 state. The PDG averages for their masses and widths are shown by the blue, red, and green stars,  
 4256 respectively, in figure 7.4.

<sup>[e]</sup> As discussed in section 5.9.1, the intensities of leakage waves are overestimated by potentially more than a factor two due the leakage effect. Hence, the relative intensities of leakage waves cannot be directly compared to those of other waves, especially to those of non-leakage waves. However, the relative intensity of the  $1^+ 0^+ K^*(892) \pi S$  of about 22.7 % is significantly larger than the 10.7 % of the second-largest leakage wave, which is the  $0^- 0^+ K^*(892) \pi P$  wave, and is much larger than the relative intensity of 3.7 % of the largest non-leakage wave, which is the  $1^+ 0^+ \rho(770) K S$  wave. Hence, we can reliably state that the  $1^+ 0^+ K^*(892) \pi S$  wave is the largest wave in our wave set.

<sup>[f]</sup> In the quark-model picture, there is a spin-triplet and a spin-singlet SU(3)-nonet for states with  $J^P = 1^+$  and an orbital angular momentum of  $L = 1$  in the  $q\bar{q}'$  system. The  $K_1(1270)$  and  $K_1(1400)$  states are assumed to be mixtures of these two SU(3) eigenstates [144].

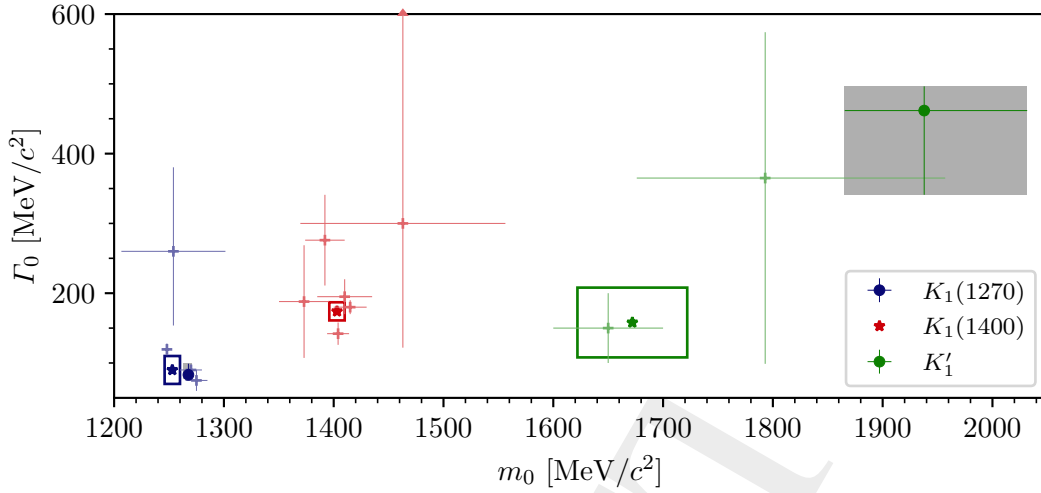


Figure 7.4: Masses  $m_0$  and widths  $\Gamma_0$  of  $K_1$  resonances. The dots represent the parameter values as obtained from the 10-wave RMF and listed in table 6.2. The thin error bars and gray boxes around the dots indicate our estimates for the total uncertainties, which we calculated by quadratically adding the statistical uncertainties to the corresponding upper and lower systematic uncertainties. One should note that the systematic uncertainties given in this work are only a lower limit on the actual systematic uncertainties (see section 6.3). The stars and colored boxes represent the PDG average values and their uncertainties, respectively [9]. The pluses in lighter color represent the central values of all previous measurements that entered the PDG averages for  $m_0$  and  $\Gamma_0$ . The error bars represent the corresponding total uncertainties calculated by quadratically adding the statistical uncertainties to the corresponding upper and lower systematic uncertainties, if given. Uncertainties that are larger than the shown  $m_0$  and  $\Gamma_0$  ranges are indicated by an arrowhead at the figure frame. In the 10-wave RMF we fixed the resonance parameters of the  $K_1(1400)$  component to the corresponding PDG average values.

#### 4257 The $K_1(1270)$

4258 Our estimate for the width of the  $K_1(1270)$  agrees well with the PDG average value, while our  
 4259 estimate for its mass is slightly larger. However, also previous measurements of the  $K_1(1270)$   
 4260 (blue pluses in figure 7.4) cluster mainly around two values for its resonance parameters. There  
 4261 is a high-mass cluster of measurements of a mass above about 1270 MeV/ $c^2$  [23, 26, 145, 146].  
 4262 Many of these measurements also yielded a small width below 100 MeV/ $c^2$ .<sup>[g]</sup> There is also a  
 4263 low-mass cluster of measurements of a mass below about 1250 MeV/ $c^2$  [27, 29, 147]. All of  
 4264 these measurements of a lower mass also yielded a large width above 100 MeV/ $c^2$ .

4265 Among the four previous measurements that entered the PDG average for the  $K_1(1270)$  resonance  
 4266 parameters, our estimates for the  $K_1(1270)$  parameters agree well with those from ref. [145],  
 4267 who measured the  $K_1(1270)$  resonance parameters from its decay to the  $\rho(770) K$  final state  
 4268 only, as in this analysis, and with those from the ACCMOR analysis [23]. Compared to our

<sup>[g]</sup> There are several previous measurements that are excluded from the PDG average, which yielded a mass above 1270 MeV/ $c^2$ , but a width above 100 MeV/ $c^2$ .

4269 analysis, ACCMOR formulated a more elaborate resonance model based on a  $K$ -matrix approach  
 4270 including two resonances and six decay channels, which they fitted simultaneously to the partial  
 4271 waves representing the  $K^*(892)\pi S$ ,  $\rho(770)KS$ ,  $K_0^*\pi P$ ,  $f_0KP$ , and  $K^*(892)\pi D$  decays.<sup>[h]</sup> The  
 4272 good agreement between the ACCMOR analysis and our results validates the application of our  
 4273 Breit-Wigner RMF model.

4274 The measurement of the  $K_1(1270)$  resonance parameters in the reaction  $\tau^- \rightarrow K^-\pi^-\pi^+\nu_\tau$  by  
 4275 CLEOII in ref. [29] yielded the largest value of all previous measurements for the width of  
 4276  $\Gamma_0 = (260_{-70}^{+90}(\text{stat.}) \pm 80(\text{sys.}))\text{MeV}/c^2$ . Even considering its large uncertainty this value is  
 4277 clearly larger than the PDG average and our estimate for the  $K_1(1270)$  width. The CLEO value  
 4278 is the result of a limited<sup>[i]</sup> Dalitz-plot analysis with a series of assumptions. The authors did not  
 4279 allow for a relative phase offset between the different resonance components, i.e. their coupling  
 4280 amplitudes were fixed to be real, which may not be the case. For example, in the COMPASS  
 4281  $\pi^-\pi^-\pi^+$  analysis a phase offset of about  $180^\circ$  was found between many ground and excited  
 4282 states [41]. Furthermore, they fixed the branching fraction ratio of  $K_1(1270) \rightarrow K^*(892)\pi$  and  
 4283  $K_1(1270) \rightarrow \rho(770)K$  to the corresponding PDG average value. Finally, contributions from  
 4284 pseudoscalar resonances in the  $K^-\pi^-\pi^+$  system were neglected, while the  $\tau^-$  may also decay  
 4285 to excited pseudoscalar kaons that further decay to  $K^-\pi^-\pi^+$  [81]. For example, the  $\tau^-$  has a  
 4286 similar branching fraction to decay to the pseudo-scalar ground state, i.e. to  $K^-\nu_\tau$ , (6.96%) and  
 4287 to  $K^-\pi^-\pi^+\nu_\tau$  (3.45%) [9]. All these potentially coarse assumptions may bias the resonance  
 4288 parameter estimates of ref. [29].

4289 The Belle collaboration [27] performed a recent analysis of the decay  $B^+ \rightarrow J/\psi K^+\pi^+\pi^-$ , which  
 4290 allowed them to study the  $K_1(1270)$  in the  $\rho(770)K$  and  $K^*(892)\pi$  decays. They obtained very  
 4291 precise and accurate resonance parameters of  $m_0 = (1248.1 \pm 3.3(\text{stat.}) \pm 1.4(\text{sys.}))\text{MeV}/c^2$   
 4292 and  $\Gamma_0 = (119.5 \pm 5.2(\text{stat.}) \pm 6.7(\text{sys.}))\text{MeV}/c^2$ . Their estimate for the mass is slightly smaller  
 4293 and their estimate for the width is slightly larger than the PDG average values and then our  
 4294 estimates. However, they fitted the resonance parameters of only the  $K_1(1270)$ . The resonance  
 4295 parameters of the other states included in the fit were fixed to the corresponding PDG averages,  
 4296 which for some have large uncertainties. Furthermore, they did not include an excited  $K_1'$  that  
 4297 may contribute to the  $1^+$  waves. All of these effects may bias their measurement for the  $K_1(1270)$   
 4298 parameters. However, they did not consider any of these effects when determining the systematic  
 4299 uncertainties. Hence, the uncertainties in ref. [27] may be underestimated. In our analysis, we  
 4300 considered more ground and excited states as in the Belle analysis. As discussed in section 6.3,  
 4301 we also give a first estimate of systematic uncertainties that may arise from excluding certain  
 4302 model components and from fixing resonance parameters to their PDG averages. Considering the  
 4303 good agreement of our measurement with the results from refs. [23, 145] and the caveats of the  
 4304 measurements in refs. [27, 29], the two clusters of measured values of the  $K_1(1270)$  resonance  
 4305 parameters may be a pure measurement effect enhanced by underestimated uncertainties.

<sup>[h]</sup> ACCMOR used an  $S$ -wave  $\pi\pi$  scattering amplitude to parameterize the  $f_0$  isobar and a Breit-Wigner amplitude with  $m_0 = 1250\text{MeV}/c^2$  and  $\Gamma_0 = 600\text{MeV}/c^2$  to parameterize the  $K_0^*$  isobar. Both parameterizations approximate the corresponding physical amplitudes only roughly (see section 5.1.4).

<sup>[i]</sup> In ref. [29], only the  $m_{K\pi\pi}$ , the  $m_{K^-\pi^+}$ , and the  $m_{\pi^-\pi^+}$  mass spectra were fitted. This was sufficient to determine the  $K_1(12700)$  contribution as they assumed that the  $K^-\pi^-\pi^+$  system consists only of axial-vector states.

4306 The authors of ref. [144] suggested that the  $K_1(1270)$  is not a single state, but arises from two  
 4307 states, i.e. from two poles of the scattering amplitude in the complex plane of the squared energy.  
 4308 From the data of the ACCMOR analysis [23], ref. [144] determines a lighter and broader state  
 4309 at  $m_0 \approx 1200 \text{ MeV}/c^2$  and  $\Gamma_0 \approx 250 \text{ MeV}/c^2$  that couples stronger to the  $K^*(892) \pi$  decay;  
 4310 and a heavier and narrower state at  $m_0 \approx 1280 \text{ MeV}/c^2$  and  $\Gamma_0 \approx 150 \text{ MeV}/c^2$  that couples  
 4311 dominantly to the  $\rho(770) K$  decay. As different production mechanisms, which may prefer  
 4312 different  $K_1(1270)$  poles, were employed and different decay modes were studied in the various  
 4313 previous measurements, the two-pole model suggest in ref. [144] may explain the two clusters of  
 4314 previous measurements of the  $K_1(1270)$  resonance parameters. Our estimates for the  $K_1(1270)$   
 4315 resonance parameters are determined from waves with  $\rho(770) K$  decay mode only and agree with  
 4316 the cluster of heavier and narrow measurements. Hence, our data would fit into this two-pole  
 4317 scenario suggestion in ref. [144].

### 4318 The $K_1(1400)$

4319 The resonance parameters of the  $K_1(1400)$  are determined rather well from previous experiments  
 4320 (red data points in figure 7.4). As for the  $K_1(1270)$ , the measurement of the  $K_1(1400)$  width in the  
 4321 reaction  $\tau^- \rightarrow K^- \pi^- \pi^+ \nu_\tau$  by CLEOII [29] yielded the largest width of all previous measurements  
 4322 of  $(300^{+370}_{-110} \text{ (stat.)} \pm 140 \text{ (sys.)}) \text{ MeV}/c^2$ . This might indicate a systematic bias towards larger  
 4323 values for the widths in the analysis in ref. [29]. Still, their parameter estimates agree within the  
 4324 large uncertainties with the PDG average values.

4325 In our analysis, the  $K_1(1400)$  is only a small contribution in the two considered  $1^+$  waves. This  
 4326 is consistent with previous observations, e.g. the PDG lists a  $\rho(770) K$  branching fraction of only  
 4327  $(3.0 \pm 3.0) \%$  [9]. In the main analysis, we fixed the resonance parameters of the  $K_1(1400)$  to the  
 4328 corresponding PDG average values. In systematic study *C*, we allowed the  $K_1(1400)$  resonance  
 4329 parameters to float. Study *C* yielded a  $K_1(1400)$  width of  $178 \text{ MeV}/c^2$ , which is in good agree-  
 4330 ment with the PDG average value of  $(174 \pm 13) \text{ MeV}/c^2$ , and a  $K_1(1400)$  mass of  $1514 \text{ MeV}/c^2$ ,  
 4331 which is about  $100 \text{ MeV}/c^2$  larger than the PDG average value of  $(1403 \pm 7) \text{ MeV}/c^2$ . The larger  
 4332 mass of may be driven by the high-mass shoulder at about  $1.5 \text{ GeV}/c^2$ , which we observe on  
 4333 the  $1^+$  waves. Given the small size of the potential  $K_1(1400)$  signal in the two considered  $1^+$   
 4334 waves and the potentially large systematic uncertainties on the results of study *C*, we conclude  
 4335 that the PDG average values used in the main analysis for the resonance parameters of the  
 4336  $K_1(1400)$  are consistent with our data. More detailed conclusions on the  $K_1(1400)$  could only  
 4337 be drawn by studying the  $1^+ 0^+ K^*(892) \pi S$  wave, which exhibits a strong potential  $K_1(1400)$   
 4338 signal. Unfortunately, this is not possible with the COMPASS data as the  $1^+ 0^+ K^*(892) \pi S$   
 4339 wave is affected by the leakage effect.

4340 **Excited  $K_1$  States**

4341 The PDG lists a higher-lying  $K_1$  state called  $K_1(1650)$  with a mass of  $(1672 \pm 50) \text{ MeV}/c^2$  and a  
 4342 width of  $(158 \pm 50) \text{ MeV}/c^2$  [9]. It is much lighter and narrower than our parameter estimates  
 4343 for a potential excited  $K_1$ , which we called  $K'_1$ .

4344 The  $K_1(1650)$  has been studied in about 10 000 events of the reaction  $K^+ p \rightarrow \phi K^+ p$  at the CERN  
 4345 Omega spectrometer [24]. In their analysis, a model consisting of the sum of a Breit-Wigner  
 4346 amplitude and a non-resonant component was fitted to only the intensity spectrum of the  $1^+$  wave,  
 4347 which is shown in figure 7.5a.<sup>[j]</sup> This fit yielded a mass of  $(1650 \pm 50) \text{ MeV}/c^2$  and a width  
 4348 of  $(150 \pm 50) \text{ MeV}/c^2$ . It is not clear whether their uncertainty estimates include systematic  
 4349 uncertainties. Given the size of their data sample and the fact that they fitted their model to only  
 4350 one intensity spectrum, a combined statistical and systematic uncertainty of only  $\pm 50 \text{ MeV}/c^2$   
 4351 appears to be rather small, compared to the uncertainties in other [34] and in our analysis.

4352 Ref. [34] presents a recent analysis of 4289 events of the decay  $B^+ \rightarrow J/\psi \phi K^+$  by LHCb,<sup>[k]</sup>  
 4353 which allows them studying strange mesons in the  $\phi K$  subsystem. They performed a partial-wave  
 4354 analysis including resonances up to  $J = 2$  in the  $\phi K$  subsystem. In contrast to, e.g., the CLEO  
 4355 analysis [29], the resonance parameters of all considered resonances were free in the fit. Two  
 4356 excited  $K_1$  states,  $K(1^+)$  and  $K'(1^+)$ , were included in the analysis in ref. [34]. Unfortunately, the  
 4357 reaction  $B^+ \rightarrow J/\psi \phi K^+$  gives access to only a limited mass range of  $1.5 \lesssim m_{\phi K} \lesssim 2.2 \text{ GeV}/c^2$ .  
 4358 Some strange mesons have nominal masses just outside this mass range, e.g. the  $K_2^*(1430)$   
 4359 or the  $K_2(2250)$ . The parameters of such strange mesons cannot be determined given the  
 4360 limited  $m_{\phi K}$  range. Hence, such states were not included in the analysis in ref. [34]. However,  
 4361 their high- or low-mass tails still may contribute to the analyzed  $m_{\phi K}$  range. Thus, omitting  
 4362 strange mesons with nominal masses just outside the accessible mass range may bias the  
 4363 estimates of ref. [34] for the resonance parameters of the included resonances. In ref. [34], these  
 4364 effects were taken into account in the systematic uncertainties. In our analysis, we can access  
 4365 the full  $m_{K\pi\pi}$  range, which is one of the major advantages of using diffractive production to  
 4366 study strange mesons. Figure 7.5b shows the  $m_{\phi K}$  spectrum (black points) together with the  
 4367 contributions from the two  $K_1$  components. For the lighter state, LHCb measured a mass of  
 4368  $(1739 \pm 59 \text{ (stat.)}_{-101}^{+153} \text{ (sys.)}) \text{ MeV}/c^2$  and a width of  $(365 \pm 157 \text{ (stat.)}_{-215}^{+138} \text{ (sys.)}) \text{ MeV}/c^2$ . The  
 4369 PDG included this measurement in the average of the  $K_1(1650)$  parameters. However, due to  
 4370 its large uncertainties, it has only a minor influence on the PDG average values. Hence, the  
 4371 PDG average values for the  $K_1(1650)$  are mainly driven by the measurement from ref. [24].  
 4372 For the heavier state, LHCb measured a mass of  $(1968 \pm 65 \text{ (stat.)}_{-172}^{+70} \text{ (sys.)}) \text{ MeV}/c^2$  and a  
 4373 width of  $(396 \pm 170 \text{ (stat.)}_{-178}^{+174} \text{ (sys.)}) \text{ MeV}/c^2$ . This heavier state contributes less strongly to  
 4374 the reaction  $B^+ \rightarrow J/\psi \phi K^+$  and has a significance of only  $1.9\sigma$ . Recently, LHCb published an  
 4375 updated analysis of the reaction  $B^+ \rightarrow J/\psi \phi K^+$  based on a three times larger sample [149]. They  
 4376 obtained consistent parameters for both excited  $K_1$  states. However, owing to the larger sample,  
 4377 they had to include resonances with nominal masses outside their accessible mass range, but  
 4378 where the tails of these states enter their accessible mass range, as discussed above.

<sup>[j]</sup> Figure 7.5a shows the total  $J^P = 1^+$  intensity, i.e. summed over both helicity states of the  $\phi$  decay.

<sup>[k]</sup> A more detailed discussion and technical aspects of the analysis in ref. [34] can be found in ref. [148].

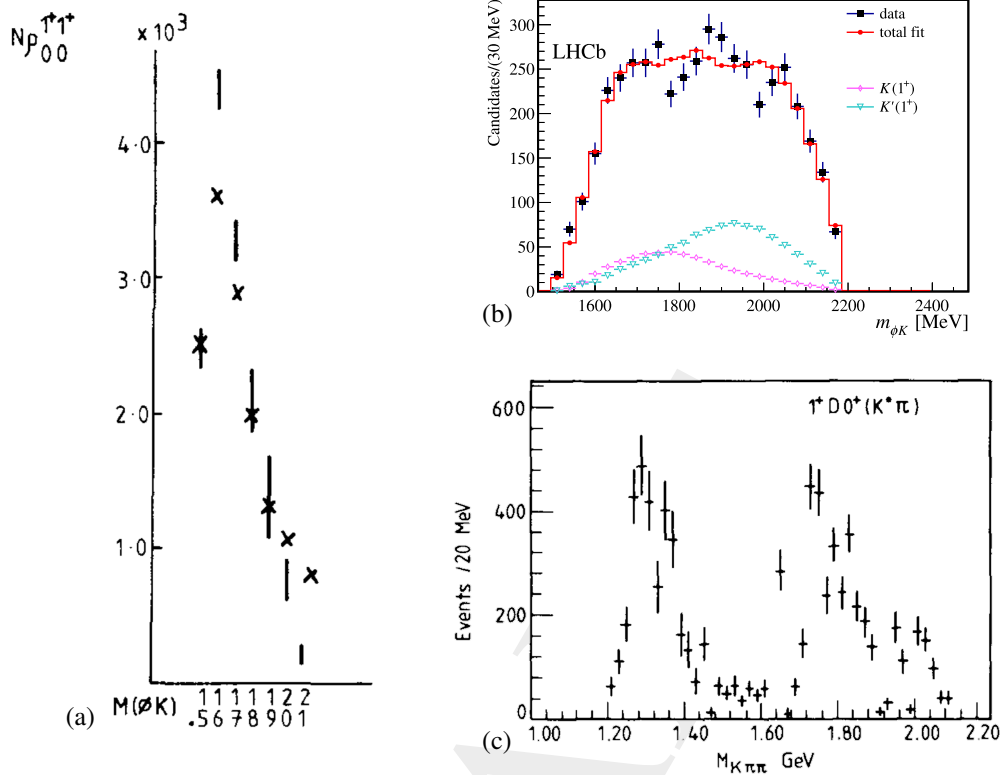


Figure 7.5: Previous studies of excited  $K_1$  states. (a) shows the intensity of the  $1^+$  partial wave (vertical lines) measured in the reaction  $K^+ p \rightarrow \phi K^+ p$  at the CERN Omega spectrometer [24]. The crosses represent the prediction of a model for the Deck process. (b) shows the invariant  $\phi K$  mass spectrum measured in the reaction  $B^+ \rightarrow J/\psi \phi K^+$  at LHCb [34]. The black data points represent the measured distribution. The red data points represent the total partial-wave model. The differently colored data points represent the contribution from the two model components representing  $K_1$  states. (c) shows the  $1^+ 0^+ K^*(892) \pi D$  wave as obtained in the ACCMOR analysis [23].

4379 Also, ACCMOR observed a potential signal with  $J^P = 1^+$  at about  $1800 \text{ MeV}/c^2$ , e.g. in the  
 4380  $1^+ 0^+ K^*(892) \pi D$  wave shown in figure 7.5c. However, they did not perform an RMF of this  
 4381 signal and hence did not determine its resonance parameters.

4382 Our parameter estimates for the  $K_1'$  component are consistent with both states considered by  
 4383 LHCb in ref. [34] and are closer to the central values of the higher-lying state. Our estimate for  
 4384 the  $K_1'$  mass is also consistent with the signal observed by ACCMOR in the  $1^+ 0^+ K^*(892) \pi D$   
 4385 wave. Furthermore, we observe a similar peak at about  $1.8 \text{ GeV}/c^2$  in this wave (see figure 7.2c).  
 4386 In summary, except for the measurement by the CERN Omega spectrometer in ref. [24], all  
 4387 previous measurements and also our measurement have indications for one or two excited  $K_1$   
 4388 states with a mass of about  $1800 \text{ MeV}/c^2$  or above. Only CERN Omega claims to have observed  
 4389 a much lighter state. As CERN Omega employed the same production mechanism as ACCMOR  
 4390 and as in our analysis, and as CERN Omega studied the same decay mode as the LHCb analysis,  
 4391 there is no clear reason why a different state may appear in the CERN Omega data. Given  
 4392 the limitations of the CERN Omega analysis, the excited  $K_1(1650)$  as listed by the PDG may

4393 actually be a state at about  $1800 \text{ MeV}/c^2$  or above, which would also be in agreement with the  
 4394 quark-model prediction from ref. [10] (see figure 1.1).

## 4395 7.2 $J^P = 2^+$ Partial Waves

4396 We included two waves with  $J^P = 2^+$  quantum numbers in the 10-wave RMF. The intensity  
 4397 spectrum of the first wave, the  $2^+ 1^+ K^*(892) \pi D$  wave, in the lowest  $t'$  bin is shown in figure 7.6a.  
 4398 It exhibits a clear peak at about  $1.4 \text{ GeV}/c^2$ . This peak is reproduced well by the RMF using, as  
 4399 expected, mainly the  $K_2^*(1430)$  component with a mass of  $(1430.1 \pm 1.5_{-2.0}^{+1.3}) \text{ MeV}/c^2$  and a width  
 4400 of  $(109 \pm 3_{-2}^{+6}) \text{ MeV}/c^2$ . We also find a small contribution of the effective background component  
 4401 in this wave.<sup>[1]</sup> The  $2^+ 1^+ K^*(892) \pi D$  wave also exhibits enhanced low- and high-mass tails,  
 4402 which are not reproduced well by the RMF as they are presumably driven by model artifacts.  
 4403 Hence, we excluded these  $m_{K\pi\pi}$  regions from the RMF. We do not find any other clear resonance  
 4404 signals, e.g. from excited  $K_2^*$  states, in the  $2^+ 1^+ K^*(892) \pi D$  wave.

4405 The second wave with  $J^P = 2^+$  that we included in the 10-wave RMF is the  $2^+ 1^+ \rho(770) K D$   
 4406 wave. Its intensity spectrum in the lowest  $t'$  bin is shown in figure 7.6d. The relative intensity  
 4407 of the  $2^+ 1^+ \rho(770) K D$  wave is about four times smaller than the one of the  $2^+ 1^+ K^*(892) \pi D$   
 4408 wave. Also the  $2^+ 1^+ \rho(770) K D$  wave exhibits a clear peak at about  $1.4 \text{ GeV}/c^2$ , which is  
 4409 reproduced well by the RMF using, as expected, mainly the  $K_2^*(1430)$  component. Compared to  
 4410 the  $2^+ 1^+ K^*(892) \pi D$  wave, we find more pronounced enhanced low- and high-mass tails. For  
 4411 such a small wave, it is expected that artifacts are relatively large. As discussed in section 6.2.2,  
 4412 the  $\pi^- \pi^- \pi^+$  background PWD predicts a large  $\pi^- \pi^- \pi^+$  background in the  $2^+ 1^+ \rho(770) K D$  wave.  
 4413 Given the consistent results we obtained from the systematic studies discussed in section 6.3 and  
 4414 especially from the pseudodata studies with and without admixed  $\pi^- \pi^- \pi^+$  background discussed  
 4415 in section 6.4, we conclude that we can reliably model the  $\pi^- \pi^- \pi^+$  background, and that it does  
 4416 not significantly bias our estimates for the resonance parameters. We do not find any other clear  
 4417 resonance signals, e.g. from excited  $K_2^*$  states, in the  $2^+ 1^+ \rho(770) K D$  wave.

4418 Figure 7.6b shows the relative phase between the  $2^+ 1^+ K^*(892) \pi D$  and the  $2^+ 1^+ \rho(770) K D$   
 4419 waves. As expected, it is almost constant, because both waves are dominated by the same  
 4420  $K_2^*(1430)$  resonance. We find a phase offset of about  $0^\circ$  between the two  $2^+$  waves, as typically  
 4421 observed for the same resonance in two partial waves. The remaining shallow phase motion  
 4422 observed in figure 7.6b may be caused by the different background contributions in both waves.

4423 Figure 7.6c shows the phase of the  $2^+ 1^+ K^*(892) \pi D$  wave relative to the  $1^+ 0^+ \rho(770) K S$  wave  
 4424 in the lowest  $t'$  bin. It exhibits a similar behaviour as in the second highest  $t'$  bin shown in

[1] In the  $2^+ 1^+ K^*(892) \pi D$  wave in figure 7.6a, the total model intensity (red curve) is similar to only the  $K_2^*(1430)$  component (blue curve), while there is also a non-negligible contribution from the effective background component (brown curve) in this wave. In fact, the  $K_2^*(1430)$  component and the non-resonant component (too small to be visible in figure 7.6a) interfere destructively in the peak region, such that the intensity  $\hat{\rho}_{aa}^{K\pi\pi}(m_{K\pi\pi}, t')$  of only the  $K^- \pi^- \pi^+$  part of the RMF model is smaller than the intensity of the total model.



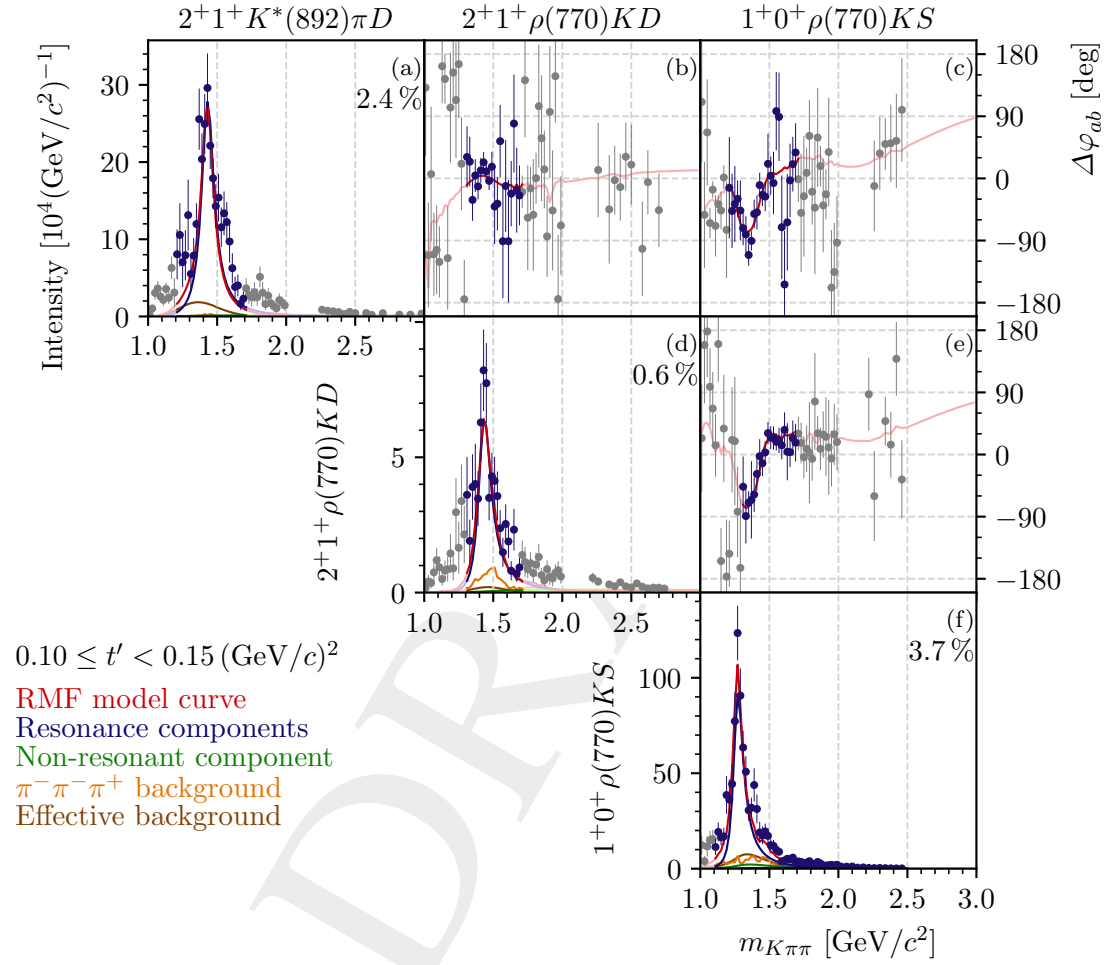


Figure 7.6: Same as figure 7.1, but for the two waves with  $J^P = 2^+$  that were included in the 10-wave RMF and the  $1^+0^+ \rho(770)KS$  wave serving as phase reference. The lowest  $t'$  bin is shown.

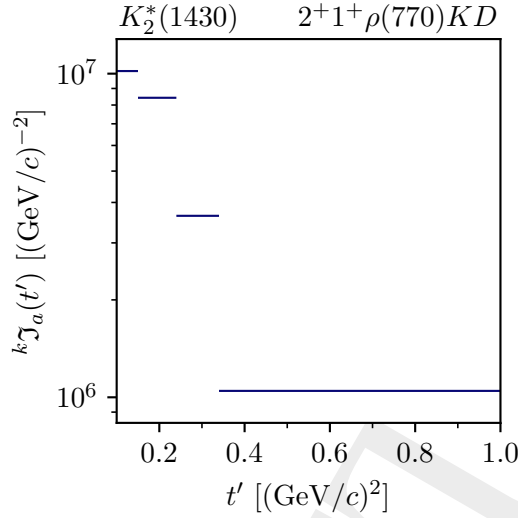


Figure 7.7: Same as figure 7.3, but for the  $K_2^*(1430)$  component in the  $2^+ 1^+ \rho(770) KD$  wave.

4425 figure 5.19: it first drops by about  $90^\circ$  around  $1.2 \text{ GeV}/c^2$  and then rises again by about  $90^\circ$   
 4426 around  $1.4 \text{ GeV}/c^2$ . Above about  $1.5 \text{ GeV}/c^2$  the relative phase is approximately constant. This  
 4427 phase motion is reproduced well by the RMF. The sharp drop of the phase is caused by the  
 4428  $K_1(1270)$  resonance in the  $1^+ 0^+ \rho(770) KS$  wave, which enters with a minus sign in the relative  
 4429 phase [see equation (5.74)]. The following rise of the phase is caused by the  $K_2^*(1430)$  resonance  
 4430 in the  $2^+ 1^+ K^*(892) \pi D$  wave. This rise is less sharp than the drop caused by the  $K_1(1270)$ ,  
 4431 which reflects the larger width of the  $K_2^*(1430)$  compared to the  $K_1(1270)$ . The phase of the  
 4432  $2^+ 1^+ \rho(770) KD$  wave relative to the  $1^+ 0^+ \rho(770) KS$  waves exhibits similar features as shown  
 4433 in figure 7.6e. In summary, we observe clear signals from the  $K_2^*(1430)$  and  $K_1(1270)$  not only  
 4434 in the intensity spectra, but also in the interferences terms represented by the relative phases.

4435 Figure 7.7 shows the  $t'$  spectrum of the  $K_2^*(1430)$  component. By construction, it is the same  
 4436 in both  $2^+$  waves up to a global factor [see equation (6.14)]. The  $t'$  spectrum of the  $K_2^*(1430)$   
 4437 exhibits an approximately exponential shape, which flattens towards  $t' = 0.1 (\text{GeV}/c)^2$ . As both  
 4438  $2^+$  waves have a spin-projection of  $M = 1$ , the shape of the  $t'$  spectrum qualitatively matches  
 4439 the expected shape for a resonance component as defined in equation (6.29). This is another  
 4440 indication for the reliable extraction of the  $K_2^*(1430)$  resonance by the RMF.

4441 Except for the  $2^+ 1^+ K^*(892) \pi D$  wave and the  $2^+ 1^+ K^*(892) \pi D$  wave, none of the five other  
 4442 waves with  $J^P = 2^+$  exhibit significant structures. They were included into the PWD model by  
 4443 the wave-set selection only in a few scattered  $(m_{K\pi\pi}, t')$  cells.

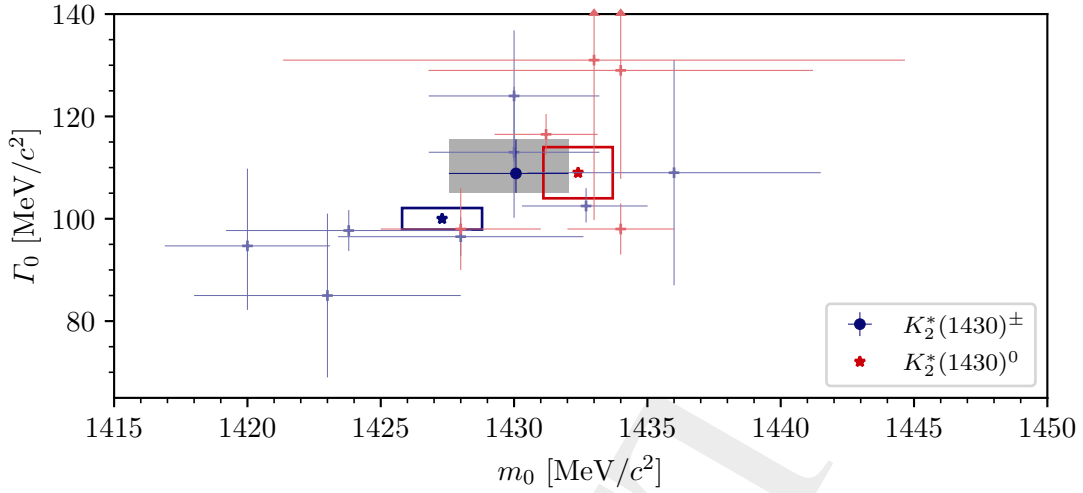


Figure 7.8: Same as figure 7.4, but showing in blue the resonance parameters of the charged  $K_2^*(1430)^\pm$  and in red the resonance parameters of the neutral  $K_2^*(1430)^0$ .<sup>[n]</sup>

## 4444 7.2.1 Discussion

4445 The PDG lists the measurements of the charged and of the neutral  $K_2^*(1430)$  separately. The  
 4446 blue and red stars with uncertainty boxes in figure 7.8 represent the PDG average values of  
 4447 the resonance parameters of the charged and neutral  $K_2^*(1430)$ , respectively. The mass and  
 4448 width values of the neutral  $K_2^*(1430)$  are slightly larger than those of the charged  $K_2^*(1430)$ .  
 4449 Our estimate for the mass of the charged  $K_2^*(1430)$  agrees with the PDG average value within  
 4450 uncertainties. However, our estimate for the width of the charged  $K_2^*(1430)$  is  $9 \text{ MeV}/c^2$  larger  
 4451 than the PDG average value, such that the corresponding uncertainty intervals do not overlap.<sup>[m]</sup>  
 4452 Interestingly, our estimate for the width of the charged  $K_2^*(1430)$  is in good agreement with the  
 4453 PDG average width value for the neutral  $K_2^*(1430)$ . Also, our mass estimate is in good agreement  
 4454 with the PDG average mass value for the neutral  $K_2^*(1430)$ .

4455 The individual measurements of the  $K_2^*(1430)$  parameters that entered the PDG averaging do  
 4456 not clearly group into two clusters of mass and width values, i.e. one for the charged and one  
 4457 for the neutral  $K_2^*(1430)$ .<sup>[n]</sup> Not only our measurement, but also other measurements of the  
 4458 charged  $K_2^*(1430)$  parameters (blue pluses in figure 7.8) yielded mass and width values that are  
 4459 in good agreement with the PDG average values for the neutral  $K_2^*(1430)$ . At the same time,  
 4460 the measurement of the neutral  $K_2^*(1430)$  in ref. [151] yielded mass and width values that are

<sup>[m]</sup> Here, we quadratically added our estimated for the statistical uncertainty to the lower systematic uncertainty.

<sup>[n]</sup> The measurement in ref. [150], which was included in the PDG average values for the neutral  $K_2^*(1430)$ , is not shown in figure 7.8 as it lies outside of the shown  $m_0$  region. It yielded a mass of  $(1471 \pm 12) \text{ MeV}/c^2$  that is much larger than the mass from any other measurement and a width of  $(143 \pm 34) \text{ MeV}/c^2$  that is among the largest values for the width from all previous measurements. The different values obtained in ref. [150] may be explained by the fact that they fitted their resonance model to only the intensity spectrum of only the  $2^+ 1^+ K^*(892) \pi D$  wave.

4461 in good agreement with the PDG average values for the charged  $K_2^*(1430)$ . However, a later  
 4462 measurement [97] of the same reaction performed by the same experiment as in ref. [151] yielded  
 4463 mass and width values that are in good agreement with the PDG average value for the neutral  
 4464  $K_2^*(1430)$ .

4465 Furthermore, the PDG considered for the averaging of the resonance parameters of the charged  
 4466  $K_2^*(1430)$  only measurements of its decay to the  $K\pi$  final state. For example, they did not consider  
 4467 the ACCMOR analysis [23], that measured the resonance parameters of the charged  $K_2^*(1430)$  in  
 4468 the  $K^-\pi^-\pi^+$  final state. Figures 7.9a and 7.9b show the intensity spectra of the  $2^+ 1^+ K^*(892)\pi D$   
 4469 and  $2^+ 1^+ \rho(770)KD$  waves, respectively, as obtained in the ACCMOR analysis in a  $t'$  range  
 4470 that is similar to our analyzed  $t'$  range. The intensity spectra exhibit the same peak at about  
 4471  $1.4 \text{ GeV}/c^2$  as in our analysis (see figures 7.9c and 7.9d). ACCMOR observed instabilities in  
 4472 the  $2^+ 1^+ K^*(892)\pi D$  wave for  $m_{K\pi\pi} \lesssim 1.3 \text{ GeV}/c^2$  [23], which are not present in our analysis.  
 4473 However, we observe an enhanced low-mass tail in the  $2^+ 1^+ \rho(770)KD$  wave below about  
 4474  $1.3 \text{ GeV}/c^2$ , which is not present in the ACCMOR analysis. Fitting a resonance model to the  
 4475 intensity spectra of both  $2^+$  waves and to their relative phases, ACCMOR obtained a mass of  
 4476  $1430 \text{ MeV}/c^2$  and a width of  $110 \text{ MeV}/c^2$  for the  $K_2^*(1430)$ . These values are nearly identical to  
 4477 those found by our analysis.

4478 In summary, the resonance parameters of the  $K_2^*(1430)$  as obtained in our analysis agree with  
 4479 many previous measurements. The PDG grouping of the measurements by the charge state of  
 4480 the  $K_2^*(1430)$  does not necessarily follow the clustering of the measured resonance parameters.  
 4481 The difference between the PDG average values of the resonance parameters of the charged and  
 4482 neutral  $K_2^*(1430)$  might have other reasons. A reason may be that for the averaging of the charged  
 4483  $K_2^*(1430)$  only measurements of the  $K\pi$  final state were considered, which may introduce a bias  
 4484 as Breit-Wigner parameters are not independent of the reaction.

### 4485 7.3 $J^P = 4^+$ Partial Waves

4486 Figures 7.10a and d show for the lowest  $t'$  bin the intensity spectra of the  $4^+ 1^+ K^*(892)\pi G$   
 4487 and  $4^+ 1^+ \rho(770)KG$  waves, respectively, which were included in the 10-wave RMF. Apart  
 4488 from these two waves, no other  $4^+$  waves exhibit clear resonance-like signals. The  $4^+ 1^+$   
 4489  $K^*(892)\pi G$  wave exhibits a peak at about  $2 \text{ GeV}/c^2$ . As discussed in section 6.2.2, the RMF  
 4490 model overall underestimates the intensity of the  $4^+ 1^+ K^*(892)\pi G$  wave, while the off-diagonal  
 4491 spin-density matrix elements for this wave are reproduced well by the RMF. The  $2 \text{ GeV}/c^2$   
 4492 peak is mainly described by the  $K_4^*(2045)$  component with a mass of  $(2059 \pm 6_{-1}^{+9}) \text{ MeV}/c^2$   
 4493 and a width of  $(188 \pm 11_{-18}^{+27}) \text{ MeV}/c^2$ . The  $K_4^*(2045)$  component sits on top of a broad bump  
 4494 from the effective background component. The non-resonant component is mainly used by the  
 4495 RMF to try to describe the enhanced intensity in the low-mass tail of the  $K_4^*(2045)$ . The non-  
 4496 resonant component contributes only little to the  $K_4^*(2045)$  mass region. The  $\pi^-\pi^-\pi^+$  background  
 4497 component does practically not contribute to the  $4^+ 1^+ K^*(892)\pi G$  wave.

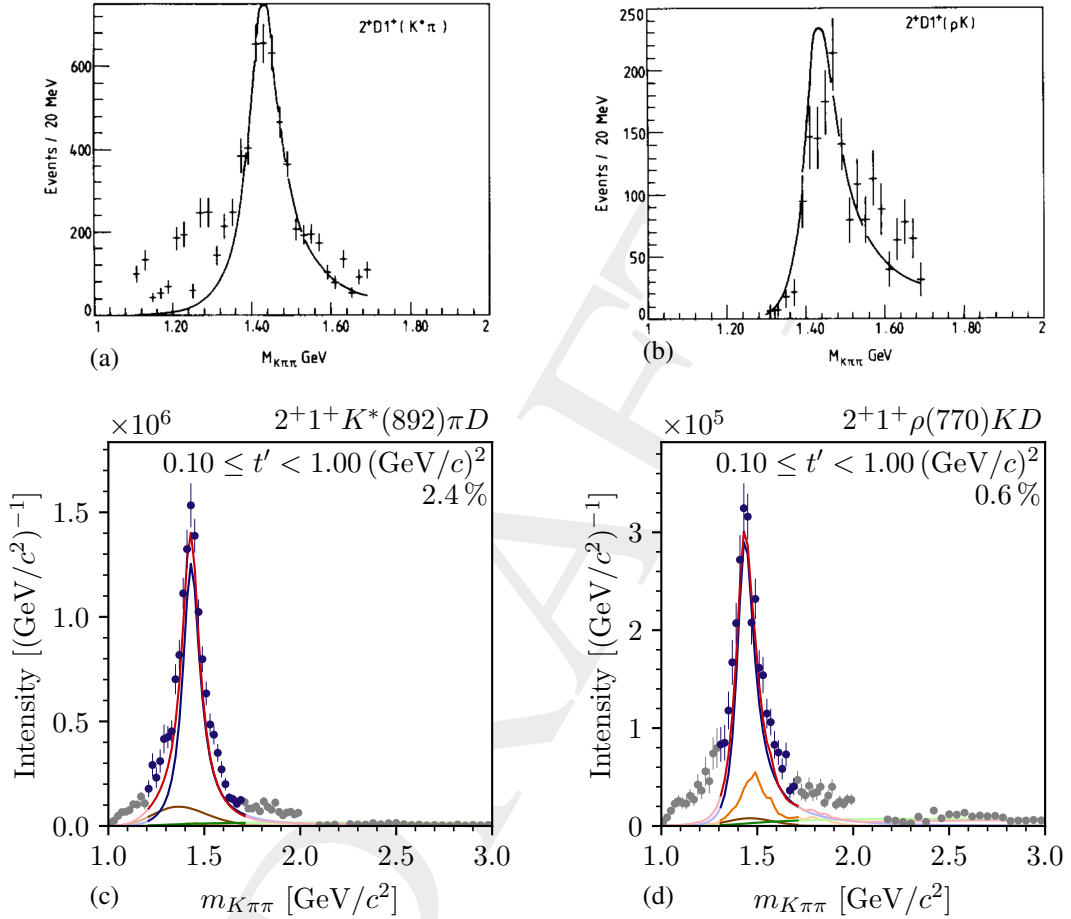


Figure 7.9: Intensity spectra of (left column) the  $2^+ 1^+ K^*(892) \pi D$  wave, and (right column) the  $2^+ 1^+ \rho(770) K D$  wave. The top row shows the results as obtained in the ACCMOR analysis in the range  $0.05 \leq t' \leq 0.7 \text{ (GeV/c)}^2$  [23]. The data points represent the results of the PWD. The curves represent the total resonance model from the ACCMOR analysis. The bottom row shows the results obtained in our analysis in the range  $0.1 \leq t' < 1.0 \text{ (GeV/c)}^2$ . Note the different mass scales of the plots. Same color code as in figure 7.2.

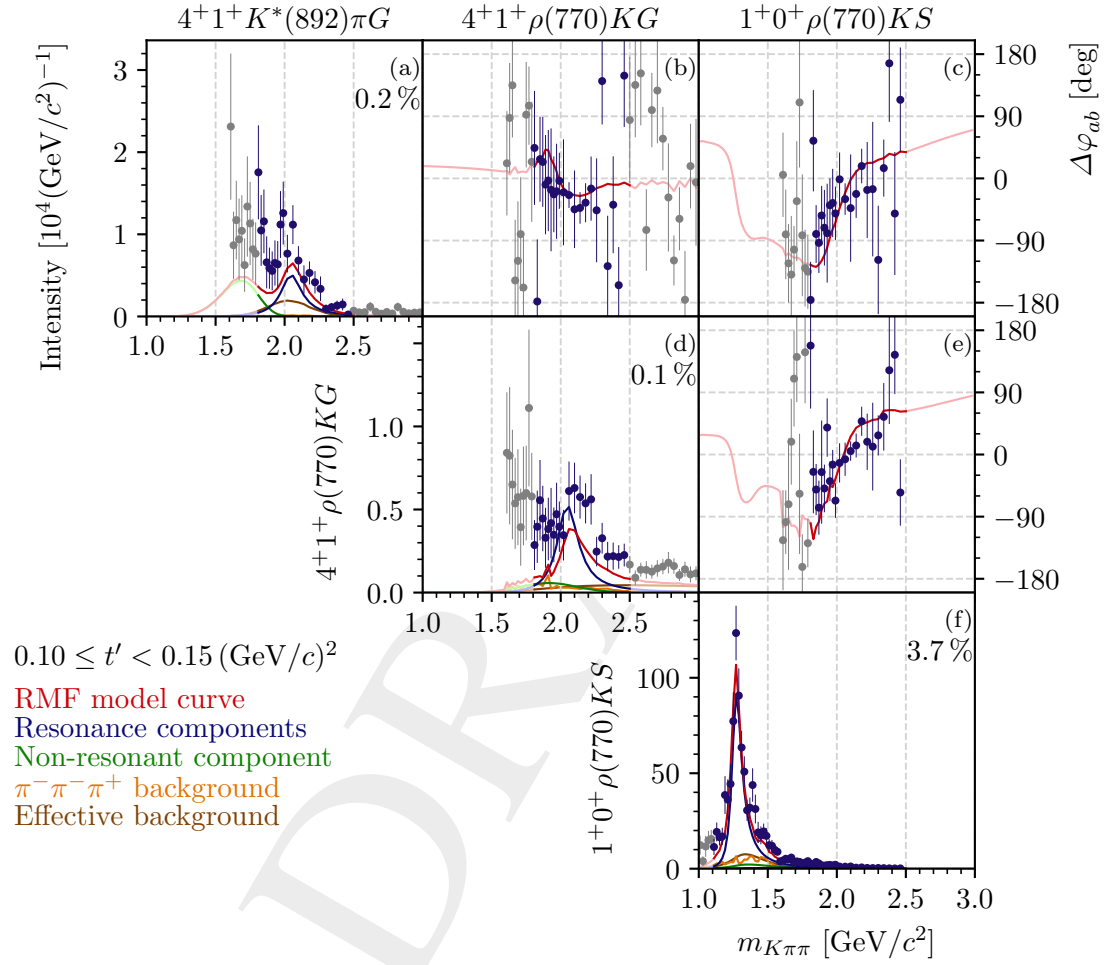


Figure 7.10: Same as figure 7.1, but for the two waves with  $J^P = 4^+$  that were included in the 10-wave RMF and the  $1^+ 0^+ \rho(770) K S$  wave serving as phase reference. The lowest  $t'$  bin is shown.

4498 The  $4^+ 1^+ \rho(770) K G$  wave has about half the relative intensity of the  $4^+ 1^+ K^*(892) \pi G$  wave.  
 4499 Its intensity spectrum exhibits a peak-like structure in the  $K_4^*(2045)$  mass region as shown in  
 4500 figure 7.10d. As for the  $4^+ 1^+ K^*(892) \pi G$  wave, the RMF overall underestimates intensity of  
 4501 the  $4^+ 1^+ \rho(770) K G$  wave, while the off-diagonal spin-density matrix elements of this wave are  
 4502 reproduced well by the RMF. The peak is mainly described by the  $K_4^*(2045)$  component, which  
 4503 destructively interferes with the small non-resonant component such that the intensity of the  
 4504 total RMF model is actually smaller than the intensity of the  $K_4^*(2045)$  component in the peak  
 4505 region. The  $\pi^- \pi^- \pi^+$  background component contributes only little to this wave. The effective  
 4506 background component is mainly used by the RMF to account for the enhanced high-mass tail  
 4507 above about  $2.2 \text{ GeV}/c^2$ .

4508 The relative phase between the  $4^+ 1^+ K^*(892) \pi G$  and  $4^+ 1^+ \rho(770) K G$  waves in the lowest  $t'$   
 4509 bin is shown in figure 7.10b. It is centered approximately around zero with a shallow drop of  
 4510 about  $50^\circ$  around  $1.9 \text{ GeV}/c^2$ , which presumably is caused by the different non-resonant and  
 4511 background contributions to these waves. Figure 7.10c shows the phase of the  $4^+ 1^+ K^*(892) \pi G$   
 4512 wave relative to the  $1^+ 0^+ \rho(770) K S$  wave, which rises by about  $120^\circ$  in the region around  
 4513  $2 \text{ GeV}/c^2$ . We observe a similar rise in the relative phase of the  $4^+ 1^+ \rho(770) K G$  wave with  
 4514 respect to the  $1^+ 0^+ \rho(770) K S$  wave as shown in figure 7.10e. All three relative phases are  
 4515 reproduced well by the RMF and are hence consistent with a dominant contribution of the  
 4516  $K_4^*(2045)$  to both  $4^+$  waves.

4517 Figure 7.11 shows the  $t'$  spectrum of the  $K_4^*(2045)$  component in the  $4^+ 1^+ \rho(770) K G$  wave.<sup>[o]</sup>  
 4518 Except for the lowest  $t'$  bin, the spectrum approximately has the expected shape according to  
 4519 equation (6.29). In the lowest  $t'$  bin, the expected suppression due to the  $(t')^{|M|}$  factor is not  
 4520 observed. This suggests that the intensity of the  $K_4^*(2045)$  component is not reliably estimated in  
 4521 the lowest  $t'$  bin.

### 4522 7.3.1 Discussion

4523 Figure 7.12 compares our estimates for the mass and width of the  $K_4^*(2045)$  (circle) to the PDG  
 4524 average values (star) and to the previous measurements that entered the PDG averaging (pluses).  
 4525 Our estimate for the width of the  $K_4^*(2045)$ , which is the so-far most precise measurement of  
 4526 this parameter, agrees well with the PDG average value and accordingly with the values from  
 4527 previous measurements. Our estimate for the mass of the  $K_4^*(2045)$  is slightly larger than the  
 4528 corresponding PDG average value. Still, both agree within their uncertainties. Our estimate for  
 4529 the mass agrees particularly well with the measurements in refs. [28, 122]. The PDG average  
 4530 value for the mass is driven by mainly the measurement in ref. [121], which yielded a low  
 4531 mass with small uncertainties of  $(2039 \pm 10) \text{ MeV}/c^2$ . However, it is not clear whether their  
 4532 uncertainties include systematic uncertainties.<sup>[p]</sup> Hence, the uncertainty quoted in ref. [121]

<sup>[o]</sup> By construction, the  $t'$  spectrum of the  $K_4^*(2045)$  component is the same in both  $4^+$  waves up to a global factor [see equation (6.14)].

<sup>[p]</sup> For example, ref. [122], where a similar reaction was under study as in ref. [121], estimated a statistical uncertainty for the  $K_4^*(2045)$  mass of  $\pm 14 \text{ MeV}/c^2$  based on a data sample of about 151 000 events; similar to the total

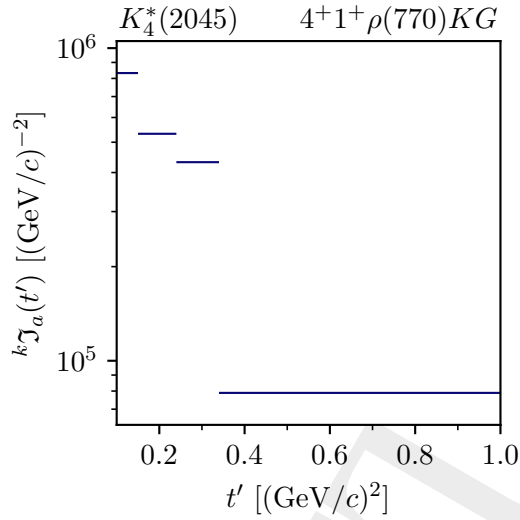


Figure 7.11: Same as figure 7.3, but for the  $K_4^*(2045)$  component in the  $4^+ 1^+ \rho(770) KG$  wave.

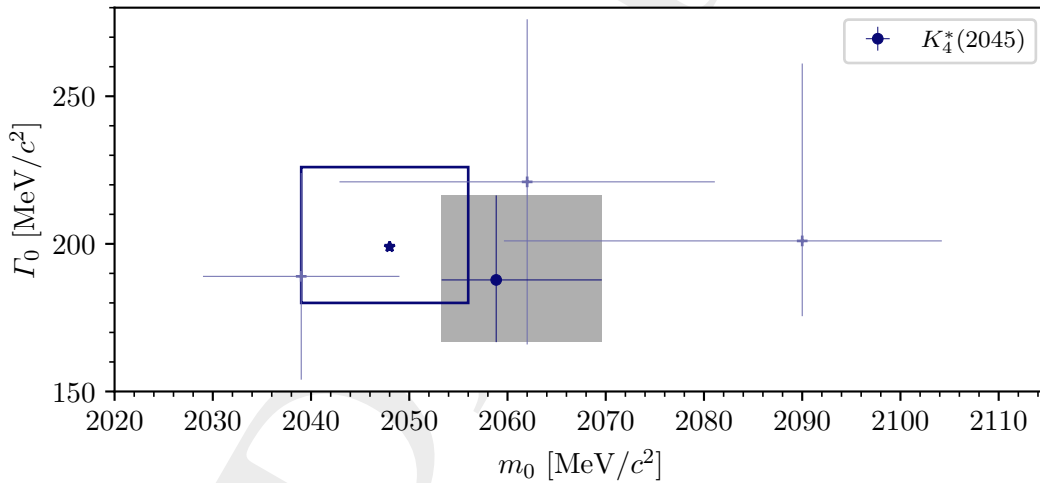


Figure 7.12: Same as figure 7.4, but for the resonance parameters of the  $K_4^*(2045)$ .

4533 might be underestimated, which would bias the PDG average value towards a smaller  $K_4^*(2045)$   
 4534 mass, i.e. away from our estimate.

4535 Despite the small intensity of the  $K_4^*(2045)$  signal at the per-mill level in our data, we were  
 4536 able to reliably extract the  $K_4^*(2045)$  component in the 10-wave RMF. This was verified in all

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uncertainty given in ref. [121] based on a data sample of only about 35 000 events. Hence, the total uncertainty given in ref. [121] might be purely statistical. Ref. [122] quotes a systematic uncertainty of a similar order of magnitude as their statistical uncertainty.



4537 performed systematic and pseudodata studies, and this is also reflected in the comparably small  
 4538 uncertainties of our estimates for the resonance-parameter of the  $K_4^*(2045)$ , which are in good  
 4539 agreement with previous measurements. Also, the overall good agreement of the shape of the  $t'$   
 4540 spectrum of the  $K_4^*(2045)$  component with the expectation indicates a reliable extraction of the  
 4541  $K_4^*(2045)$ . This supports our statement in section 6.2.2, that the imperfections in the description  
 4542 of the intensity spectra of the  $4^+$  waves by the RMF do not strongly bias the determination of the  
 4543  $K_4^*(2045)$ , because the RMF is driven mainly by the off-diagonal spin-density matrix elements.  
 4544 Hence, we are not only able to accurately measure the mass and width of the  $K_4^*(2045)$ , but the  
 4545 good agreement of our estimates for the parameters of the well-known  $K_4^*(2045)$  with previous  
 4546 measurements demonstrates that we are able to determine even signals at the per-mill level and  
 4547 with significant artifacts, e.g. in the corresponding intensity spectra.

## 4548 7.4 $J^P = 2^-$ Partial Waves

4549 We selected four waves with  $J^P = 2^-$  for the 10-wave RMF, which are shown in figures 7.13  
 4550 and 7.15 in the second-lowest  $t'$  bin, where the interesting features are seen clearly. The  
 4551 largest of these four waves is the  $2^- 0^+ K_2^*(1430) \pi S$  wave. Its intensity spectrum is shown  
 4552 in figure 7.13a and exhibits a broad peak at about  $1.8 \text{ GeV}/c^2$ , with a peak-like high-mass  
 4553 shoulder at about  $2.2 \text{ GeV}/c^2$ . The peak position moves with  $t'$  from about  $1.74 \text{ GeV}/c^2$  in the  
 4554 lowest  $t'$  bin to about  $1.87 \text{ GeV}/c^2$  in the highest  $t'$  bin (cf. figures 7.14a and 7.14b). Overall,  
 4555 the RMF reproduces well the intensity spectra of the  $2^- 0^+ K_2^*(1430) \pi S$  wave in all four  $t'$   
 4556 bins. The shift of the position of the  $1.8 \text{ GeV}/c^2$  peak with  $t'$  is reproduced by the RMF as  
 4557 a complex interplay of the various components, which changes with  $t'$ . Overall, the RMF  
 4558 describes the peak by an interference of the  $K_2(1770)$  component with a mass of  $(1715 \pm 4_{-6}^{+1}) \text{ MeV}/c^2$   
 4559 and a width of  $(139 \pm 7_{-7}^{+14}) \text{ MeV}/c^2$ , the  $K_2(1820)$  component with a mass of  
 4560  $(1848 \pm 5_{-20}^{+6}) \text{ MeV}/c^2$  and a width of  $(250 \pm 10_{-23}^{+17}) \text{ MeV}/c^2$ , and the non-resonant component.  
 4561 The  $K_2(1820)$  component dominates the total intensity of the RMF model. In addition, in the two  
 4562 lowest  $t'$  bins shown in figures 7.13a and 7.14a, the low-mass tail of the  $1.8 \text{ GeV}/c^2$  peak is mainly  
 4563 described by an unexpectedly strongly peaking effective background component, similar to the  
 4564 one observed in the  $1^+ 1^+ \rho(770) K S$  wave (see figure 7.1c). In the highest  $t'$  bin, the effective  
 4565 background component vanishes and the peak is mainly described by the  $K_2(1820)$  component  
 4566 (see figure 7.14b). The high-mass shoulder of the  $2^- 0^+ K_2^*(1430) \pi S$  wave is described well by  
 4567 the RMF using the  $K_2(2250)$  component with a mass of  $(2230 \pm 11_{-61}^{+7}) \text{ MeV}/c^2$  and a width of  
 4568  $(266 \pm 29_{-16}^{+225}) \text{ MeV}/c^2$ . Overall, there is only a small contribution of the  $\pi^- \pi^- \pi^+$  background  
 4569 component to the  $2^- 0^+ K_2^*(1430) \pi S$  wave.

4570 The  $2^- 0^+ f_2(1270) K S$  wave has a relative intensity of about 1.1 %, which is similar to the one  
 4571 of the  $2^- 0^+ K_2^*(1430) \pi S$  wave. The intensity spectrum of the  $2^- 0^+ f_2(1270) K S$  wave in the  
 4572 second-lowest  $t'$  bin is shown in figure 7.13d and exhibits a clear peak at about  $1.7 \text{ GeV}/c^2$ , i.e.  
 4573 at slightly lower mass than the peak in the  $2^- 0^+ K_2^*(1430) \pi S$  wave. The peak is reproduced  
 4574 well by the RMF with a dominant contribution of the  $K_2(1770)$  component. Also, the  $2^- 0^+$   
 4575  $f_2(1270) K S$  wave exhibits a high-mass shoulder at about  $2.2 \text{ GeV}/c^2$ . The RMF is able to

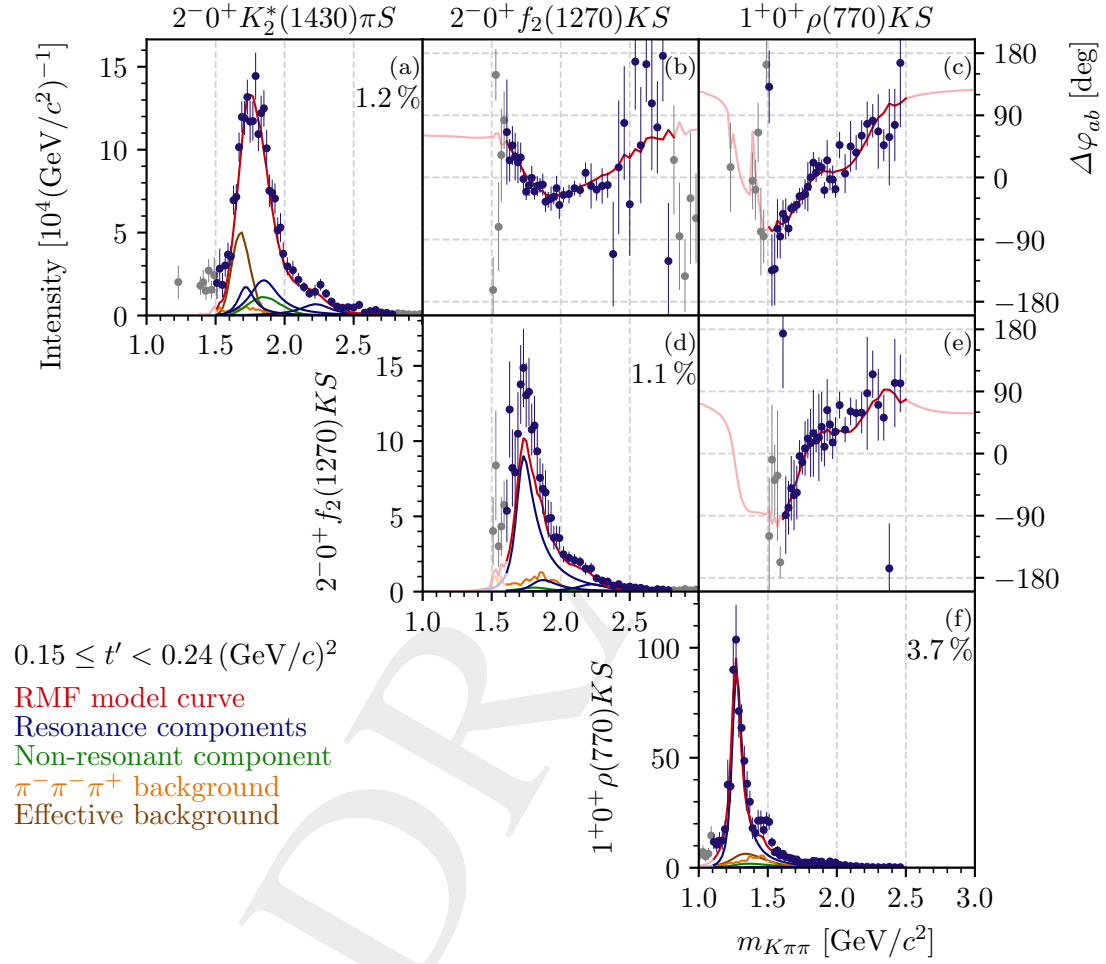


Figure 7.13: Same as figure 7.1, but for the  $J^P = 2^-$  waves with  $K_2^*(1430)$  or  $f_2(1270)$  isobars that were included in the 10-wave RMF and the  $1^{+0+} \rho(770) KS$  wave serving as phase reference. The second-lowest  $t'$  bin is shown.

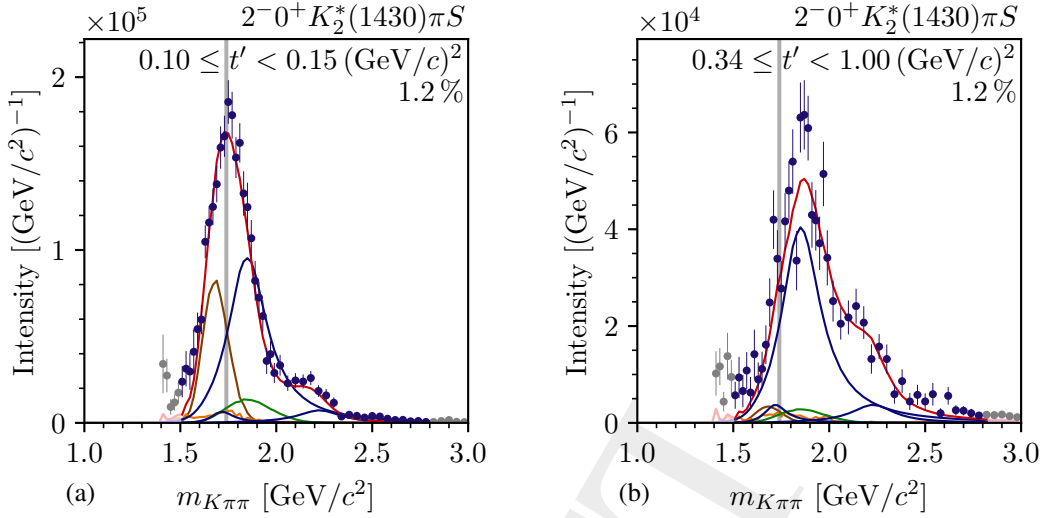


Figure 7.14: Same as figure 7.2, but for the intensity spectra of the  $2^- 0^+ K_2^*(1430) \pi S$  wave (a) in the lowest  $t'$  bin and (b) in the highest  $t'$  bin. The gray vertical lines at  $m_{K\pi\pi} = 1.74 \text{ GeV}/c^2$  indicate for comparison the peak position in the lowest  $t'$  bin.

4576 reproduce this shoulder using the  $K_2(2250)$  component. The non-resonant,  $\pi^- \pi^- \pi^+$  background,  
4577 and effective background components contribute only little to the  $2^- 0^+ f_2(1270) K S$  wave.

4578 The phase of the  $2^- 0^+ K_2^*(1430) \pi S$  wave relative to the  $1^+ 0^+ \rho(770) K S$  wave in the second-  
4579 lowest  $t'$  bin is shown in figure 7.13c. It rises by about  $90^\circ$  in the mass region of the  $1.8 \text{ GeV}/c^2$   
4580 peak. After a short plateau, it rises again in the mass region of the high-mass shoulder. The  
4581 relative phases of the  $2^- 0^+ K_2^*(1430) \pi S$  wave are reproduced well by the RMF, which supports  
4582 the resonance interpretation of the  $1.8 \text{ GeV}/c^2$  peak and the high-mass shoulder. The relative  
4583 phase of the  $2^- 0^+ f_2(1270) K S$  wave with respect to the  $1^+ 0^+ \rho(770) K S$  wave shows similar  
4584 features (see figure 7.13e), and is also reproduced well by the RMF. Figure 7.13b shows the  
4585 relative phase between the  $2^- 0^+ K_2^*(1430) \pi S$  wave and the  $2^- 0^+ f_2(1270) K S$  wave in the  
4586 second-lowest  $t'$  bin. It drops by about  $90^\circ$  around  $1.7 \text{ GeV}/c^2$  and slowly rises again by about  
4587  $30^\circ$  above about  $1.9 \text{ GeV}/c^2$ . The drop of the relative phase can be explained by the  $K_2(1770)$   
4588 resonance contributing more dominantly to the  $2^- 0^+ f_2(1270) K S$  wave, while the following  
4589 slow rise of the relative phase hints towards more dominant contributions of the  $K_2(1820)$  and  
4590 the  $K_2(2250)$  to the  $2^- 0^+ K_2^*(1430) \pi S$  wave. Both phase motions are reproduced well by the  
4591 RMF and are hence consistent with the resonance interpretation of the signals in the  $2^- 0^+$   
4592  $K_2^*(1430) \pi S$  and  $2^- 0^+ f_2(1270) K S$  waves by the RMF.

4593 The  $2^- 0^+ K^*(892) \pi F$  wave has about half the relative intensity of the  $2^- 0^+ K_2^*(1430) \pi S$  wave.  
4594 Its intensity spectrum exhibits a peak at about  $1.75 \text{ GeV}/c^2$  as exemplarily shown in figure 7.15a  
4595 for the second-lowest  $t'$  bin. This peak is reproduced by the RMF by an interference between  
4596 the  $K_2(1770)$  and  $K_2(1820)$  components and a broad non-resonant component. Here; in contrast  
4597 to the  $K_2^*(1430)$  and  $f_2(1270)$  waves, which are dominated either by the  $K_2(1820)$  component  
4598 or by the  $K_2(1770)$  component; the  $t'$ -summed intensities of both resonance components are of

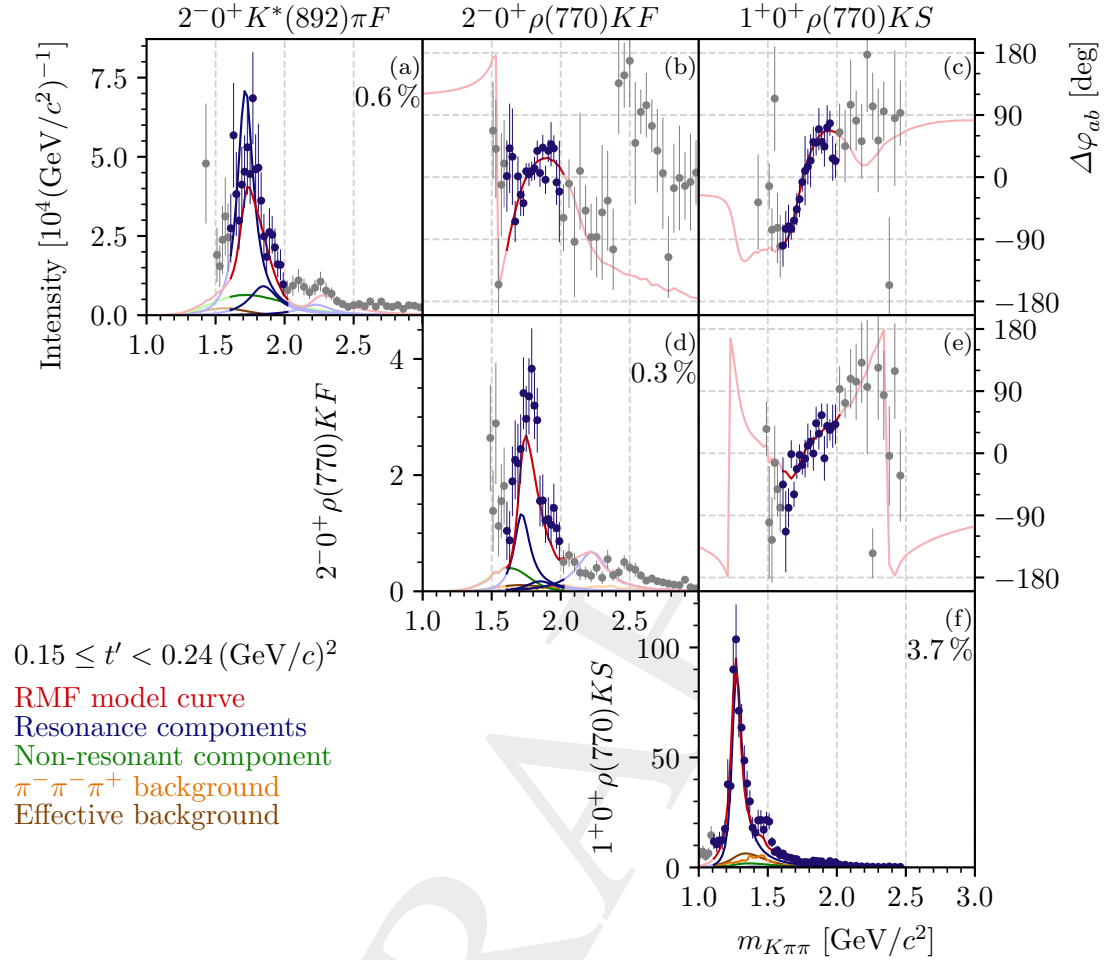


Figure 7.15: Same as figure 7.1, but for the  $J^P = 2^-$  waves with  $K^*(892)$  or  $\rho(770)$  isobars that were included in the 10-wave RMF and the  $1^+0^+ \rho(770)KS$  wave serving as phase reference. The second-lowest  $t'$  bin is shown.

4599 a similar order of magnitude. The  $\pi^- \pi^- \pi^+$  background and effective background components  
 4600 contribute only little to the  $2^-0^+ K^*(892)\pi F$  wave. The high-mass tail above about  $2 \text{ GeV}/c^2$   
 4601 changes its shape from  $t'$ -bin to  $t'$ -bin.<sup>[q]</sup> We were not able to model the high-mass tail in the  
 4602 RMF. Hence, we excluded this wave in the region  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$  from the RMF. Below  
 4603 about  $1.6 \text{ GeV}/c^2$ , the  $2^-0^+ K^*(892)\pi F$  wave exhibits an enhanced low-mass tail as observed  
 4604 also for other small waves and discussed in section 5.5. Hence, we also excluded this wave in the  
 4605 region  $m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$  from the RMF.

4606 The  $2^-0^+ \rho(770)KF$  wave is the smallest of the four  $2^-$  waves included in the 10-wave RMF.  
 4607 It has about a quarter of the relative intensity of the  $2^-0^+ K_2^*(1430)\pi S$  wave. Similar to the

<sup>[q]</sup> For example, while there is almost no enhanced high-mass tail in the lowest  $t'$  bin (not shown), the enhanced high-mass tail in the second-lowest  $t'$  bin has two peaks at about  $2.1 \text{ GeV}/c^2$  and  $2.3 \text{ GeV}/c^2$ .

4608  $2^- 0^+ K^*(892)\pi F$  wave, the intensity spectrum of the  $2^- 0^+ \rho(770)KF$  wave exhibits a peak at  
 4609 about  $1.75 \text{ GeV}/c^2$  (see figure 7.15d). This peak is described by the RMF by an interference of  
 4610 the  $K_2(1770)$  and  $K_2(1820)$  components and the high-mass tail of the non-resonant component.  
 4611 Like for the  $K^*(892)$  wave, the  $t'$ -summed intensities of both resonance components are of a  
 4612 similar order of magnitude. Summed over all  $t'$  bins, the RMF yielded a small contribution from  
 4613 the effective background component and a vanishing contribution from the  $\pi^- \pi^- \pi^+$  background  
 4614 component to the  $2^- 0^+ \rho(770)KF$  wave. As for the  $2^- 0^+ K^*(892)\pi F$  wave, we observe  
 4615 enhanced low- and high-mass tails in the regions  $m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$  and  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$ ,  
 4616 which we could not model in the RMF. Hence, we excluded this wave in these mass regions  
 4617 from the RMF.

4618 The phases of the  $2^- 0^+ K^*(892)\pi F$  and  $2^- 0^+ \rho(770)KF$  waves relative to the  $1^+ 0^+ \rho(770)KS$   
 4619 wave rise by nearly  $180^\circ$  in the mass region of the  $K_2(1770)$  and  $K_2(1820)$  resonances as shown  
 4620 in figures 7.15c and e, respectively. The RMF is able to reproduce these phase motions well.  
 4621 Above  $2 \text{ GeV}/c^2$ , we do not observe a rise of the relative phase of the  $2^- 0^+ K^*(892)\pi F$  wave  
 4622 that would indicate a contribution of the  $K_2(2250)$  to this wave. Thus, the high-mass tail of the  
 4623  $2^- 0^+ K^*(892)\pi F$  wave might not arise from the  $K_2(2250)$ , but might be, for example, a model  
 4624 artifact. The relative phase of the  $2^- 0^+ \rho(770)KF$  wave rises by about  $30^\circ$  above  $2 \text{ GeV}/c^2$ .  
 4625 Still, we were not able to model this wave in the region  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$  by the  $K_2(2250)$   
 4626 component. The relative phase between the  $2^- 0^+ K^*(892)\pi F$  wave and the  $2^- 0^+ \rho(770)KF$   
 4627 wave in the second-lowest  $t'$  bin is shown in figure 7.15b. It is centered around approximately  
 4628 zero in the fitted mass region and rises around  $1.7 \text{ GeV}/c^2$  by about  $60^\circ$ . This phase motion  
 4629 is caused by the different strengths with which the various components in the two  $2^-$  waves  
 4630 interfere and is reproduced by the RMF.

4631 Figure 7.16 shows the  $t'$  spectra of the three  $K_2$  components included in the 10-wave RMF in  
 4632 the  $2^- 0^+ K_2^*(1430)\pi S$  wave. All four  $2^-$  waves have  $M = 0$  quantum number. Therefore, the  
 4633 shape of the  $t'$  spectra of each of the three  $K_2$  components by construction is the same in all four  
 4634  $2^-$  waves because of equation (6.14). In the second-lowest  $t'$  bin, the fit assigns less intensity to  
 4635 the  $K_2(1820)$  component than expected from the other  $t'$  bins, which approximately follow the  
 4636 expected exponential shape (see figure 7.16b). Also, the intensity of the  $K_2(1770)$  component  
 4637 does not follow the expected shape in the two lowest  $t'$  bins (see figure 7.16a). This is due  
 4638 to a different interference pattern between both components in the two lowest  $t'$  bins, which  
 4639 result in a similar description of the data. Hence, the yields of individual components are not  
 4640 determined as reliable as the resonance parameters by the RMF. This holds especially in cases  
 4641 where the resonance components overlap in mass as it is the case for the  $K_2(1770)$  and  $K_2(1820)$   
 4642 components. The  $t'$  spectrum of the  $K_2(2250)$  component exhibits the expected exponential  
 4643 shape as shown in figure 7.16c. This indicates a reliable extraction of the  $K_2(2250)$  from our  
 4644 data.

4645 The  $2^-$  waves represent the largest spin-parity sector in the 238-wave set. In the following, we  
 4646 show a selection of further  $2^-$  waves with potentially interesting signals. The  $t'$ -summed intensity  
 4647 spectrum of the  $2^- 0^+ K^*(892)\pi P$  wave is shown in figure 7.17a. The  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$   
 4648 region of this wave is strongly affected by the leakage effect. Above this region, the  $2^- 0^+$   
 4649  $K^*(892)\pi P$  wave exhibits a peak between about  $1.7 \text{ GeV}/c^2$  and  $1.8 \text{ GeV}/c^2$ , similar to the

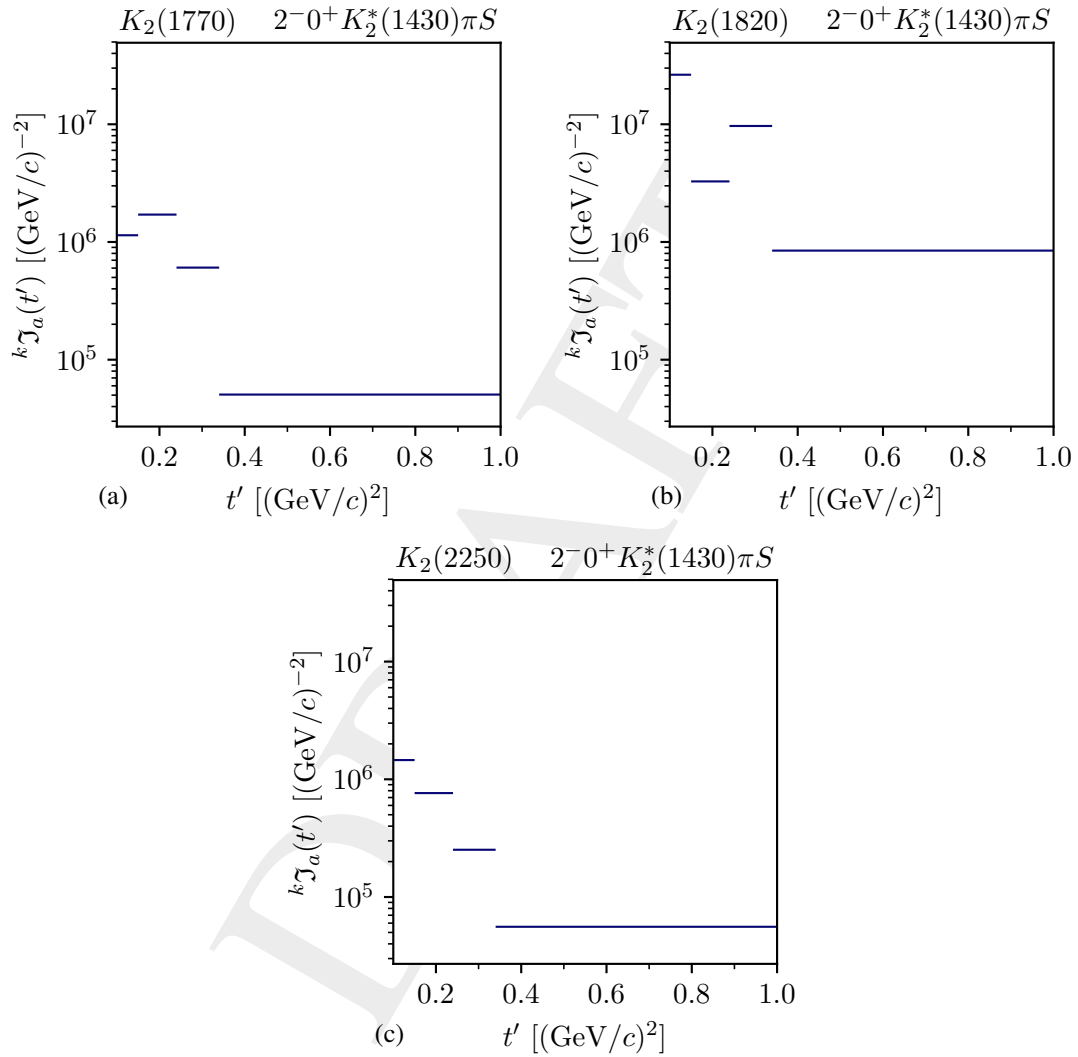


Figure 7.16: Same as figure 7.3 but for (a) the  $K_2(1770)$  component, (b) the  $K_2(1820)$  component, and (c) the  $K_2(2250)$  component in the  $2^- 0^+ K_2^*(1430)\pi S$  wave.

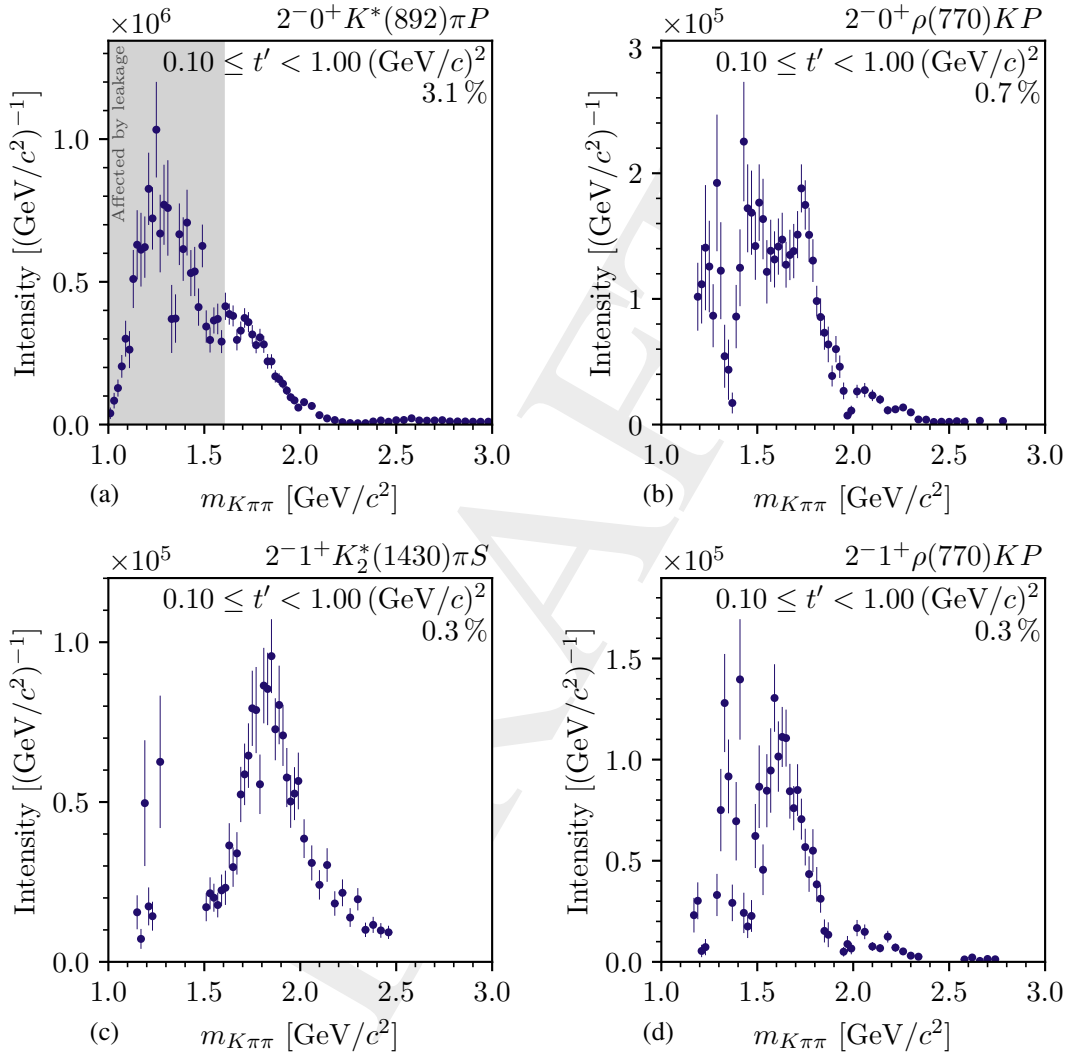


Figure 7.17: Same as figure 7.2, but for four selected partial waves with  $J^P = 2^-$  that were not included in the 10-wave RMF.

4650  $2^- 0^+ K^*(892) \pi F$  wave, which was included in the 10-wave RMF. The intensity of the peak  
4651 is about twice as large as the intensity of the  $1.75 \text{ GeV}/c^2$  peak in the  $2^- 0^+ K^*(892) \pi F$  wave,  
4652 which is expected because of the higher energy needed to produce the larger orbital angular  
4653 momentum of the  $F$  wave. Also, the  $2^- 0^+ \rho(770) K P$  wave shows a narrow peak between about  
4654  $1.7 \text{ GeV}/c^2$  and  $1.8 \text{ GeV}/c^2$  as shown in figure 7.17b. Similar to the two waves with  $K^*(892)$   
4655 isobar, the peak in the  $2^- 0^+ \rho(770) K P$  wave has about twice the intensity of the  $1.75 \text{ GeV}/c^2$   
4656 peak in the  $2^- 0^+ \rho(770) K F$  wave. Although the  $2^- 0^+ \rho(770) K P$  wave does not exhibit artifacts  
4657 that could directly be related to the leakage effect in our studies, its intensity spectrum exhibits a  
4658 strongly enhanced intensity for  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$ , which presumably is an analysis artifact.<sup>[†]</sup>  
4659 The  $2^- 1^+ \rho(770) K P$  wave, i.e. the same wave but with  $M = 1$ , is shown in figure 7.17d. It has  
4660 about half the intensity of the  $M = 0$  wave, which is consistent with the expectation that waves  
4661 with a higher spin projection  $M$  are suppressed. The  $2^- 1^+ \rho(770) K P$  wave exhibits much fewer  
4662 artifacts in the low-mass region than the  $M = 0$  wave. It also exhibits a clear peak, which however  
4663 sits at a lower mass of about  $1.6 \text{ GeV}/c^2$ . This shift may be caused by a different composition  
4664 of the various possible contributions to this wave. A potential origin of this shift could only be  
4665 studied by including this wave in an RMF, which was not possible here due to the remaining  
4666 artifacts in this wave. All of these three waves; i.e. the  $2^- 0^+ K^*(892) \pi P$ ,  $2^- 0^+ \rho(770) K P$ , and  
4667  $2^- 1^+ \rho(770) K P$  waves; exhibit non-zero intensity for  $m_{K\pi\pi} \geq 2 \text{ GeV}/c^2$ . However, no clear  
4668 signal from the  $K_2(2250)$  can be observed in any of these three waves. Finally, the  $t'$ -summed  
4669 intensity spectrum of the  $2^- 1^+ K_2^*(1430) \pi S$  wave is shown in figure 7.17c. It has about a  
4670 quarter of the intensity of its partner wave with  $M = 0$  in the 10-wave RMF, which is the  $2^- 0^+$   
4671  $K_2^*(1430) \pi S$  wave. The  $2^- 1^+ K_2^*(1430) \pi S$  wave exhibits a clear peak at about  $1.8 \text{ GeV}/c^2$ ,  
4672 similar to its  $M = 0$  partner wave. However, we do not observe a pronounced high-mass shoulder,  
4673 which indicates that the  $K_2(2250)$  is suppressed in the  $M = 1$  wave with respect to  $M = 0$  wave. A  
4674 similar effect was observed for the  $\pi_2(2005)$  resonance in the COMPASS  $\pi^- \pi^- \pi^+$  analysis in the  
4675  $2^- 0^+ f_2(1270) \pi S$  and  $2^- 1^+ f_2(1270) \pi S$  waves [41]. In summary, the  $2^-$  sector comprises  
4676 many waves with interesting signals in addition to the four wave selected for the 10-wave RMF.  
4677 However, most of them exhibit artifacts or are small. Hence, they were not included in the  
4678 10-wave RMF.

#### 4679 7.4.1 Discussion

4680 The PDG [9] lists three states with  $J^P = 2^-$  quantum numbers: the established  $K_2(1770)$   
4681 and  $K_2(1820)$ , which are close in mass; and the  $K_2(2250)$ , which needs further confirmation.  
4682 Figure 7.18 shows the PDG average values for the masses and widths of these states as blue, red,  
4683 and green stars, respectively.

<sup>[†]</sup> For example, the intensity of the  $2^- 0^+ \rho(770) K P$  wave in the region  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$  strongly changes in the various systematic studies as shown in figure G.2b. Especially, it seems to be sensitive to the choice of the wave-set.



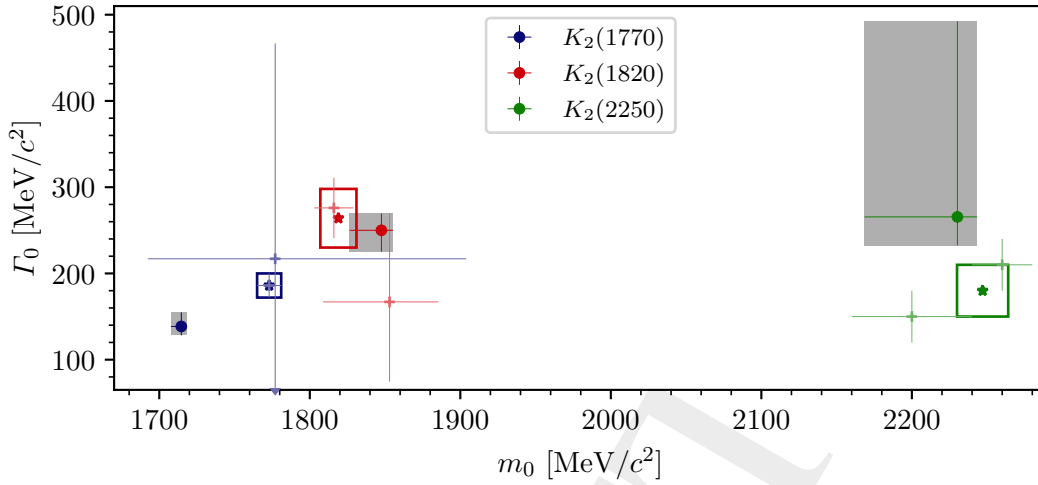


Figure 7.18: Same as figure 7.4, but for the resonance parameters of the  $K_2$  resonances.

#### 4684 The $K_2(1770)$ and the $K_2(1820)$

4685 The different signals in the four waves with  $J^P = 2^-$  included in the 10-wave RMF, and especially  
 4686 the large phase motions in the relative phases between these waves indicate a complicated  
 4687 interference of various components in the  $1.8 \text{ GeV}/c^2$  mass region. However, our approach to  
 4688 simultaneously model these four waves in all  $t'$  bins in one RMF gives us the possibility to  
 4689 reliably separate these contributions and to measure their parameters, i.e. the masses and widths  
 4690 of the  $K_2(1770)$  and  $K_2(1820)$ .

4691 Our estimate for the mass of the  $K_2(1770)$  (blue point) is smaller than the PDG average value.  
 4692 We also obtained a slightly smaller width compared to the PDG average value. Our estimate  
 4693 for the width the  $K_2(1820)$  (red point) is in good agreement with the PDG average value. Our  
 4694 estimate for its mass is slightly larger than the PDG average value, but they still agree within  
 4695 their uncertainties.

4696 Only two measurements entered the PDG averaging for the resonance parameters of the  $K_2(1770)$   
 4697 and the  $K_2(1820)$ , i.e. the measurement of the LASS experiment of the reaction  $K^- p \rightarrow$   
 4698  $K^- \omega p$  [35] and the measurement of the LHCb experiment of the reaction  $B^+ \rightarrow J/\psi \phi K^+$  [34],  
 4699 which was already discussed in section 7.1.1. LASS quotes very small uncertainties for their  
 4700 estimates of the  $K_2(1770)$  mass and width. Especially, they are much smaller than the uncer-  
 4701 tainties of the LHCb measurement. Consequently, the LASS measurement dominates the PDG  
 4702 average values for the  $K_2(1770)$ . However, it is not clear whether the uncertainties quoted by  
 4703 LASS in ref. [35] include systematic effects. Thus, the total uncertainties of the PDG average  
 4704 values for the resonance parameters of the  $K_2(1770)$  might be underestimated. Furthermore, as  
 4705 discussed in section 6.3, it was not possible to perform a full set of systematic studies within the  
 4706 scope of this work. Therefore, also our estimate for the systematic uncertainty of the mass of the

4707  $K_2(1770)$  might be underestimated. This may cause the discrepancy between our estimate for  
 4708 the  $K_2(1770)$  mass and the PDG average value. It should also be noted that our estimates for the  
 4709 resonance parameters of the  $K_2(1770)$  are in agreement with the LHCb measurement within their  
 4710 large uncertainties. In addition, our estimate for the mass of the  $K_2(1770)$  is in better agreement  
 4711 with the prediction of  $1709 \text{ MeV}/c^2$  from a quark-model calculation in ref. [10] (see figure 1.1),  
 4712 than the PDG average value. This further supports our estimate for this parameter.

4713 There are other previous studies of the  $2^-$  sector in the mass region below about  $2 \text{ GeV}/c^2$  [24,  
 4714 37, 152, 153]. However, they typically considered only one  $K_2$  state, which yielded a mass  
 4715 of this state of about  $1770 \text{ MeV}/c^2$ , i.e. similar to the PDG average value for the  $K_2(1770)$ . To  
 4716 compare to these results, we performed in systematic study *E* an RMF where we included only  
 4717 one  $K_2$  component for the mass region below  $2 \text{ GeV}/c^2$  (see section 6.3). This study yielded a  
 4718 mass of this state of about  $1740 \text{ MeV}/c^2$ , which is more consistent with previous observations  
 4719 (see table 6.4). This demonstrates the sensitivity of the obtained resonance parameters on the  
 4720 employed RMF model. Furthermore, study *E* yielded a reduced  $\chi^2$  of 0.844, which is slightly  
 4721 worse than the reduced  $\chi^2$  value of 0.826 obtained in the main analysis. Hence, our data prefer  
 4722 two  $K_2$  resonances for the mass region below  $2 \text{ GeV}/c^2$ . However, given the limited precision of  
 4723 our data, we cannot exclude the hypothesis of a single  $K_2$  in the mass region below  $2 \text{ GeV}/c^2$ .  
 4724 Also, the results from LASS “clearly prefer the model with two  $J^P = 2^-$  resonances” [35],<sup>[s]</sup> while  
 4725 they cannot exclude the single- $K_2$  hypothesis and LHCb [34] determined the significance of the  
 4726  $K_2(1770)$  to be  $5.0\sigma$  and that of the  $K_2(1820)$  to be  $3.0\sigma$ . Thus, none of the measurements of the  
 4727  $2^-$  sector, including our analysis, could individually exclude the single- $K_2$  hypothesis. However,  
 4728 many analyses prefer the two- $K_2$  hypothesis. Therefore,  $K_2(1770)$  and  $K_2(1820)$  are both now  
 4729 considered established states, which is also supported by our measurement. Furthermore, also  
 4730 quark-model calculations predict two  $K_2$  states in this mass region [10].

4731 In addition to the measurements discussed above, also ACCMOR studied four  $2^-$  waves in  
 4732 their analysis of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  [23]. Analogously to our analysis, they  
 4733 studied the  $2^- 0^+ K_2^*(1430) \pi S$  and  $2^- 0^+ f_2(1270) K S$  waves shown in figures 7.19a and 7.19b,  
 4734 respectively. Both waves exhibit similar signals as found in this analysis (cf. figures 7.13a and  
 4735 d). In addition, ACCMOR studied the  $2^- 0^+ K^*(892) \pi P$  wave shown in figure 7.19c, which  
 4736 is affected by the leakage effect in our analysis. In exchange for this wave, we used the  $2^- 0^+$   
 4737  $K^*(892) \pi F$  wave, which exhibits an even clearer signal. The  $2^- 0^+ K^*(892) \pi F$  wave was not  
 4738 considered in the ACCMOR analysis. ACCMOR also included the  $2^- 0^+ \rho(770) K P$  wave in  
 4739 their wave set. However, a signal in this wave “is barely significant” [23] in their data. We  
 4740 observe a peak in this wave (see figure 7.17b) and an even clearer signal in the  $2^- 0^+ \rho(770) K F$   
 4741 wave (see figure 7.15d), which was also not considered in the ACCMOR analysis. Since the  
 4742 COMPASS  $K^- \pi^- \pi^+$  sample is about 3.6 times larger than the one used in the ACCMOR analysis,  
 4743 our parameter estimates are not only more precise, but we were also able to study more waves  
 4744 including waves at the per-mil level such as the  $2^- 0^+ K^*(892) \pi F$  and  $2^- 0^+ \rho(770) K F$  waves.  
 4745 These waves exhibit more clean resonance signals, which also mitigates systematic effects. From  
 4746 their fits, ACCMOR obtained only rough estimates for the resonance parameters of the  $K_2(1770)$

<sup>[s]</sup> In ref. [35], fitting a model with only a single  $K_2$  component to their data yielded a low mass value of the  $K_2$  state of  $(1728 \pm 7) \text{ MeV}/c^2$ , which surprisingly is in better agreement with our estimate for the mass of the  $K_2(1770)$ .

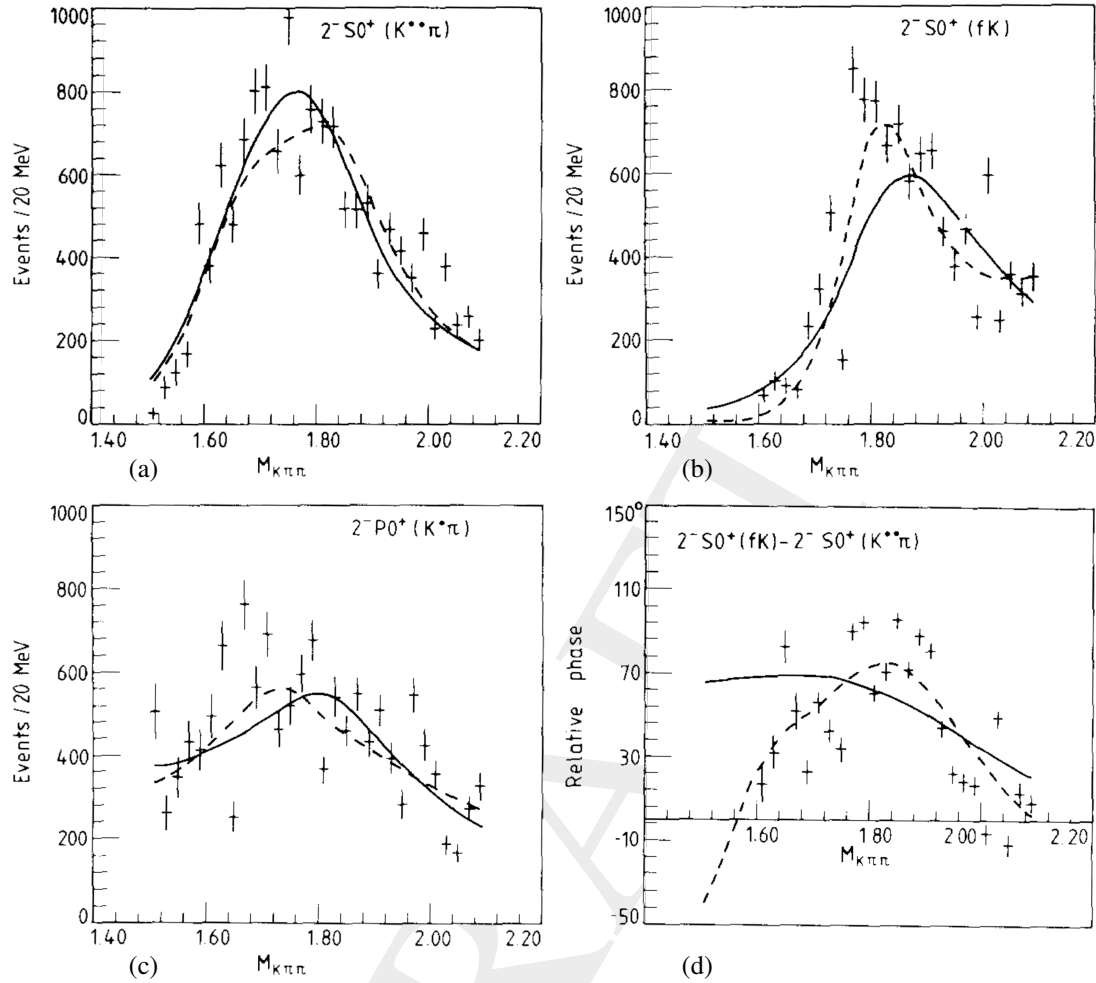


Figure 7.19: Intensities and phases of three  $2^-$  waves as obtained from a partial-wave decomposition performed by the ACCMOR collaboration [23] in the range  $0.0 \leq t' \leq 0.7 (\text{GeV}/c)^2$  (data points). (a), (b), and (c) show the intensity spectra of the  $2^- 0^+ K_2^*(1430) \pi S$ ,  $2^- 0^+ f_2(1270) K S$ , and  $2^- 0^+ K^*(892) \pi P$  waves, respectively. (d) shows the relative phase between the  $2^- 0^+ f_2(1270) K S$  wave and the  $2^- 0^+ K_2^*(1430) \pi S$  wave. The solid curves represent the results of an RMF with a single resonance component and a background component to these waves. The dashed curves represent the results of an RMF of two resonance components and a background component to these waves.

4747 and  $K_2(1820)$ , which were excluded from the PDG averaging. While their estimates for the mass  
 4748 and width of the  $K_2(1820)$  are in good agreement with our results, they obtained for the  $K_2(1770)$   
 4749 a larger mass of about  $1780 \text{ MeV}/c^2$  and a larger width of about  $210 \text{ MeV}/c^2$  with respect to our  
 4750 analysis.

4751 ACCMOR also tested the one- $K_2$  hypothesis (solid curves in figure 7.19) and the two- $K_2$   
 4752 hypothesis (dashed curves in figure 7.19). While models based on both hypotheses reproduce  
 4753 the  $2^- 0^+ K_2^*(1430) \pi S$  and  $2^- 0^+ K^*(892) \pi P$  waves fairly well (see figures 7.19a and 7.19c),  
 4754 the description of the  $2^- 0^+ f_2(1270) K S$  wave is improved when including two  $K_2$  components

(see figure 7.19b). In particular, ACCMOR observed a rise in the relative phase between the  $2^- 0^+ f_2(1270) K S$  wave and the  $2^- 0^+ K_2^*(1430) \pi S$  wave in the mass region of the peak (see figure 7.19d), similar to the one observed in our analysis (cf. figure 7.13b). This phase motion cannot be reproduced with only one  $K_2$  component. ACCMOR concluded, that “fits with two resonances are slightly better” [23], but they also could not exclude the one- $K_2$  hypothesis.

## 4760 The $K_2(2250)$

4761 In the mass region above  $2 \text{ GeV}/c^2$ , the PDG lists one state with  $J^P = 2^-$ , i.e. the  $K_2(2250)$ .  
 4762 We find a potential signal from the  $K_2(2250)$  and no evidence for additional states in this mass  
 4763 region. Our estimate for the mass of the  $K_2(2250)$  agrees with the PDG average value and also  
 4764 with the values from previous measurements (see green point, star, and pluses in figure 7.18).  
 4765 However, our estimate for the width of the  $K_2(2250)$  is about  $90 \text{ MeV}/c^2$  larger than the PDG  
 4766 average value and is also larger than all previous measurements. Still, our estimate for the  
 4767  $K_2(2250)$  width agrees with the PDG average value within two times their uncertainties.<sup>[†]</sup>  
 4768 Except for the measurement in ref. [152], which did not enter the PDG averaging, all previous  
 4769 measurements studied the  $K_2(2250)$  in its decay to the  $\Lambda \bar{p}$  or  $\bar{\Lambda} p$  final state [30, 31, 36, 154, 155].  
 4770 However, the  $K_2(2250)$  is close in mass to the phase-space threshold of the  $\bar{\Lambda} \bar{p}$  final states and  
 4771 the obtained resonance parameters may be sensitive to the employed model for kinematic effects  
 4772 such as the centrifugal-barrier factors. We studied, for the first time,<sup>[‡]</sup> the  $K_2(2250)$  decaying  
 4773 to  $K_2^*(1430)\pi$  and  $f_2(1270)K$  in a partial-wave analysis. For the first time, we simultaneously  
 4774 studied resonances in the mass regions below and above  $2 \text{ GeV}/c^2$  in one RMF. This allowed  
 4775 us to consistently take into account the high-mass tails of the  $K_2(1770)$  and  $K_2(1820)$  when  
 4776 modeling the mass region of the  $K_2(2250)$  and the low-mass tail of the  $K_2(2250)$  when modeling  
 4777 the mass region of the  $K_2(1770)$  and  $K_2(1820)$ . In summary, we gained a new view on the  
 4778  $K_2(2250)$  in our analysis, which may contribute to establish this state.

## 4779 7.5 $J^P = 3^-$ Partial Waves

4780 The main 10-wave RMF does not include waves from the  $J^P = 3^-$  sector. However, the  $K_3^*(1780)$   
 4781 with  $J^P = 3^-$  is a well-known state. In order to study this state in our data, we present studies  
 4782 extending the 10-wave RMF by  $3^-$  waves. We find potential resonance-like signals only in  
 4783 two  $3^-$  waves, i.e. in the  $3^- 1^+ K^*(892)\pi F$  and  $3^- 1^+ \rho(770) K F$  waves. These waves are small  
 4784 with relative intensities of about 0.3 % and 0.1 %, respectively, i.e. only at the per-mill level.

<sup>[†]</sup> In our analysis, the width of the  $K_2(2250)$  has a large systematic uncertainty. Further systematic studies, which are missing, might reveal larger uncertainties towards a lower value. This would bring our estimate for the width of the  $K_2(2250)$  in better agreement with the PDG average value.

<sup>[‡]</sup> According to the PDG listing [9], the  $K_2(2250)$  was studied so far only in  $\bar{\Lambda} \bar{p}$  final states, except for the measurement in ref. [152]. In ref. [152], where the  $K_2(2250)$  was studied in the  $K_S K_S K_L$  system in the reaction  $\pi C \rightarrow K_S K_S K_L + Y$ , no partial-wave analysis was performed, but only a cut-based analysis was performed followed by fitting the mass spectra of the  $K_S K_S K_L$  and  $K_S K_S$  systems.

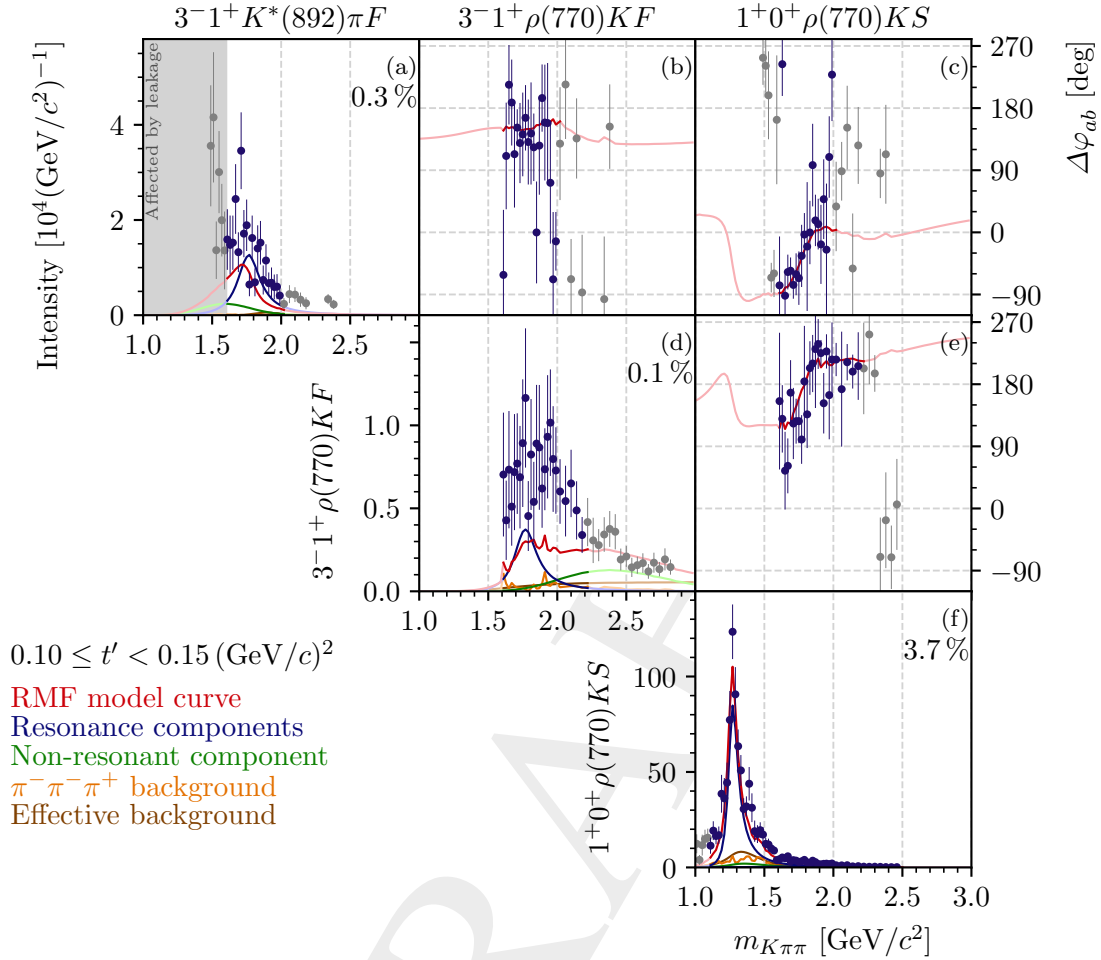


Figure 7.20: Same as figure 7.1, but showing the results of an extended RMF, where the  $3^- 1^+ K^*(892) \pi F$  and  $3^- 1^+ \rho(770) K F$  waves were included in addition to the waves of the 10-wave RMF. The  $1^+ 0^+ \rho(770) K S$  wave serves as phase reference. The lowest  $t'$  bin is shown.

4785 As exemplarily shown in figure 7.20a for the lowest  $t'$  bin, the intensity spectrum of the  $3^- 1^+$   
4786  $K^*(892) \pi F$  wave exhibits a peak at about  $1.8 \text{ GeV}/c^2$  and practically zero intensity above about  
4787  $2 \text{ GeV}/c^2$ . The mass region below  $1.6 \text{ GeV}/c^2$  cannot be interpreted in terms of physics signals,  
4788 because it is affected by the leakage effect. In contrast, the intensity spectrum of the  $3^- 1^+$   
4789  $\rho(770) K F$  wave exhibits a broad bump peaking at about  $2.0 \text{ GeV}/c^2$  with a high-mass tail  
4790 reaching up to almost  $3 \text{ GeV}/c^2$  (see figure 7.20d).

4791 The phase of the  $3^- 1^+ K^*(892) \pi F$  wave relative to the  $1^+ 0^+ \rho(770) K S$  wave is shown for  
4792 the lowest  $t'$  bin in figure 7.20c. It rises between  $1.5$  and  $2.0 \text{ GeV}/c^2$  by about  $140^\circ$ , which is  
4793 consistent with a resonance causing the peak in the intensity spectrum of the  $3^- 1^+ K^*(892) \pi F$   
4794 wave. Interestingly, also the phase of the  $3^- 1^+ \rho(770) K F$  wave relative to the  $1^+ 0^+ \rho(770) K S$   
4795 wave rises in the same mass region by about  $120^\circ$  (see figure 7.20e). The relative phase between

4796 the  $3^- 1^+ K^*(892)\pi F$  wave and the  $3^- 1^+ \rho(770)KF$  wave is approximately constant with a  
 4797 phase offset of about  $140^\circ$ . Both observations point towards the same resonance contributing to  
 4798 both  $3^-$  waves, even if their intensity spectra are significantly different.

4799 In order to perform a first study of a possible resonance content in the  $3^- 1^+ K^*(892)\pi F$  and  
 4800  $3^- 1^+ \rho(770)KF$  waves, we performed an extended RMF including these two waves in addition  
 4801 to the waves of the 10-wave RMF. We modeled the  $3^-$  waves by a  $K_3^*(1780)$  component in  
 4802 addition to non-resonant and background components (see appendix E.2 for details). This  
 4803 extended RMF yielded resonance parameters for the  $K_1$ ,  $K_2$ ,  $K_2^*$ , and  $K_4^*$  components that agree  
 4804 with the results from the 10-wave RMF.<sup>[v]</sup> The extended RMF describes the main features of the  
 4805 intensity spectrum of the  $3^- 1^+ K^*(892)\pi F$  wave reasonably well as shown by the red curve in  
 4806 figure 7.20a. The fit yields a large contribution of the  $K_3^*(1780)$  component. The extended RMF  
 4807 cannot reproduce the broad bump in the intensity spectrum of the  $3^- 1^+ \rho(770)KF$  wave (see  
 4808 figure 7.20d). However, the extended RMF describes well all the off-diagonal spin-density matrix  
 4809 elements of the  $3^- 1^+ K^*(892)\pi F$  and  $3^- 1^+ \rho(770)KF$  waves as exemplary shown in figure 7.21.  
 4810 The good description of the off-diagonal spin-density matrix elements by the extended RMF can  
 4811 also be seen in the relative phases of the  $3^- 1^+ K^*(892)\pi F$  and  $3^- 1^+ \rho(770)KF$  waves, which  
 4812 are all reproduced well by the RMF (see figures 7.20b, c, and e). The imperfect description of  
 4813 only the intensity spectrum of the  $3^- 1^+ \rho(770)KF$  wave, which is at per-mill level, is similar  
 4814 to the one observed for the  $4^+$  waves (see section 7.3). Following the same argumentation, we  
 4815 can still use this wave to study the  $K_3^*(1780)$ . The RMF yields a considerable contribution of the  
 4816  $K_3^*(1780)$  also to the  $3^- 1^+ \rho(770)KF$  wave.

### 4817 7.5.1 Discussion

4818 The  $K_3^*(1780)$  was observed by various previous experiments [22, 97, 156, 157]. Our rough esti-  
 4819 mate for its mass of  $1790 \text{ MeV}/c^2$ <sup>[w]</sup> agrees with the PDG average value of  $(1779 \pm 8) \text{ MeV}/c^2$ .  
 4820 Our rough estimate for its width of  $210 \text{ MeV}/c^2$  is slightly larger than the PDG average value  
 4821 of  $(161 \pm 17) \text{ MeV}/c^2$  [9]. However, the latter is mainly determined by the measurement in  
 4822 ref. [157], which obtained a width of only  $(135 \pm 22) \text{ MeV}/c^2$ . Other measurements, such as a  
 4823 recent study of the decay  $\psi(3686) \rightarrow K^+ K^- \eta$  performed by BES III [156] or a measurement  
 4824 by LASS [97] obtained a width of about  $200 \text{ MeV}/c^2$ , i.e. in good agreement with our rough  
 4825 estimate. Hence, we conclude that we observe clear indications for the  $K_3^*(1780)$  contributing to  
 4826 the  $3^- 1^+ K^*(892)\pi F$  and  $3^- 1^+ \rho(770)KF$  waves consistent with previous observations of this  
 4827 known state. This means, that the  $K_4^*(2045)$  is not the only known state at the per-mill level that  
 4828 we can extract, which further supports the robustness of our analysis.

<sup>[v]</sup> Except for the value of the  $K_2(2250)$  width, all resonance parameters obtained from this extended RMF are consistent with the results from the 10-wave RMF within the corresponding uncertainties. The extended RMF yielded a  $55 \text{ MeV}/c^2$  smaller width of the  $K_2(2250)$ . This discrepancy is slightly larger than the corresponding negative uncertainty of  $33 \text{ MeV}/c^2$  as obtained from the 10-wave RMF. However, our estimates for the systematic uncertainties may be underestimated (see section 6.3). Thus, we consider the results from this extended RMF to agree with the results from the 10-wave RMF.

<sup>[w]</sup> As no systematic studies of the extended RMFs were performed, we only quote rough values for our estimates on the resonance parameters rounded to a precision of  $10 \text{ MeV}/c^2$ , and we do not give the corresponding uncertainties.

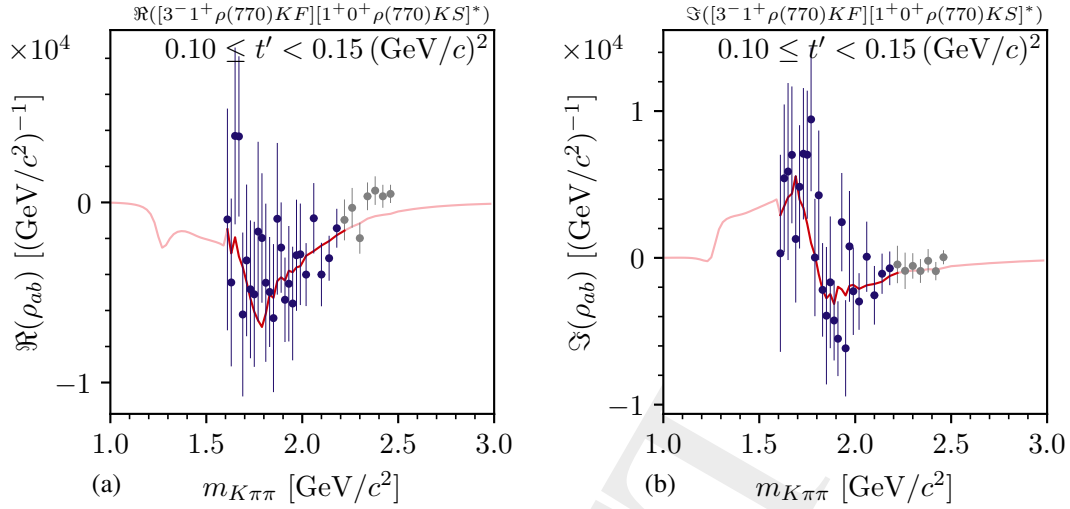


Figure 7.21: Same as figure 7.2, but showing the results of an extended RMF, where the  $3^- 1^+ K^*(892) \pi F$  and  $3^- 1^+ \rho(770) K F$  waves and the waves of the 10-wave RMF were included, for (a) the real part and (b) the imaginary part of the off-diagonal spin-density matrix element of the  $3^- 1^+ \rho(770) K F$  and the  $1^+ 0^+ \rho(770) K S$  waves in the lowest  $t'$  bin.

## 4829 7.6 $J^P = 0^-$ Partial Waves

4830 Among the  $0^-$  waves included in the 238-wave set, the  $0^- 0^+ \rho(770) K P$  wave exhibits the  
 4831 clearest potential signals of excited pseudoscalar kaons. The intensity spectrum of this wave  
 4832 in the second-lowest  $t'$  bin, where the interesting features are seen clearly, is shown in figure  
 4833 7.22a. It exhibits a peak at about  $1.4 \text{ GeV}/c^2$  followed by a second peak at about  $1.7 \text{ GeV}/c^2$   
 4834 and a small bump at about  $1.9 \text{ GeV}/c^2$ . In the  $1.4 \text{ GeV}/c^2$  region, the intensities have large  
 4835 uncertainties, which indicates that we cannot reliably determine the contribution of this wave  
 4836 in this mass region. This may be caused by the large leakage effect on other  $J^P = 0^-$  waves as  
 4837 discussed below, which may influence also the  $0^- 0^+ \rho(770) K P$  wave via its correlation with the  
 4838 other  $0^-$  waves.

4839 The phase of the  $0^- 0^+ \rho(770) K P$  wave relative to the  $1^+ 0^+ \rho(770) K S$  wave is shown in figure  
 4840 7.22b. Similar to the intensity, it is not well determined in the  $1.4 \text{ GeV}/c^2$  region. In the mass  
 4841 region of the  $1.7 \text{ GeV}/c^2$  peak, we observe a rise in this relative phase of about  $60^\circ$ . Also the  
 4842 phase of the  $0^- 0^+ \rho(770) K P$  wave relative to the  $2^+ 1^+ \rho(770) K S$  wave rises in this mass  
 4843 region (see figure 7.22c). Together, the peak in the intensity and the rise of the phases of the  
 4844  $0^- 0^+ \rho(770) K P$  wave relative to various other waves indicate the presence of a resonance at  
 4845 about  $1.7 \text{ GeV}/c^2$ . We do not observe a clear phase motion in the relative phases of the  $0^- 0^+$   
 4846  $\rho(770) K P$  wave in the mass region of the  $1.9 \text{ GeV}/c^2$  bump. However, in this mass region there  
 4847 are also resonances in the reference waves, such as the  $K_1^+$ , which may partly compensate the  
 4848 phase motion caused by a potential  $K$  resonance at about  $1.9 \text{ GeV}/c^2$ .

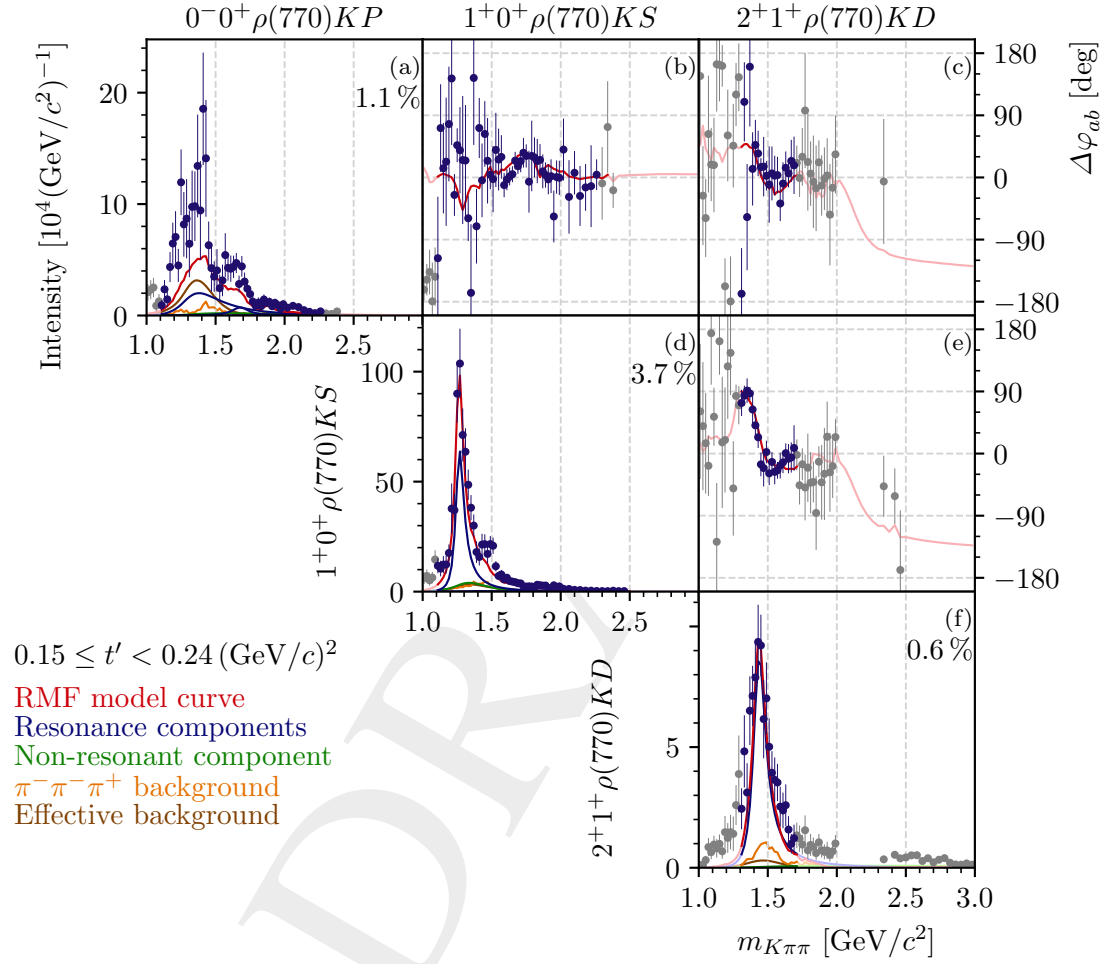


Figure 7.22: Same as figure 7.1, but showing the results of an extended RMF, where the  $0^- 0^+ \rho(770) KP$  wave was included in addition to the waves of the 10-wave RMF. The  $1^+ 0^+ \rho(770) KS$  and  $2^+ 1^+ \rho(770) KD$  waves serve as phase references. The second-lowest  $t'$  bin is shown.



4849 In order to perform a first study of a possible resonance content in the  $0^- 0^+ \rho(770) K P$  wave, we  
 4850 performed an extended RMF including this wave in addition to the waves of the 10-wave RMF.  
 4851 We modeled this  $0^-$  wave by three  $K$  resonance components; i.e. the  $K(1460)$ , the  $K(1630)$ ,  
 4852 and the  $K(1830)$ ; in addition to non-resonant and background components (see appendix E.2  
 4853 for details). This extended RMF yielded resonance parameters for the  $K_1$ ,  $K_2$ ,  $K_2^*$ , and  $K_4^*$   
 4854 components that agree with the results from the 10-wave RMF.<sup>[x]</sup> While this extended RMF  
 4855 reproduces reasonably well the off-diagonal spin-density matrix elements of the  $0^- 0^+ \rho(770) K P$   
 4856 wave, the description of the intensity spectrum of this wave by the RMF is imperfect. In particular,  
 4857 it fails to reproduce the overall magnitude of the intensity in this wave, similar to the results  
 4858 for the  $3^-$  waves (see section 7.5) and for the  $4^+$  waves (see section 7.3). Given the small yield  
 4859 of the potential  $K(1830)$  signal, we performed another extended RMF where we omitted the  
 4860  $K(1830)$  component from the RMF model. This RMF yielded an only slightly worse reduced  $\chi^2$   
 4861 value of 0.840 compared to 0.837 when including the  $K(1830)$  component. Also, the resonance  
 4862 parameters of the  $K(1460)$  and  $K(1630)$  components are not strongly affected when omitting the  
 4863  $K(1830)$  component. Hence, the  $K(1830)$  component describes an only weak signal in the  $0^- 0^+$   
 4864  $\rho(770) K P$  wave.

4865 The largest wave of the  $0^-$  sector is the  $0^- 0^+ K^*(892) \pi P$  wave. Its  $t'$ -summed intensity spectrum  
 4866 is shown in figure 7.23a. The  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$  region of this wave is affected by the leakage  
 4867 effect. Hence, we cannot study the  $K(1460)$  in this wave. At about  $1.6 \text{ GeV}/c^2$ , the  $0^- 0^+$   
 4868  $K^*(892) \pi P$  wave exhibits a shoulder, which may arise from the  $K(1630)$ . However, as this  
 4869 shoulder is just at the border of the mass region affected by the leakage effect, we cannot draw  
 4870 hard conclusions on a  $K(1630)$  signal in the  $0^- 0^+ K^*(892) \pi P$  wave. The intensity spectrum of  
 4871 the  $0^- 0^+ K^*(892) \pi P$  wave also exhibits a bump between  $1.8 \text{ GeV}/c^2$  and  $1.9 \text{ GeV}/c^2$ , which  
 4872 may arise from the  $K(1830)$ . In order to validate this hypothesis, the  $0^- 0^+ K^*(892) \pi P$  wave  
 4873 would have to be included in an RMF, but the leakage effect prohibits this.

4874 The last  $0^-$  wave in our analysis that exhibits potential resonance-like signals is the  $0^- 0^+$   
 4875  $[K\pi]_S^{K\pi} \pi S$  wave shown in figure 7.23b. Also in this wave, the  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$  region of is  
 4876 affected by the leakage effect. Above this mass region, its intensity spectrum exhibits a broad  
 4877 peak at about  $1.7 \text{ GeV}/c^2$  with a long high-mass tail that extends beyond  $2 \text{ GeV}/c^2$ . This peak  
 4878 may arise from the  $K(1630)$  and the  $K(1830)$  may contribute to the high-mass tail. However, we  
 4879 were not able to describe the  $0^- 0^+ [K\pi]_S^{K\pi} \pi S$  wave together with the  $0^- 0^+ \rho(770) K P$  wave in  
 4880 one RMF. Hence, the signals in both waves may not be fully compatible within the limitations of  
 4881 our Breit-Wigner RMF model.

<sup>[x]</sup> Except for the value of the  $K_1(1270)$  width, all resonance parameters obtained from this extended RMF are consistent with the results from the 10-wave RMF within the corresponding uncertainties. The extended RMF yielded a  $12 \text{ MeV}/c^2$  smaller width of the  $K_1(1270)$ . This deviation is slightly larger than the corresponding negative uncertainty of  $6 \text{ MeV}/c^2$  as obtained from the 10-wave RMF. However, our estimates for the systematic uncertainties may be underestimated (see section 6.3). Thus, we consider the results from this extended RMF to agree with the results from the 10-wave RMF.

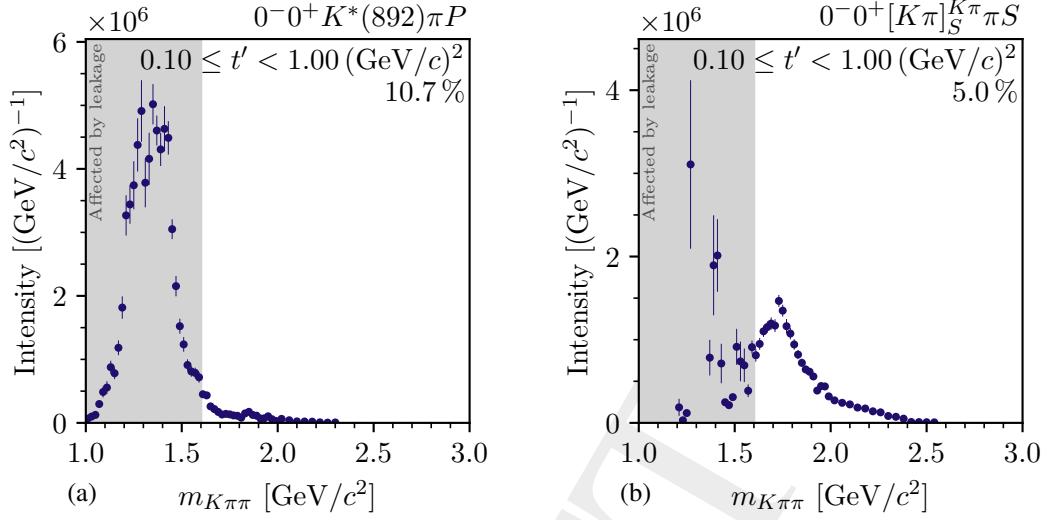


Figure 7.23: Same as figure 7.2, but showing the  $t'$ -summed intensity spectra of (a) the  $0^- 0^+ K^*(892) \pi P$  wave and (b) the  $0^- 0^+ [K\pi]_S^{K\pi} \pi S$  wave.

### 4882 7.6.1 Discussion

4883 Unfortunately, many of the  $J^P = 0^-$  waves are affected by the leakage effect. Consequentially,  
 4884 we can study excited pseudoscalar states reliably only in the  $0^- 0^+ \rho(770) K P$  wave. The PDG  
 4885 lists three excited pseudoscalar states: the  $K(1460)$ , the  $K(1630)$ , and the  $K(1830)$ . While  
 4886 the  $K(1460)$  is considered an established state, the  $K(1830)$  and the  $K(1630)$  still need further  
 4887 confirmation.

#### 4888 The $K(1460)$

4889 The  $K(1460)$  has been studied in an analysis of the decay  $D^0 \rightarrow K^\mp \pi^\pm \pi^+ \pi^-$  by LHCb [26],  
 4890 as well as in the ACCMOR analysis [23] and in the analysis of data from SLAC in ref. [158],  
 4891 which both analyzed the same reaction as in our work. The PDG does not provide average  
 4892 values for the  $K(1460)$  resonance parameters. Our rough estimate for its mass of  $1360 \text{ MeV}/c^2$   
 4893 is smaller than the masses observed by the previous experiments, which are in the range of  $1400$   
 4894 to  $1480 \text{ MeV}/c^2$  [9]. Our rough estimate for its width of  $420 \text{ MeV}/c^2$  is larger than the widths  
 4895 observed by previous experiments, which are in the range of  $250$  to  $340 \text{ MeV}/c^2$  [9]. However,  
 4896 given the large uncertainties of measured spin-density matrix elements of the  $0^- 0^+ \rho(770) K P$   
 4897 wave in the  $1.4 \text{ GeV}/c^2$  mass region and the fact that we considered only one  $0^-$  wave, our  
 4898 estimates for the  $K(1460)$  resonance parameters have large statistical uncertainties and may have  
 4899 systematic uncertainties. Hence, we consider our results on the  $K(1460)$  to not contradict the  
 4900 previous measurements.

4901 **The  $K(1830)$** 

4902 So far, the  $K(1830)$  has been studied by the CERN  $\mathcal{Q}'$  spectrometer in the reaction  $K^- p \rightarrow$   
 4903  $K^- K^- K^+ p$  [37] and by LHCb in the analysis of the decay  $B^+ \rightarrow J/\psi \phi K^+$  [34]. Our rough  
 4904 estimate for the  $K(1830)$  mass of  $1870 \text{ MeV}/c^2$  is in good agreement with the mass estimate  
 4905 by LHCb. Our rough estimate for its width of  $80 \text{ MeV}/c^2$  is smaller than the width estimate of  
 4906  $(168 \pm 90_{-104}^{+280}) \text{ MeV}/c^2$  by LHCb, but still consistent within their large uncertainties. CERN  $\mathcal{Q}'$   
 4907 gives only rough estimates for the resonance parameters of the  $K(1830)$  without uncertainties.  
 4908 Hence, our rough estimates for the  $K(1830)$  resonance parameters are consistent with the results  
 4909 from the limited set of previous studies of this state.

4910 **The  $K(1630)$** 

4911 While the PDG lists three excited pseudoscalar states, quark-model calculations [10, 159] predict  
 4912 only two states (see figure 1.1). The lower-mass quark-model state can be associated with the  
 4913  $K(1460)$ , and the higher-mass quark-model state can probably be associated with the  $K(1830)$ .  
 4914 Hence, the  $K(1630)$  is a candidate for a supernumerary state with respect to the quark model,  
 4915 which points towards a possible exotic nature of the  $K(1630)$ .

4916 The  $K(1630)$  was studied so far only in the reaction  $\pi^- p \rightarrow (K_S^0 \pi^+ \pi^-) X^+ \pi^- X^0$  by a single  
 4917 bubble-chamber experiment at CERN [160, 161]. While the PDG lists the  $K(1630)$  as a  $K$  state,  
 4918 i.e. with  $J^P = 0^-$ , its quantum numbers are not yet well determined [161]. Our rough estimate  
 4919 of  $1680 \text{ MeV}/c^2$  for the  $K(1630)$  mass is similar to the value of  $(1629 \pm 7) \text{ MeV}/c^2$  obtained in  
 4920 ref. [160]. However, we obtained a larger value of  $150 \text{ MeV}/c^2$  for its width compared to the  
 4921  $16_{-16}^{+19} \text{ MeV}/c^2$  [9] obtained in ref. [160]. However, one would expect a much larger width for an  
 4922 excited pseudoscalar state.

4923 In the ACCMOR analysis, a model consisting of a single Breit-Wigner component for the  $K(1460)$   
 4924 and a simple background component was fitted to the  $0^- 0^+ \rho(770) K P$ ,  $0^- 0^+ K^*(892) \pi P$ , and  
 4925  $0^- 0^+ [\pi\pi]_S K S$  waves [23]. While their model reproduces well the  $0^- 0^+ K^*(892) \pi P$  and  $0^- 0^+$   
 4926  $[\pi\pi]_S K S$  intensities and relative phases, it is not able to perfectly reproduce the intensity and  
 4927 the relative phase of the  $0^- 0^+ \rho(770) K P$  wave at a mass of about  $1.7 \text{ GeV}/c^2$ , i.e. in the mass  
 4928 region in which we potentially observe the  $K(1630)$  in the same wave (cf. curve and data points  
 4929 in figure 7.24a). For example, ACCMOR also observed a rise in the relative phase of the  $0^- 0^+$   
 4930  $\rho(770) K P$  wave around about  $1.7 \text{ GeV}/c^2$  similar to what we find in our analysis. However,  
 4931 their model with only the  $K(1460)$  could not reproduce this rise. Thus, it seems that signs of the  
 4932  $K(1630)$  are visible already in the ACCMOR analysis, but they did not consider this state in their  
 4933 RMF.

4934 In the LHCb analysis in ref. [26], the authors performed a model-independent partial-wave  
 4935 analysis (MIPWA), which is similar to our so-called freed-isobar analysis that is presented in  
 4936 chapter 8 and which allowed them to extract the amplitude for the  $J^P = 0^- K^- \pi^- \pi^+$  system in

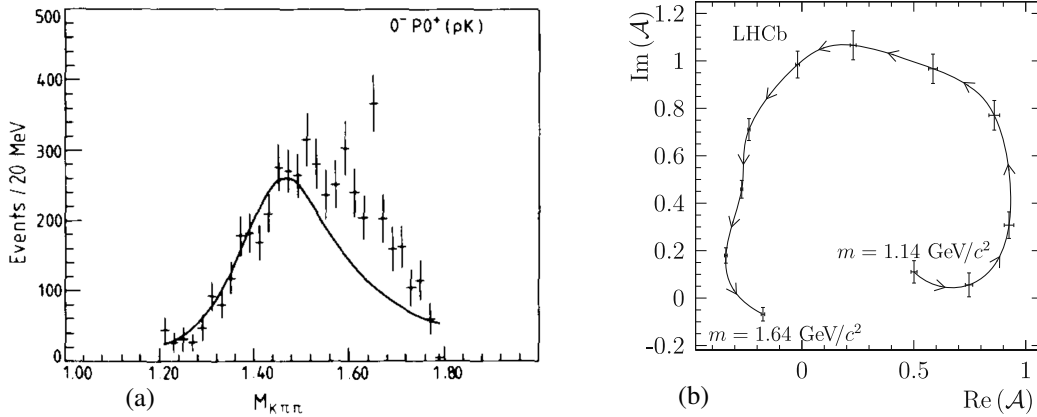


Figure 7.24: Results from previous studies of excited pseudoscalar resonances. (a) shows the intensity spectrum of the  $0^- 0^+ \rho(770) K P$  wave as obtained in the ACCMOR analysis in the range  $0 \leq t' \leq 0.7 (\text{GeV}/c)^2$  [23]. The curve represents the results of a fit of a model consisting of one Breit-Wigner component and a simple background component to this wave and to the  $0^- 0^+ K^*(892) \pi P$  and  $0^- 0^+ [\pi\pi]_S K S$  waves. (b) shows the Argand diagram of the amplitude for the  $K^- \pi^- \pi^+$  system being in a  $J^P = 0^-$  state as obtained from a model-independent partial-wave analysis by LHCb [26]. The curve shows a cubic spline that interpolates between the data points.

4937 bins of  $m_{K\pi\pi}$  instead of imposing a Breit-Wigner shape for it. They used this approach to confirm  
 4938 the resonance nature of the  $K(1430)$ . Figure 7.24b shows the Argand diagram as obtained from  
 4939 their MIPWA. In addition to the clear circle caused by the  $K(1460)$ , the last three data points  
 4940 might indicate the beginning of another circle at about  $1.6 \text{ GeV}/c^2$ , which might be related  
 4941 to the  $K(1630)$ . Unfortunately, LHCb could not study the  $0^-$  amplitude beyond  $1.64 \text{ GeV}/c^2$   
 4942 because of the limited kinematic reach of their analysis given by the  $D^0$  mass. This clearly shows  
 4943 the advantage of studying strange mesons in diffractive production where the full mass range  
 4944 and hence the complete spectrum of strange mesons is accessible in a single self-consistent  
 4945 analysis. Hence, we can directly count the number of appearing states unambiguously, while  
 4946 determining the number of states from multiple measurements that studied only a single state  
 4947 requires assigning these measurements to the corresponding states, which may be ambiguous to  
 4948 the measurement uncertainties. The three signals we observe in the  $0^- 0^+ \rho(770) K P$  wave point  
 4949 towards a supernumerary, excited pseudoscalar state in the  $1.7 \text{ GeV}/c^2$  mass region. However,  
 4950 further systematic studies are needed in order to establish this state.

## 4951 7.7 $J^P = 3^+$ Partial Waves

4952 Among the waves with  $J^P = 3^+$ , the  $3^+ 0^+ K_3^*(1780) \pi S$  and  $3^+ 1^+ K_2^*(1430) \pi P$  waves exhibit  
 4953 the clearest signals of a potential  $K_3$  resonance. Both waves have a relative intensity at the  
 4954 per-mill level of only about 0.1%. The intensity spectrum of the  $3^+ 0^+ K_3^*(1780) \pi S$  wave in the  
 4955 second-lowest  $t'$  bin, where the interesting features are seen clearly, is shown in figure 7.25a.  
 4956 It exhibits a narrow peak at about  $2.1 \text{ GeV}/c^2$  with a high-mass shoulder at about  $2.5 \text{ GeV}/c^2$ .

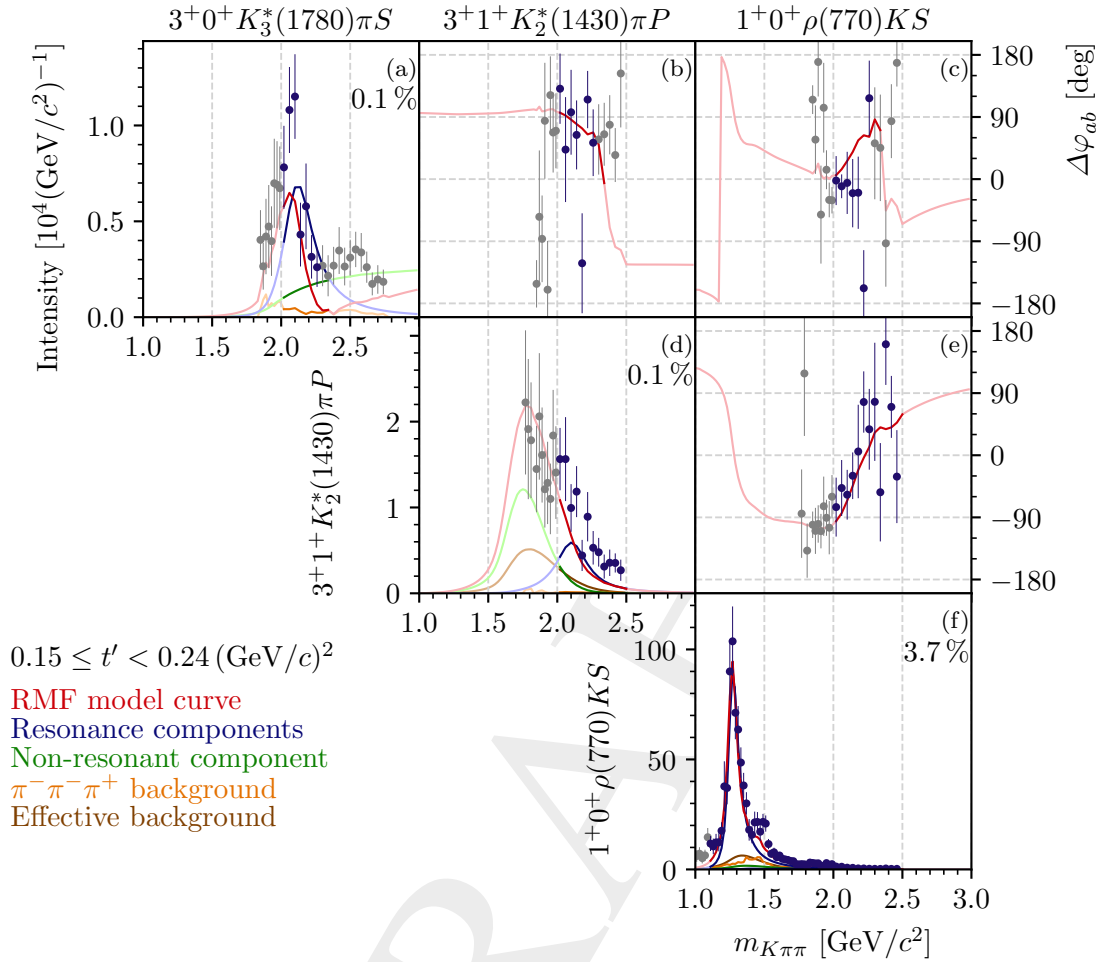


Figure 7.25: Same as figure 7.1, but showing the results of an extended RMF, where the  $3^+ 0^+ K_3^*(1780)\pi S$  and  $3^+ 1^+ K_2^*(1430)\pi P$  waves were included in addition to the waves of the 10-wave RMF. The  $1^+ 0^+ \rho(770)KS$  wave serves as phase reference. The second-lowest  $t'$  bin is shown.

4957 The intensity spectrum of the  $3^+ 1^+ K_2^*(1430)\pi P$  wave continuously falls from about 1.8 to  
 4958  $2.5 \text{ GeV}/c^2$ , i.e. in the mass region in which this wave was included in the 238-wave set (see  
 4959 figure 7.25d).

4960 Figure 7.25e shows the phase of the  $3^+ 1^+ K_2^*(1430)\pi P$  wave relative to the  $1^+ 0^+ \rho(770)KS$   
 4961 wave in the second-lowest  $t'$  bin. We observe a clear rise by about  $130^\circ$  between about 1.9 and  
 4962  $2.4 \text{ GeV}/c^2$ , even though there is no clear peak visible in the corresponding intensity spectrum.  
 4963 The phase of the  $3^+ 0^+ K_3^*(1780)\pi S$  wave relative to the  $1^+ 0^+ \rho(770)KS$  wave exhibits large  
 4964 fluctuations (see figure 7.25c). Overall, it exhibits only the tendency of a rise between 2.0 and  
 4965  $2.4 \text{ GeV}/c^2$ , even though there is a clear peak visible in the corresponding intensity spectrum.  
 4966 Hence, we find indications for a resonance at about  $2.1 \text{ GeV}/c^2$  in both  $3^+$  waves, i.e. in the  
 4967 intensity of the  $3^+ 0^+ K_3^*(1780)\pi S$  wave and in the relative phase of the  $3^+ 1^+ K_2^*(1430)\pi P$

4968 wave. The relative phase between the  $3^+ 0^+ K_3^*(1780)\pi S$  wave and the  $3^+ 1^+ K_2^*(1430)\pi P$  wave  
 4969 in the second-lowest  $t'$  bin is shown in figure 7.25b. It exhibits no clear phase motion below  
 4970  $2.2 \text{ GeV}/c^2$ , as expected if both waves are dominated by the same resonance.

4971 In order to perform a first study of a possible resonance content in the  $3^+ 0^+ K_3^*(1780)\pi S$  and  
 4972  $3^+ 1^+ K_2^*(1430)\pi P$  waves, we performed an extended RMF including both  $3^+$  waves in addition  
 4973 to the waves of the 10-wave RMF. We modeled the  $3^+$  waves by the  $K_3(2320)$  component  
 4974 in addition to non-resonant and background components (see appendix E.2 for details). The  
 4975 extended RMF yielded resonance parameters for the  $K_1$ ,  $K_2$ ,  $K_2^*$ , and  $K_4^*$  components that are  
 4976 consistent with the results from the 10-wave RMF. The model curve of the extended RMF has a  
 4977 peak in the intensity spectrum of the  $3^+ 0^+ K_3^*(1780)\pi S$  wave, similar to the one observed in  
 4978 the measured intensity spectrum (see figure 7.25a). This peak is dominated by the  $K_3(2320)$   
 4979 component. The continuously falling intensity spectrum of the  $3^+ 1^+ K^*(892)\pi P$  wave is repro-  
 4980 duced by the extended RMF by large contributions of the non-resonant and effective background  
 4981 components together with the  $K_3(2320)$  component. Also, the relative phases of both  $3^+$  waves  
 4982 are reproduced well by the extended RMF. <sup>[y]</sup>

### 4983 7.7.1 Discussion

4984 The PDG lists one strange meson with  $J^P = 3^+$ , the  $K_3(2320)$ , which is not considered an  
 4985 established state [9]. So far, it has been seen by only two experiments in the  $\Lambda\bar{p}$  and  $\bar{\Lambda}p$   
 4986 final states [30, 31]. <sup>[z]</sup> The analysis in ref. [30] yielded a width of  $(150 \pm 30) \text{ MeV}/c^2$  and the  
 4987 analysis in ref. [31] yielded a width of about  $250 \text{ MeV}/c^2$ . <sup>[aa]</sup> The latter one agrees well with  
 4988 our rough estimate of  $270 \text{ MeV}/c^2$ . On average, both experiments measured a  $K_3(2320)$  mass  
 4989 of  $(2324 \pm 24) \text{ MeV}/c^2$  [9], which is slightly larger than our rough estimate of  $2120 \text{ MeV}/c^2$ .  
 4990 Interestingly, the mass of the  $K_3(2320)$  as obtained from the  $\Lambda\bar{p}$  and  $\bar{\Lambda}p$  final states agrees with  
 4991 the quark-model prediction from ref. [10] for the first excitation of the  $\bar{K}_3$  spectrum, while our  
 4992 estimate from  $K_3^*(1780)\pi$  and  $K_2^*(1430)\pi$  final states is in good agreement with the predicted  
 4993 ground states (see figure 1.1). Hence, different states may appear in our analysis and in the  
 4994 analyses in refs. [30, 31], due to the different decay modes that are studied. However, the  
 4995 assignment of our measurement and of the measurements in refs. [30, 31] to the corresponding  
 4996 quark-model states may be ambiguous, because the systematic uncertainties on our estimates  
 4997 for the  $K_3(2320)$  resonance parameter may be large. Also, the systematic uncertainties on the  
 4998 estimates for the  $K_3(2320)$  resonance parameter from refs. [30, 31] may be large, because it is not  
 4999 clear whether the authors of refs. [30, 31] used centrifugal-barrier factors to model the threshold  
 5000 behavior. <sup>[ab]</sup> Omitting the centrifugal-barrier factors biases the mass estimates towards larger

<sup>[y]</sup> In general, the extended RMF reproduces well the off-diagonal spin-density matrix elements of the  $3^+ 0^+$   
 $K_3^*(1780)\pi S$  and  $3^+ 1^+ K_2^*(1430)\pi P$  waves (not shown).

<sup>[z]</sup> According to the PDG listing [9].

<sup>[aa]</sup> In ref. [31], the value of the  $K_3(2320)$  width was not optimized in a fit to data, but tuned by hand.

<sup>[ab]</sup> The authors of refs. [30, 31] only give the statement that they fit a relativistic Breit-Wigner to the partial waves, but they do not give the exact formula. Hence, it is not clear whether their model includes centrifugal barrier factors. Ref. [30] does not make any statement about centrifugal barrier factors and ref. [31] only states that they “have imposed correct threshold behavior by drawing smooth curves  $\propto p^L$  through the moments ...” [31].

5001 values, in particular for the  $K_3(2320)$ , because its mass is close to the phase-space threshold  
 5002 of the  $(\bar{\Lambda}p)$  final state and because of the large orbital angular momentum involved in the  $(\bar{\Lambda}p)$   
 5003 decay.

## 5004 7.8 $J^P = 4^-$ Partial Waves

5005 The  $4^- 0^+ K_2^*(1430)\pi D$  wave exhibits the cleanest resonance-like signal with  $J^P = 4^-$ . This  
 5006 wave has a relative intensity of only about 0.1 %. The corresponding intensity spectrum is shown  
 5007 in figure 7.26a exemplarily for the lowest  $t'$  bin. It exhibits a broad peak at about  $2.3 \text{ GeV}/c^2$ . In  
 5008 the same mass region, we observe a rise by about  $100^\circ$  of the phase of the  $4^- 0^+ K_2^*(1430)\pi D$   
 5009 wave relative to the  $1^+ 0^+ \rho(770)KS$  wave as shown in figure 7.26b. Both, the intensity peak  
 5010 and the rise of the relative phase, indicate the presence of a  $K_4$  resonance at about  $2.3 \text{ GeV}/c^2$ .

5011 In order to perform a first study of a possible resonance content in the  $4^- 0^+ K_2^*(1430)\pi D$  wave,  
 5012 we performed an extended RMF including this  $4^-$  wave in addition to the waves of the 10-wave  
 5013 RMF. We modeled this  $4^-$  wave by one resonance component, i.e. the  $K_4(2500)$ , in addition to  
 5014 non-resonant and background components (see appendix E.2 for details). This extended RMF  
 5015 yielded resonance parameters for the  $K_1$ ,  $K_2$ ,  $K_2^*$ , and  $K_4^*$  components that are consistent with the  
 5016 results from the 10-wave RMF. The model curve of extended RMF has a peak in the intensity  
 5017 spectrum of the  $4^- 0^+ K_2^*(1430)\pi D$  wave similar to the one observed in the measured intensity  
 5018 spectrum (see figure 7.26a). However, the RMF underestimates the total intensity in this wave,  
 5019 similar to other waves at the per-mill level (see section 7.3). In addition to a broad effective  
 5020 background component, the RMF assigns a large intensity to the  $K_4(2500)$  component. The rise  
 5021 in the phase of the  $4^- 0^+ K_2^*(1430)\pi D$  wave relative to the  $1^+ 0^+ \rho(770)KS$  wave is reproduced  
 5022 well by the extended RMF.

### 5023 7.8.1 Discussion

5024 The PDG lists the  $K_4(2500)$  as a not-established state [9]. So far, it has been seen by only a single  
 5025 experiment in the reaction  $K^+p \rightarrow \bar{\Lambda}pp$  [31].<sup>[ac]</sup> They measured a mass of  $(2490 \pm 20) \text{ MeV}/c^2$ ,  
 5026 which is larger than our rough estimate of  $2260 \text{ MeV}/c^2$ , and a width of about  $250 \text{ MeV}/c^2$   
 5027 similar to our rough estimate of  $300 \text{ MeV}/c^2$ .<sup>[ad]</sup> Similar to the discussion of the  $K_3(2320)$  in  
 5028 section 7.7, the mass of the  $K_4(2500)$  as obtained from the  $\bar{\Lambda}p$  final state agrees better with  
 5029 a quark-model prediction from ref. [10] for the first excitation of the  $K_4$  spectrum, while our  
 5030 estimate is in good agreement with the predicted ground states. However, the assignment of our  
 5031 measurement and of the measurement in refs. [31] to the corresponding quark-model states may  
 5032 be ambiguous, as already discussed for the  $K_3(2320)$ .

<sup>[ac]</sup> According to the PDG listing [9].

<sup>[ad]</sup> In ref. [31], the value of the  $K_4(2500)$  width was not optimized in a fit to data, but tuned by hand.

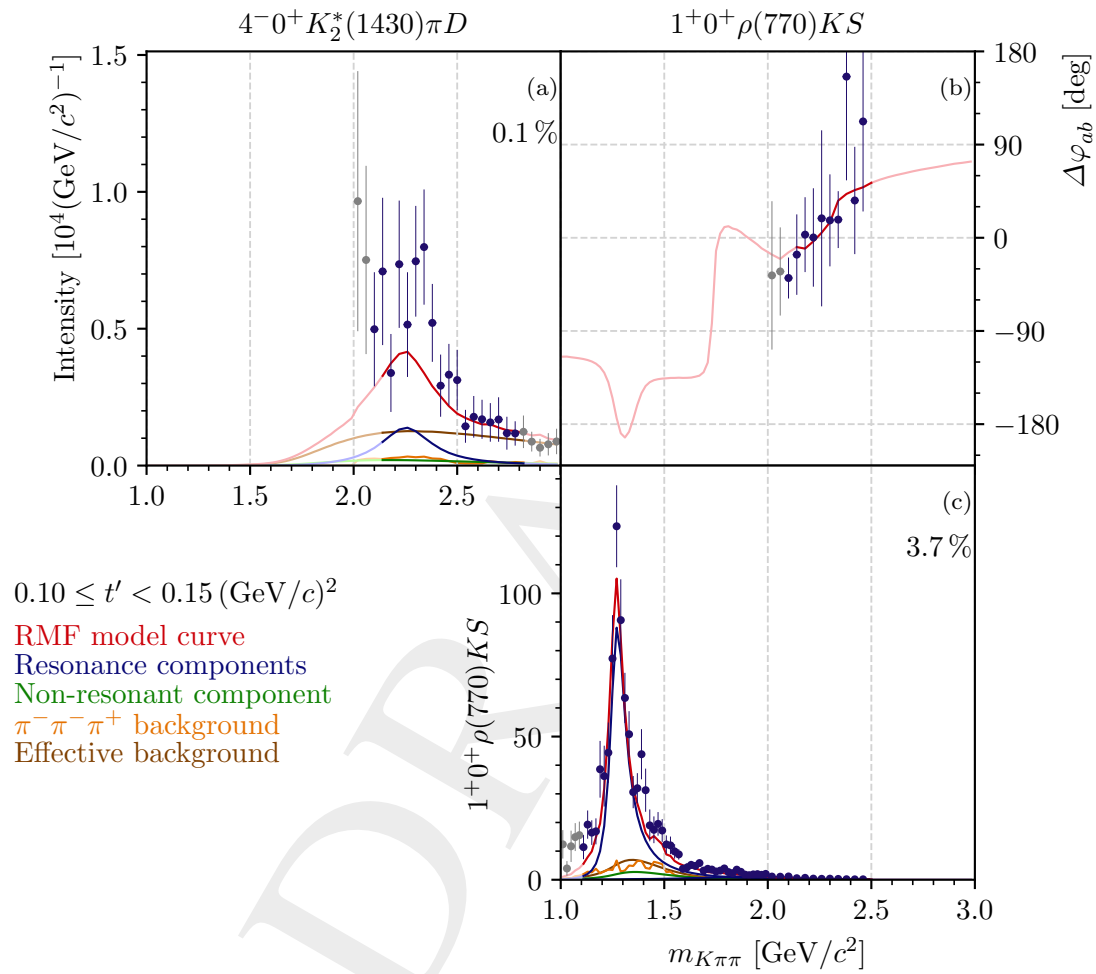


Figure 7.26: Same as figure 7.1, but showing the results of an extended RMF, where the  $4^- 0^+ K_2^*(1430)\pi D$  wave was included in addition to the waves of the 10-wave RMF. The  $1^+ 0^+ \rho(770) K S$  wave serves as phase reference. The lowest  $t'$  bin is shown.



## 5033 7.9 Further Interesting Partial Waves

5034 In this section we summarize our findings in partial waves with  $J^P$  quantum numbers that are  
 5035 not discussed in sections 7.1 to 7.8. The PDG lists two excited  $K^*$  state, i.e. the  $K^*(1410)$   
 5036 and the  $K^*(1680)$  [9]. Both are considered as established states.<sup>[ae]</sup> In our analysis, the  $1^-$   
 5037 waves are strongly affected by the leakage effect. Thus, we cannot study the  $K^*(1410)$  in our  
 5038 analysis as it lies in the affected mass region. Figure 7.27a exemplarily shows the  $t'$ -summed  
 5039 intensity spectrum of the  $1^- 1^+ \rho(770) K P$  wave. It exhibits an enhancement between about  
 5040 1.6 and 1.9 GeV/ $c^2$ , i.e. in the mass region of the  $K^*(1680)$ . However, this enhancement is not  
 5041 accompanied by a clear rise of the relative phases of this wave (not shown), which would indicate  
 5042 a  $K^*(1680)$  signal in this wave. In general, we do not observe any clear resonance-like signals in  
 5043  $J^P = 1^-$  waves in our data. Hence, we did not study  $1^-$  waves in RMFs.

5044 The last group of partial waves that were not yet discussed are waves with high spins or  $J \geq 5$ .  
 5045 The PDG lists only one state with  $J \geq 5$ , the  $K_5^*(2380)$ , which has been seen so far only by the  
 5046 LASS experiment in the  $K^- \pi^+$  final state [122]. In our analysis, we observe in all corresponding  
 5047  $5^-$  waves negligible intensity over the analyzed mass range (not shown). Hence, we do not  
 5048 observe a  $K_5^*(2380)$  in our data. In general, the partial waves with  $J \geq 5$  that were selected  
 5049 by the wave-set selection procedure in section 5.2 have only small intensity at the per-mill  
 5050 level. Most of these high-spin waves have a  $K^- \pi^+$  isobar such as the  $K^*(892)$ . Figures 7.27b  
 5051 to 7.27d show exemplarily the  $t'$ -summed intensity spectra of three selected waves. Typically, the  
 5052  $m_{K\pi\pi} \lesssim 2$  GeV/ $c^2$  regions exhibit a noncontinuous intensity spectrum, e.g. at about 1.9 GeV/ $c^2$   
 5053 in figure 7.27c. We assume this mass region of the high-spin waves to be dominated by artifacts,  
 5054 because of three reasons: (i) it is partly affected by the leakage effect, (ii) the intensity spectra  
 5055 are sensitive to systematic effects, and (iii) we do not expect a state with  $J \geq 5$  in this low-mass  
 5056 region. Above about 2 GeV/ $c^2$ , the high-spin waves typically exhibit a broad bump in their  
 5057 intensity spectra. These broad intensity bumps are not accompanied by any clear phase motions.  
 5058 In general, we observe no evidence for resonances in the high-spin waves. However, more  
 5059 detailed studies might be able to reveal small resonance signals.

5060 A possible explanation for the broad intensity bumps in the high-spin waves is that these waves  
 5061 are dominated by non-resonant contributions such as contributions from Deck-like reactions,  
 5062 which are described in section 2.1.1. We discussed the importance of high-spin waves to describe  
 5063 non-resonant contributions already when discussing the narrow peaks at  $\cos \theta_{GJ}^{K\pi} = +1$  and  
 5064  $\cos \theta_{GJ}^{\pi\pi} = -1$  shown in figure 5.24. From the COMPASS  $\pi^- \pi^- \pi^+$  analysis, where similar Deck-  
 5065 like non-resonant contributions appear, it is known that these contributions cause broad bumps in  
 5066 the intensity spectra of partial waves with high spin, which are not accompanied by pronounced  
 5067 phase motions [11, 124]. We expect qualitatively similar contributions from Deck-like reactions  
 5068 also in our analysis. Furthermore, given the much larger mass of the  $K^-$  compared to the  $\pi^-$ , we  
 5069 assume the contributions from Deck-like reactions with pion exchange shown in figure 2.2a to be  
 5070 dominant compared to the ones with kaon exchange shown in figure 2.2b. Deck-like reactions

<sup>[ae]</sup> Waves with  $J^P = 1^-$  would be interesting to study, not only because they may exhibit excitations of the  $K^*(892)$  ground state, but also because one of these excited states may be the strange partner of the spin-exotic  $\pi_1(1600)$  resonance, which was observed e.g. in the COMPASS  $\pi^- \pi^- \pi^+$  analysis [41].

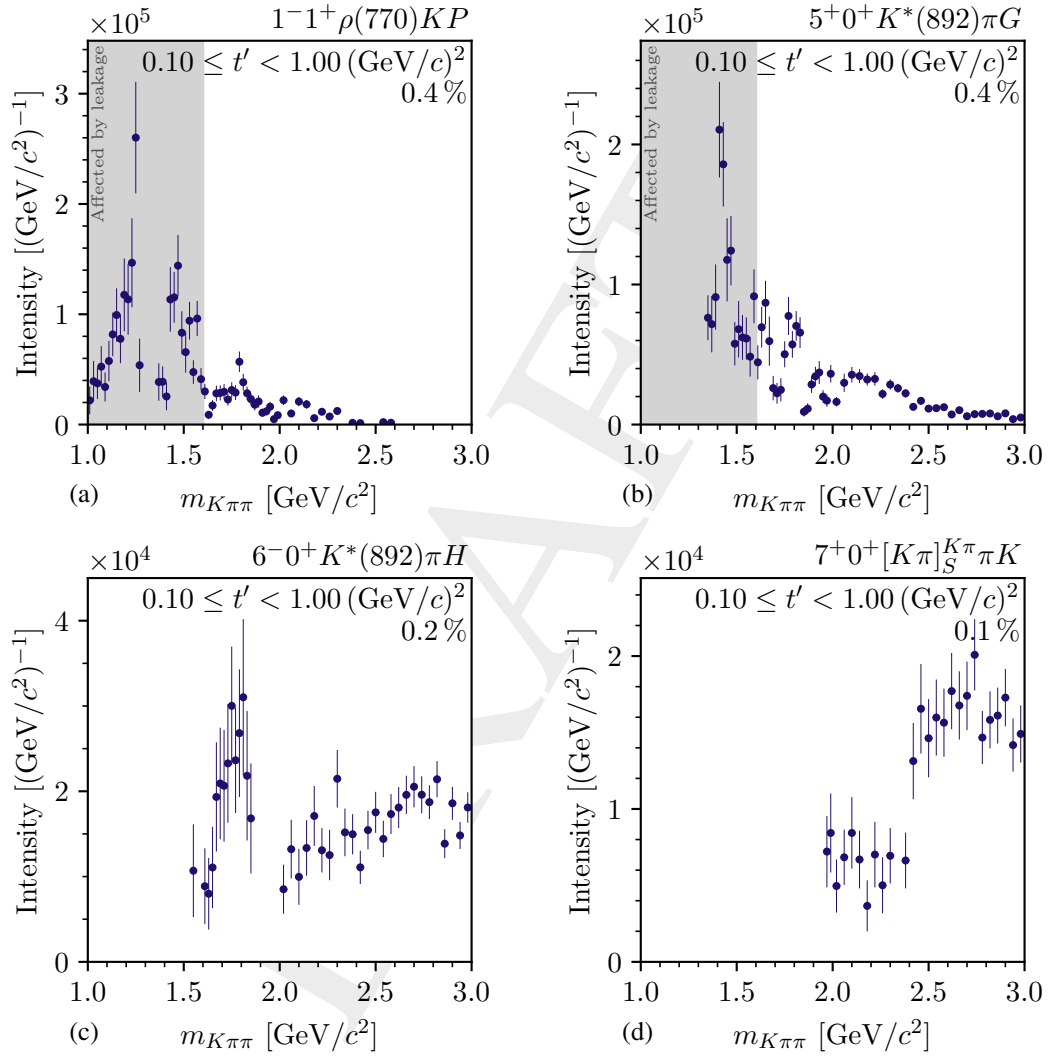


Figure 7.27: Same as figure 7.2, but showing the  $t'$ -summed intensity spectra of the  $1^- 1^+ \rho(770) K P$  wave and of three high-spin waves with  $J \geq 5$ .

5071 with pion exchange proceed via  $K^- \pi^+$  isobars. Hence, the fact the most of the high-spin waves  
5072 have a  $K^- \pi^+$  isobar supports the hypothesis that the high-spin waves are dominated by Deck-like  
5073 reactions.

DRAFT



## 8 The Freed-Isobar Analysis

5075 The main focus of our analysis is the study of strange mesons appearing in the  $K^- \pi^- \pi^+$  system  
 5076 as it was done in the conventional PWD and in the RMFs discussed in chapters 5 to 7. However,  
 5077 non-strange and strange light mesons appear also as isobars in the  $\pi^- \pi^+$  and  $K^- \pi^+$  subsystems,  
 5078 respectively. So far, this fact was used in the conventional PWD to disentangle the various decay  
 5079 modes of the strange mesons into the  $K^- \pi^- \pi^+$  system by employing fixed parameterizations  
 5080 for the dynamic amplitudes of the corresponding isobars (see section 5.1.4). However, the  
 5081 appearance of light mesons in the  $\pi^- \pi^+$  and  $K^- \pi^+$  subsystems allows us to also study these  
 5082 states. Therefore, we performed so-called freed-isobar PWD fits. The freed-isobar approach  
 5083 was developed and successfully applied already in the COMPASS  $\pi^- \pi^- \pi^+$  analysis [11, 39,  
 5084 42, 125] and is similar to approaches called (Quasi-)Model-Independent-Partial-Wave-Analysis  
 5085 (Q)MIPWA applied in the analysis of multi-body heavy-meson and  $\tau$  decays [26, 162].

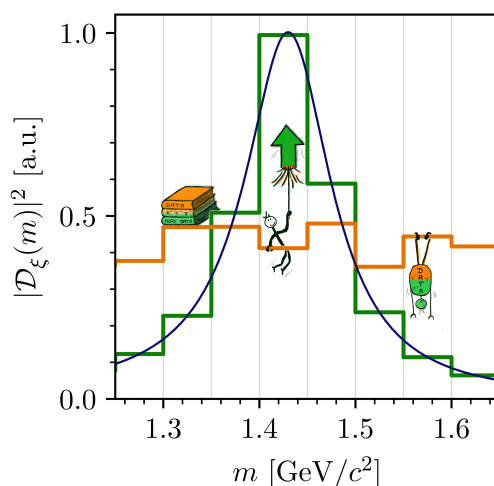


Figure 8.1: Schematic illustration of the freed-isobar method. The blue curve shows the intensity of a relativistic Breit-Wigner amplitude as used for the fixed isobar dynamic amplitudes as a function of the two-body mass. The horizontal orange lines represent the piecewise constant functions before the PWD fit to the data. The vertical gray lines indicate the mass bins. The horizontal green lines represent the piecewise constant functions after the PWD fit. In this illustration, the bins were chosen to be much wider than in the actual analysis for better visualisation. From ref. [163].

5086 In the freed-isobar PWD the fixed parameterizations for the dynamic amplitudes of the isobars  
5087 (blue curve in figure 8.1) are replaced by piecewise constant functions in the two-body mass  
5088 (orange lines in figure 8.1). The function values in the two-body mass bins are adopted to the  
5089 data during the PWD fit. This parameterization is hence very flexible and does not make any  
5090 assumptions on the resonance content in the particular two-body subsystem. In this way, we  
5091 measure the amplitudes of  $\pi^- \pi^+$  and  $K^- \pi^+$  subsystems in the freed-isobar PWDs (green lines in  
5092 figure 8.1). Although the dynamic amplitudes of the isobars are free in the freed-isobar PWDs,  
5093 still the isobar model is employed. This means we consider the decay of a  $K^- \pi^- \pi^+$  intermediate  
5094 state with well-defined quantum numbers  $J^P M^e$  into a bachelor particle and into a  $\pi^- \pi^+$  or  
5095  $K^- \pi^+$  isobar two-body subsystem, which has a well-defined relative orbital angular momentum  
5096  $l$  between both particles. The species of isobar resonances appearing in the studied  $\pi^- \pi^+$  and  
5097  $K^- \pi^+$  subsystems are fully determined by  $l$ , i.e. their spin equals to  $l$ ; their parity equals to  $(-1)^l$ ;  
5098 and their isospin equals to  $1/2$  for  $K^- \pi^+$  isobars,  $1$  for  $\pi^- \pi^+$  isobars with odd spin, and  $0$  for  
5099  $\pi^- \pi^+$  isobars with even spin. The bachelor particle and the isobar system have a well-defined  
5100 relative orbital angular momentum  $L$ . Thus, in a freed-isobar PWD, we measure the  $[\pi\pi]_l$  and  
5101  $[K\pi]_l$  isobar amplitudes as a function of the invariant mass, i.e.  $m_{\pi^- \pi^+}$  and  $m_{K^- \pi^+}$ , respectively,  
5102 of the isobar system in a certain partial wave. We do this independently for each  $(m_{K\pi\pi}, t')$  cell.  
5103 This means, for each  $(m_{K\pi\pi}, t')$  cell we measure an independent isobar amplitude. The formalism  
5104 of the freed-isobar PWD is presented in appendix F.

5105 As the freed-isobar approach increases drastically the number of free parameters of the PWD  
5106 model, its application is possible only for high-precision data samples as it is the case for the  
5107 COMPASS  $\pi^- \pi^- \pi^+$  sample. Compared to the COMPASS  $\pi^- \pi^- \pi^+$  sample, our  $K^- \pi^- \pi^+$  sample  
5108 is about 70 times smaller.<sup>[a]</sup> Hence, we cannot free the dynamic amplitudes of multiple isobars  
5109 simultaneously as it was done in the COMPASS  $\pi^- \pi^- \pi^+$  analysis [125]. Still, our  $K^- \pi^- \pi^+$   
5110 sample is sufficiently large to perform proof-of-principle tests of the freed-isobar approach for  
5111 single isobars. We performed four independent freed-isobar PWDs. In each, we freed only  
5112 a single isobar dynamic amplitude; i.e. the  $[\pi\pi]_P$ ,  $[K\pi]_P$ ,  $[K\pi]_D$ , and  $[K\pi]_S$  amplitudes; in a  
5113 single partial wave, while keeping the other partial waves as in the conventional 238-wave PWD.  
5114 Finally, we performed RMFs to the two-body mass dependence of the measured freed-isobar  
5115 amplitudes in order to study their resonance content. As we performed no systematic studies  
5116 yet, we cannot give systematic uncertainties for the parameter estimates of the isobar resonance.  
5117 Hence, we give no uncertainties, and we quote the resonance parameters only rounded to a  
5118 precision of  $1 \text{ MeV}/c^2$ . The results of the four freed-isobar analyses are discussed in sections 8.1  
5119 to 8.4.

<sup>[a]</sup> Here, we refer to the size of the COMPASS  $\pi^- \pi^- \pi^+$  sample as used for the first freed-isobar PWD presented in ref. [39]. Compared to the COMPASS  $\pi^- \pi^- \pi^+$  sample that was obtained in the improved analysis that will be presented in ref. [43], our  $K^- \pi^- \pi^+$  sample is about 150 times smaller.

## 8.1 The $[\pi\pi]_P$ Amplitude

Among the isobars resonances that were considered in the conventional PWD (see table 5.2), the  $\rho(770)$  is one of the best known states. Thus, studying the corresponding dynamic amplitude in the freed-isobar analysis and comparing the results to previous measurements of the  $\rho(770)$  parameters allows us to verify the freed-isobar approach for our  $K^-\pi^-\pi^+$  sample. The  $\rho(770)$  dominantly decays to two pions, where the pion pair is in a  $P$  wave, i.e. the pions have one unit of orbital angular momentum. Hence, our goal is to determine the  $[\pi\pi]_P$  amplitude by employing the freed-isobar PWD. The largest partial-wave with a  $\rho(770)$  isobar is the  $1^+0^+ \rho(770) K S$  wave (see section 7.1). Thus, we performed a freed-isobar PWD, where we replaced the  $1^+0^+ \rho(770) K S$  wave included in the conventional 238-wave PWD by a freed  $1^+0^+ [\pi\pi]_P K S$  wave.

Figure 8.2 shows the measured  $[\pi\pi]_P$  freed-isobar amplitude in two exemplarily selected  $m_{K\pi\pi}$  bins in the lowest  $t'$  bin. The intensity spectrum of the  $[\pi\pi]_P$  freed-isobar amplitude in the  $m_{K\pi\pi}$  region of the  $K_1$  double peak exhibits a clear peak at  $m_{\pi^-\pi^+} \approx 0.75 \text{ GeV}/c^2$  (see figure 8.2a). The high-mass part of the peak is cut off by the phase-space border. As shown in figure 8.2b, the corresponding Argand diagram of the real and imaginary parts of the  $[\pi\pi]_P$  freed-isobar amplitude exhibits a circle, which is characteristic for a Breit-Wigner like resonance. Figure 8.2c exemplarily shows the intensity spectrum of the  $[\pi\pi]_P$  freed-isobar amplitude at higher  $m_{K\pi\pi}$ . It also exhibits a peak at  $m_{\pi^-\pi^+} \approx 0.75 \text{ GeV}/c^2$ , which is, however, more noisy. The corresponding Argand diagram does not show a clear circle starting at the origin. However, a circle-like shape may be recognized, whose starting point is shifted away from the origin. Such a shift may be caused by a background contribution to this amplitude.

The red curves in figure 8.2 represent the result of an RMF to the measured  $[\pi\pi]_P$  freed-isobar amplitude, which we modeled by a single Breit-Wigner component. The RMF reproduces well the  $[\pi\pi]_P$  amplitude in the  $m_{K\pi\pi}$  region of the  $K_1$  double peak. We obtained a mass of about  $766 \text{ MeV}/c^2$  and a  $\rho(770)$  width of about  $148 \text{ MeV}/c^2$ . Both values are close to the corresponding PDG average values of  $(769.0 \pm 0.9) \text{ MeV}/c^2$  and  $(150.9 \pm 1.7) \text{ MeV}/c^2$  [9]. In the higher  $m_{K\pi\pi}$  region shown in figures 8.2c and 8.2d, the RMF cannot reproduce the  $[\pi\pi]_P$  freed-isobar amplitude as the RMF model consists of only a Breit-Wigner resonance component without a background component. However, one should note that the  $m_{\pi^-\pi^+}$  position of the peak in the intensity spectrum agrees well with the expected position of the  $\rho(770)$  peak also in the higher  $m_{K\pi\pi}$  region shown in figures 8.2c and 8.2d. Furthermore, the agreement between the RMF and the measured  $[\pi\pi]_P$  freed-isobar amplitude is better again for  $m_{K\pi\pi} \gtrsim 1.7 \text{ GeV}/c^2$ . We cannot observe clear indications for excited  $\rho$  states in the measured  $[\pi\pi]_P$  freed-isobar amplitude.

In summary, the  $[\pi\pi]_P$  freed-isobar amplitude from the  $1^+0^+ [\pi\pi]_P K S$  partial wave exhibits a clear  $\rho(770)$ -like signal, whose mass and width agree with previous measurements. This proves that the freed-isobar approach works in principle, even for our comparatively small  $K^-\pi^-\pi^+$  sample. Furthermore, this demonstrates the applicability of the isobar model and of the  $\rho(770)$  Breit-Wigner parameterization with mass and width taken from the PDG in the conventional

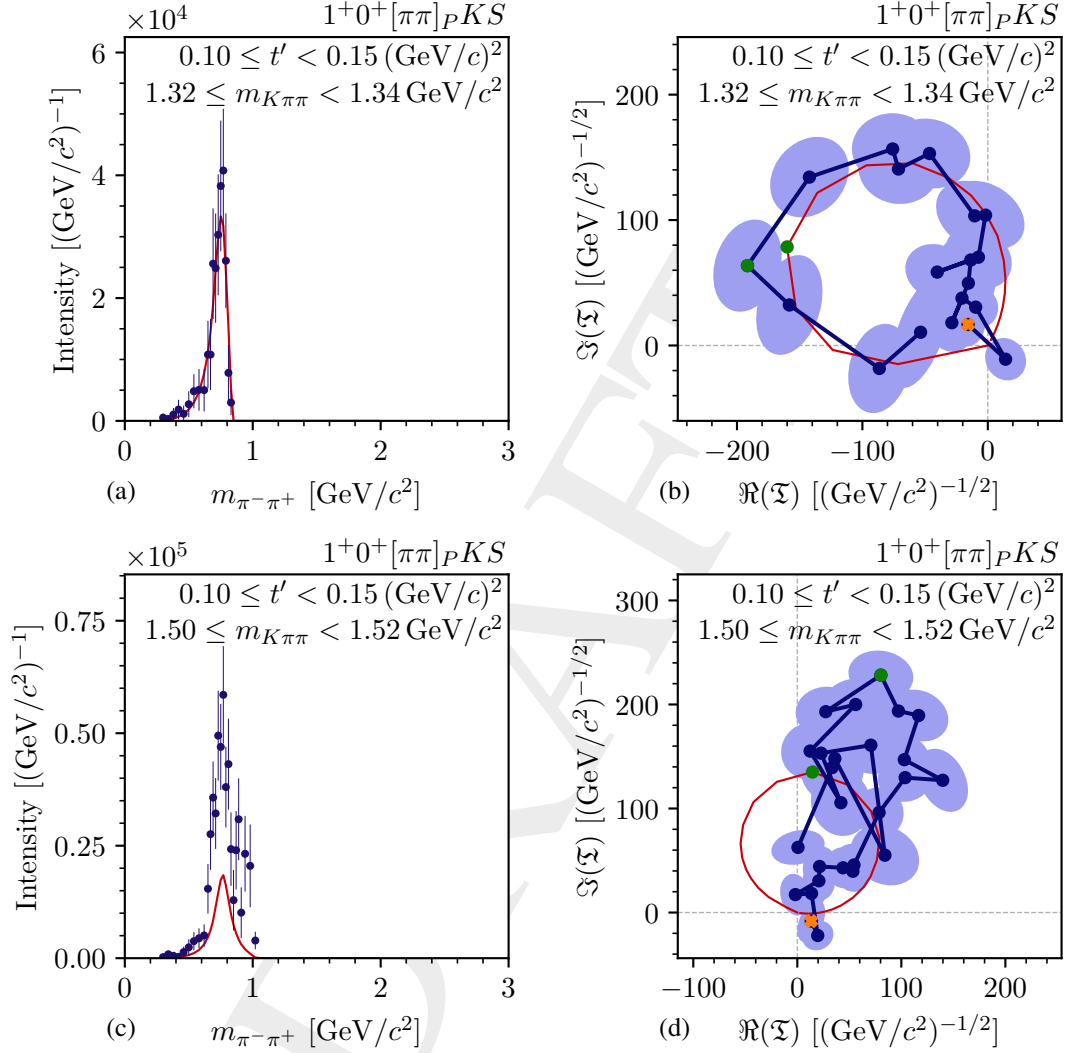


Figure 8.2: Intensities (left column) and Argand diagram (right column), i.e. real vs. imaginary parts of the  $[\pi\pi]_P$  freed-isobar amplitude in the  $1^+0^+[\pi\pi]_P K S$  wave at  $m_{K\pi\pi} \approx 1.33 \text{ GeV}/c^2$  (top row) and  $m_{K\pi\pi} \approx 1.51 \text{ GeV}/c^2$  (bottom row) in the lowest  $t'$  bin. The blue data points represent the result of the freed-isobar PWD. In (b) and (d), the blue shaded areas represent the corresponding uncertainty ellipses and the orange crosses indicate the data point that corresponds to the lowest  $m_{\pi^-\pi^+}$  bin, i.e. the start point of the Argand diagram. The red curves are the model curves from an RMF to the measured  $[\pi\pi]_P$  freed-isobar amplitude. The green data points and the corresponding green points on the model curves indicate the  $m_{\pi^-\pi^+}$  bin that is closest to the nominal mass of the  $\rho(770)$  resonance as obtained in the RMF.



5160 fixed-isobar PWD. Additional effects, such as final-state interactions, i.e. rescattering within the  
 5161 three-body final state,<sup>[b]</sup> seem to have only a minor influence on the dynamic amplitude of the  
 5162 isobars in the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . Hence, the freed-isobar analysis of the  $[\pi\pi]_P$   
 5163 amplitude confirms in a model-independent way our observation of the  $K_1(1270)$  and  $K'_1$  decays  
 5164 to the  $\rho(770)K$  final state, which are discussed in section 7.1.

## 5165 8.2 The $[K\pi]_P$ Amplitude

5166 Besides the  $\rho(770)$ , also the  $K^*(892)$  is a well-known state, which decays dominantly to the  
 5167  $K^- \pi^+$  final state where both are in a  $P$  wave. We study the corresponding  $[K\pi]_P$  freed-isobar  
 5168 amplitude in the largest partial wave with a  $K^*(892)$  isobar, which is the  $1^+ 0^+ K^*(892) \pi S$  wave.  
 5169 Hence, we performed a freed-isobar PWD, where we replaced the  $1^+ 0^+ K^*(892) \pi S$  and  $1^+ 0^+$   
 5170  $K^*(1680) \pi S$  waves included in the conventional 238-wave PWD by a freed  $1^+ 0^+ [K\pi]_P \pi S$   
 5171 wave. However, one should note that both replaced waves are affected by the leakage effect in the  
 5172 conventional PWD. Thus, the leakage effect may also bias the results of the freed-isobar PWD  
 5173 for the  $[K\pi]_P$  amplitude.

5174 Figure 8.3 shows the measured  $[K\pi]_P$  freed-isobar amplitude in two exemplarily selected  $m_{K\pi\pi}$   
 5175 bins in the lowest  $t'$  bin. The intensity spectrum of the  $[K\pi]_P$  freed-isobar amplitude exhibits  
 5176 a clear narrow peak at  $m_{K^- \pi^+} \approx 0.9 \text{ GeV}/c^2$  as shown in figure 8.3a for the  $m_{K\pi\pi}$  region of the  
 5177  $K_1(1400)$ . The corresponding Argand diagram exhibits a circle as expected for the  $K^*(892)$   
 5178 resonance (see figure 8.3b). Figures 8.3c and 8.3d show the  $[K\pi]_P$  amplitude in a higher  $m_{K\pi\pi}$   
 5179 bin. Also here, we observe a clear  $K^*(892)$  peak in the intensity spectrum and a circle in the  
 5180 Argand diagram. In addition, we observe a small high-mass shoulder at  $m_{K^- \pi^+} \approx 1.2 \text{ GeV}/c^2$ .

5181 The red curves in figure 8.3 represent the result of an RMF to the measured  $[K\pi]_P$  freed-isobar  
 5182 amplitude, which we modeled by a single Breit-Wigner component. The RMF reproduces well  
 5183 the intensity spectra of the  $[K\pi]_P$  freed-isobar amplitude over the analyzed  $m_{K\pi\pi}$  range. Also,  
 5184 the Argand diagrams are overall reproduced well. However, at higher  $m_{K\pi\pi}$ , the Argand diagram  
 5185 of the  $[K\pi]_P$  freed-isobar amplitude appears to be rotated and shifted with respect to the RMF  
 5186 curve (see figure 8.3d). As for the  $[\pi\pi]_P$  freed-isobar amplitude discussed in section 8.1, this  
 5187 rotation and shift may indicate small background contributions to the measured  $[K\pi]_P$  freed-  
 5188 isobar amplitude. For  $m_{K^- \pi^+} > 1 \text{ GeV}/c^2$ , the  $[K\pi]_P$  intensity exhibits an enhancement over  
 5189 the RMF curve, which includes only the  $K^*(892)$ . However, in additional RMFs we could not  
 5190 model sufficiently well this  $m_{K^- \pi^+}$  region by the excited  $K^*(1410)$  and  $K^*(1680)$ , which are both  
 5191 listed as established states by the PDG [9]. Hence, we do not observe clear signals of excited  
 5192  $K^*$  states in the measured  $[K\pi]_P$  freed-isobar amplitude. We obtained a mass for the  $K^*(892)$   
 5193 component of about  $895 \text{ MeV}/c^2$  and a width of about  $49 \text{ MeV}/c^2$ . Both values agree well with  
 5194 the corresponding PDG average values of  $(895.55 \pm 0.20) \text{ MeV}/c^2$  and  $(47.3 \pm 0.5) \text{ MeV}/c^2$ ,  
 5195 respectively.

<sup>[b]</sup> See ref. [164] for a discussion on effects from final-state interactions on the amplitudes of two-body subsystems in three-body decays of heavy mesons.

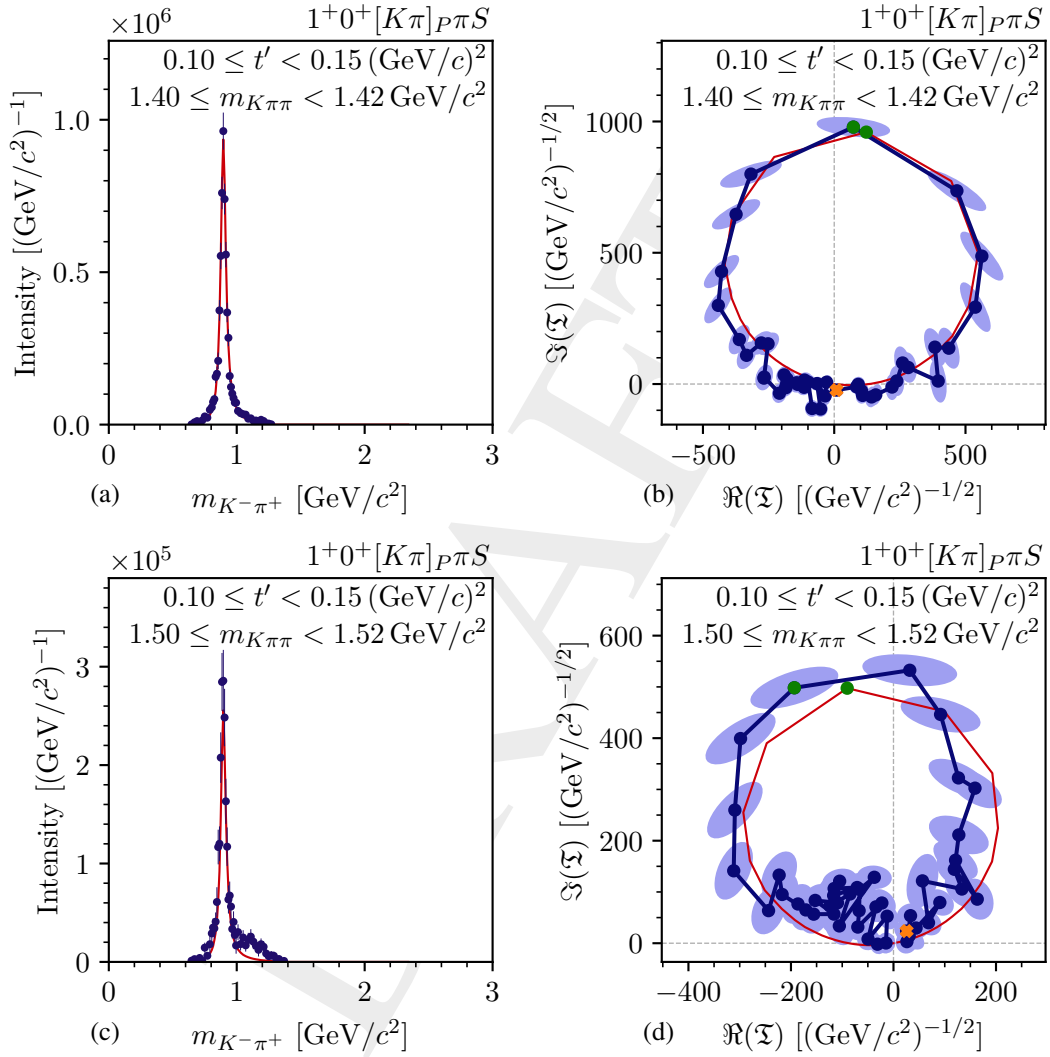


Figure 8.3: Same as figure 8.2, but showing the  $[K\pi]_P$  freed-isobar amplitude from the freed  $1^+0^+[K\pi]_P\pi S$  wave at  $m_{K\pi\pi} \approx 1.41 \text{ GeV}/c^2$  (top row) and  $m_{K\pi\pi} \approx 1.51 \text{ GeV}/c^2$  (bottom row) in the lowest  $t'$  bin.

5196 In summary, we observe a clear  $K^*(892)$  signal in the  $[K\pi]_P$  freed-isobar amplitude as determined  
 5197 from the freed-isobar PWD, whose mass and width agree with previous measurements, and we  
 5198 do not observe pronounced signals from excited  $K^*(1410)$  or  $K^*(1680)$ . This further confirms the  
 5199 applicability of the freed-isobar approach to our  $K^-\pi^-\pi^+$  sample and demonstrates that the PDG  
 5200 average values for the  $K^*(892)$  mass and width used in the conventional PWD are consistent with  
 5201 our data. This good agreement is somewhat surprising and means that the leakage effect does not  
 5202 seem to induce a large bias on the shape of the measured  $[K\pi]_P$  freed-isobar amplitude.

### 5203 8.3 The $[K\pi]_D$ Amplitude

5204 In our analysis, the  $K_2^*(1430)$  appears not only in the  $K^-\pi^-\pi^+$  system in partial waves with  
 5205  $J^P = 2^+$  (see section 7.2), but also in the  $K^-\pi^+$  subsystem as an isobar. In order to study the  
 5206  $K_2^*(1430)$  also in the  $K^-\pi^+$  subsystem, we measured the  $[K\pi]_D$  amplitude in a freed-isobar  
 5207 analysis. The largest wave in the 238-wave set with a  $K_2^*(1430)$  isobar is the  $2^- 0^+ K_2^*(1430)\pi S$   
 5208 wave. However, it still has a small relative intensity of only 1.2%. We performed a freed-isobar  
 5209 PWD, where we replaced the  $2^- 0^+ K_2^*(1430)\pi S$  wave included in the conventional 238-wave  
 5210 PWD by a freed  $2^- 0^+ [K\pi]_D \pi S$  wave.

5211 Figure 8.4 shows the measured  $[K\pi]_D$  freed-isobar amplitude in an exemplarily selected  $m_{K\pi\pi}$  bin  
 5212 at the  $K_2(1770)$  in the lowest  $t'$  bin. The intensity spectrum of the  $[K\pi]_D$  freed-isobar amplitude  
 5213 exhibits a clear peak at  $m_{K^-\pi^+} \approx 1.4 \text{ GeV}/c^2$ . The corresponding Argand diagram show a circle  
 5214 as expected for the  $K_2^*(1430)$  resonance.

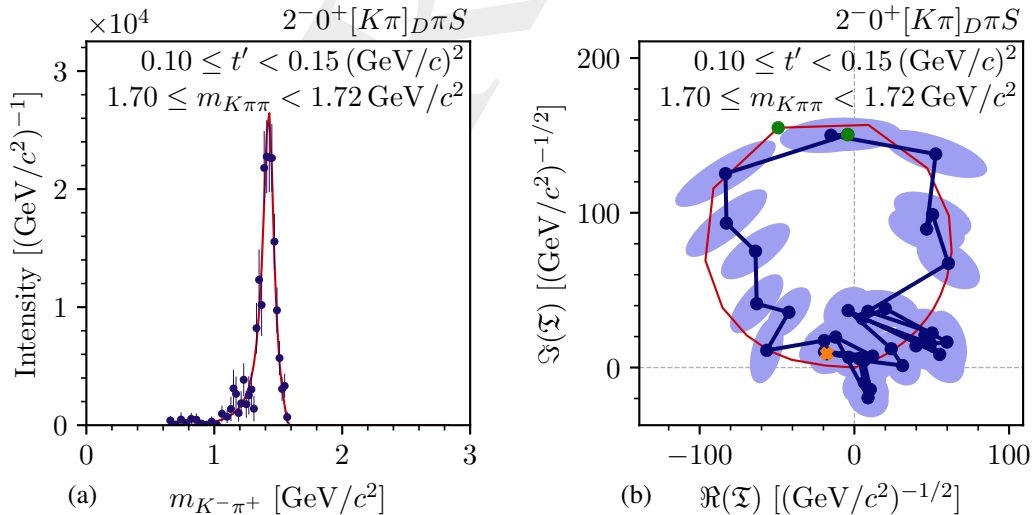


Figure 8.4: Same as figure 8.2, but showing the  $[K\pi]_D$  freed-isobar amplitude from the freed  $2^- 0^+ [K\pi]_D \pi S$  wave at  $m_{K\pi\pi} \approx 1.73 \text{ GeV}/c^2$  in the lowest  $t'$  bin.

5215 The red curves in figure 8.4 represent the result of an RMF to the measured  $[K\pi]_D$  freed-isobar  
 5216 amplitude, which we modeled by a single Breit-Wigner component. The RMF reproduces  
 5217 well the intensity spectra of the  $[K\pi]_D$  freed-isobar amplitude over the analyzed  $m_{K\pi\pi}$  range as  
 5218 exemplarily shown in figure 8.4a. Also, the Argand diagrams are reproduced well. From the  
 5219 freed-isobar analysis, we obtained a mass of the  $K_2^*(1430)$  component of about  $1430 \text{ MeV}/c^2$   
 5220 and a width of about  $106 \text{ MeV}/c^2$ , which are in good agreement with our estimates for the mass  
 5221 and width of the  $K_2^*(1430)$  in the  $K^- \pi^- \pi^+$  decay as obtained from the conventional PWD (see  
 5222 section 7.2). Given that we study the neutral  $K_2^*(1430)$  in the  $K^- \pi^+$  decay and the charged  
 5223  $K_2^*(1430)$  in the  $K^- \pi^- \pi^+$  decay and considering that both measurements yielded the same mass,  
 5224 we do not observe a significant mass difference between the neutral and the charged  $K_2^*(1430)$   
 5225 as indicated by the PDG average values (see discussion in section 7.2). We do not observe any  
 5226 pronounced signal from an excited  $K_2^*(1980)$  in our data.

5227 In summary, the  $[K\pi]_D$  freed-isobar amplitude exhibits a clear  $K_2^*(1430)$  signal. This demon-  
 5228 strates that the freed-isobar approach works even for small waves at the percent level, such as  
 5229 the  $2^- 0^+ K_2^*(1430) \pi S$  wave, and confirms the partial waves with a  $K_2^*(1430)$  resonance in the  
 5230 conventional PWD.

## 5231 8.4 The $[K\pi]_S$ Amplitude

5232 Among the isobar subsystems that can be studied in the freed-isobar analysis, the  $[K\pi]_S$  freed-  
 5233 isobar amplitude is of special interest. It plays a major role in multi-body final states with a  $K\pi$   
 5234 subsystem as the  $K^- \pi^- \pi^+$  final state studied here, but also in many other analyses [26, 162, 165,  
 5235 166]. At the same time, the analytical structure of the  $[K\pi]_S$  amplitude is complicated and not  
 5236 yet well-known. It is hence in the focus of theoretical investigations [98, 101, 167].

5237 The largest wave in the 238-wave set with a  $[K\pi]_S^{K\pi}$  isobar is the  $0^- 0^+ [K\pi]_S^{K\pi} \pi S$  wave with a  
 5238 relative intensity of 5.0%. Hence, we performed a freed-isobar PWD, where we replaced the  
 5239  $0^- 0^+ [K\pi]_S^{K\pi} \pi S$  and  $0^- 0^+ [K\pi]_S^{K\eta} \pi S$  waves included in the conventional 238-wave PWD by a  
 5240 freed  $0^- 0^+ [K\pi]_S \pi S$  wave.

5241 Figure 8.5 shows the measured  $[K\pi]_S$  freed-isobar amplitude in three exemplarily selected  
 5242  $(m_{K\pi\pi}, t')$  cells. At  $m_{K\pi\pi} \approx 1.73 \text{ GeV}/c^2$ , the  $[K\pi]_S$  intensity spectrum shown in figure 8.5a  
 5243 exhibits a peak at  $m_{K^- \pi^+} \approx 1.4 \text{ GeV}/c^2$  with a pronounced low-mass shoulder reaching down to  
 5244 the phase-space border. The corresponding Argand diagram is shown in figure 8.5b. It exhibits  
 5245 a deformed half-circle in the  $m_{K^- \pi^+}$  region of the  $1.4 \text{ GeV}/c^2$  peak. In the  $m_{K^- \pi^+}$  region of the  
 5246 low-mass shoulder, the amplitude in the Argand diagram moves only slowly with a bulge. Both,  
 5247 the intensity spectrum and the Argand diagram show similarities to the fixed  $[K\pi]_S^{K\pi}$  isobar  
 5248 dynamic amplitude used in the conventional PWD (see figure 5.5).<sup>[c]</sup> Hence, the  $1.4 \text{ GeV}/c^2$

<sup>[c]</sup> The measured  $[K\pi]_S$  freed-isobar amplitude also includes phase-space effects, in contrast to the fixed  $[K\pi]_S^{K\pi}$  isobar dynamic amplitude shown in figure 5.5. However, these phase-space effects are only slowly changing with mass and not introduce peaks.

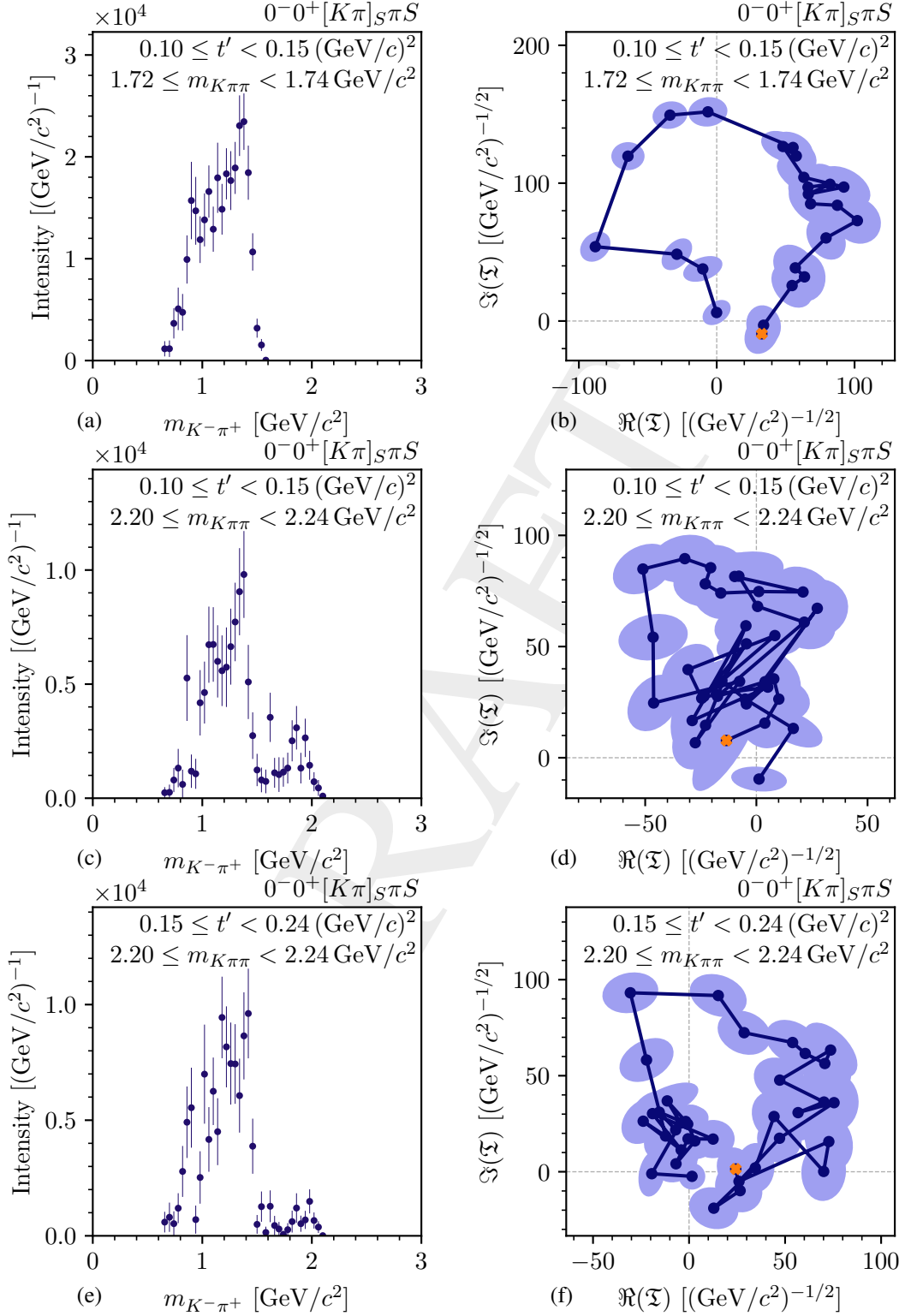


Figure 8.5: Same as figure 8.2, but showing the  $[K\pi]_S$  freed-isobar amplitude in the  $0^-0^+[K\pi]_S\pi\pi S$  wave at  $m_{K\pi\pi} \approx 1.73 \text{ GeV}/c^2$  (top row) and  $m_{K\pi\pi} \approx 2.22 \text{ GeV}/c^2$  (middle row) in the lowest  $t'$  bin and at  $m_{K\pi\pi} \approx 2.22 \text{ GeV}/c^2$  in the second-lowest  $t'$  bin (bottom row).

5249 peak indicates a  $K_0^*(1430)$  signal in our data and the low-mass shoulder is presumably driven by  
 5250 the  $K_0^*(700)$ .

5251 At higher  $m_{K\pi\pi}$ , we still observe the same features in the intensity spectra and the Argand diagram  
 5252 for  $m_{K^-\pi^+} \lesssim 1.6 \text{ GeV}/c^2$  as exemplarily shown in figures 8.5c to 8.5f for  $m_{K\pi\pi} \approx 2.22 \text{ GeV}/c^2$  in  
 5253 the two lowest  $t'$  bins. In the—now accessible— $m_{K^-\pi^+} \gtrsim 1.6 \text{ GeV}/c^2$  region, the intensity spectra  
 5254 of the  $[K\pi]_S$  freed-isobar amplitude exhibit another peak at about  $1.9 \text{ GeV}/c^2$  (see figures 8.5c  
 5255 and 8.5e). This peak is accompanied by structures at the end of the Argand diagrams, which  
 5256 are clearest in the  $(m_{K\pi\pi}, t')$  cell shown in figure 8.5f. However, due to the limited precision  
 5257 of our  $K^-\pi^-\pi^+$  sample, we cannot resolve a clear circle at  $m_{K^-\pi^+} \approx 1.9 \text{ GeV}/c^2$ , which would  
 5258 clarify the resonance character of the intensity peak. Still, the peak at  $m_{K^-\pi^+} \approx 1.9 \text{ GeV}/c^2$  is an  
 5259 indication for a possible  $K_0^*(1950)$  isobar signal in our data.

5260 In summary, the similarities of the measured  $[K\pi]_S$  freed-isobar amplitude to the fixed model used  
 5261 for the  $[K\pi]_S^{K\pi}$  and  $[K\pi]_S^{K\eta}$  dynamic amplitudes indicate the observation of  $K_0^*(700)$ ,  $K_0^*(1430)$ ,  
 5262 and possibly  $K_0^*(1950)$  signals in our data. Since in particular the  $K_0^*(700)$  and  $K_0^*(1430)$  are  
 5263 overlapping due to their large widths, the modeling of the  $[K\pi]_S$  freed-isobar amplitude would  
 5264 require a more elaborate RMF model than a simple sum of Breit-Wigner amplitudes. With the  
 5265 help of such a more elaborate model, we could also measure the properties of the  $K_0^*$  states, i.e.  
 5266 their pole parameters. Furthermore, the freed  $0^- 0^+$   $[K\pi]_S \pi S$  wave has an isotropic distribution  
 5267 in all decay angles.<sup>[d]</sup> As an isotropic distribution is less characteristic and thus harder to  
 5268 distinguish, e.g. from background, we expect the  $[K\pi]_S$  wave to be more likely affected by  
 5269 systematic effects or analysis artifacts. This would need to be studied in dedicated systematic  
 5270 and pseudodata studies, which are beyond the scope of this work. However, the first glimpse on  
 5271 the  $[K\pi]_S$  freed-isobar amplitude presented in this section, as well as the consistent results from  
 5272 the three other freed-isobar analyses, demonstrate that the COMPASS  $K^-\pi^-\pi^+$  sample has the  
 5273 potential to also deepen our knowledge about the  $[\pi\pi]_P$ ,  $[K\pi]_P$ ,  $[K\pi]_D$ , and  $[K\pi]_S$  systems.

<sup>[d]</sup> The orbital angular momentum  $L$  in the isobar-bachelor system is 0 as well as the orbital angular momentum in the  $K^-\pi^+$  isobar subsystem.

## 9 Conclusions and Outlook

5275 We employed the diffractive-scattering reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  to explore the excitation  
 5276 spectrum of strange mesons based on a data sample that was collected during the 2008 and 2009  
 5277 diffraction data-taking campaigns of the COMPASS experiment. The event selection was based  
 5278 on an unpublished study of this reaction at COMPASS [44] and was considerably improved. One  
 5279 of the major challenges of this event selection is the separation of beam kaons from the about 36  
 5280 times larger pion contribution in the beam. To this end, we developed a novel likelihood-based  
 5281 approach that exploits the full information from both CEDAR detectors. Our approach yields  
 5282 an excellent performance for beam-kaon identification with an efficiency of about 85 %—about  
 5283 twice as large as the efficiency of the previously used method—while maintaining a low impurity  
 5284 from pions of about 3 %. Our optimized event selection yields the so far world’s largest  $K^- \pi^- \pi^+$   
 5285 sample of 720 949 events, which is about 3.6 times larger than the previously world’s largest  
 5286  $K^- \pi^- \pi^+$  sample obtained by the WA3 experiment at CERN [23].

5287 Based on this data sample, we performed a partial-wave decomposition (PWD), where we extract  
 5288 the  $m_{K\pi\pi}$  and  $t'$  dependence of the transition amplitudes of partial waves with well-defined  
 5289 quantum numbers and decay modes of the  $K^- \pi^- \pi^+$  system. We inferred the set of partial waves  
 5290 that need to be included in the PWD model from the data. To this end, we started with a large  
 5291 pool of 596 allowed waves considering spins up to  $J = 7$ . To select those waves that significantly  
 5292 contribute to the data, we added regularization terms to the likelihood function that are based  
 5293 on model-selection techniques to select those waves that significantly contribute to the data. In  
 5294 comparison to previous analyses applying model-selection techniques [67, 108], we extended the  
 5295 approach by incorporating effects from the experimental acceptance in the regularization terms  
 5296 and by imposing continuity in  $m_{K\pi\pi}$  for the selected wave sets. Both extensions clearly improved  
 5297 the selected wave sets. Furthermore, we improved the estimates for the parameter values and  
 5298 their uncertainties determined from the PWD by using Bootstrapping techniques starting at the  
 5299 event-sample level. In addition, we performed first studies of applying the freed-isobar technique,  
 5300 which allowed us to study for the first time the amplitudes of the  $K^- \pi^+$  and  $\pi^- \pi^+$  subsystems in  
 5301 the diffractively produced  $K^- \pi^- \pi^+$  final state.

5302 We observe artificially enhanced partial-waves intensities in a limited set of partial waves for  
 5303  $m_{K\pi\pi} \lesssim 1.6 \text{ GeV}/c^2$ . These artifacts are caused by the loss of information due to the limited  
 5304 kinematic coverage of our final-state particle identification. This so-called leakage effect limits  
 5305 the physics reach of our analysis. However, we could clearly identify waves affected by the  
 5306 leakage effect using three different approaches, which yielded consistent results. This allowed us  
 5307 to still study strange mesons in the large set of non-leakage waves, which covers a variety of  $J^P$   
 5308 sectors and decay modes.

5309 We searched for strange mesons and measured their masses and widths by performing resonance-  
 5310 model fits (RMFs) to the spin-density matrix elements of selected waves, which were extracted  
 5311 by the conventional and the freed-isobar PWDs. For the main analysis, we selected a subset  
 5312 of 10 partial waves, which included 7 resonance components. We extended this 10-wave RMF  
 5313 model in dedicated studies of further resonances. To construct the RMF models, we employed  
 5314 Breit-Wigner amplitudes. It is worth stressing that we obtained our estimates for the masses and  
 5315 widths of the strange mesons by fitting simultaneously a large set of partial waves from different  
 5316  $J^P$  sectors taking into account all interference terms between these partial waves. We also freed  
 5317 the mass and width parameters for all studied strange-meson resonances,<sup>[a]</sup> in contrast to many  
 5318 previous analyses [23, 24, 26, 27, 30].

5319 One of the major challenges of our analysis is the treatment of incoherent background in our  
 5320  $K^-\pi^-\pi^+$  sample. We developed an ansatz where we effectively treat these incoherent background  
 5321 contributions at the level of the PWD and explicitly model them in the RMFs. The largest  
 5322 incoherent background of about 6.7 % arises from events of the reaction  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$ .  
 5323 We take into account this background component by employing a high-quality model obtained  
 5324 by the analysis of the COMPASS  $\pi^-\pi^-\pi^+$  sample [43].

5325 Finally, we performed extensive studies to verify our analysis approach and to estimate systematic  
 5326 effects. We performed a variety of pseudodata studies of the PWD and RMF. With these studies  
 5327 we showed the self-consistency of our analysis. For example, we performed an input-output  
 5328 studied by applying our full analysis chain to a pseudodata sample that includes resonances  
 5329 with known masses and widths. Then we measured these masses and widths again in the RMF.  
 5330 Especially noteworthy, we demonstrated that we can separate  $K^-\pi^-\pi^+$  signals from  $\pi^-\pi^-\pi^+$   
 5331 background by mixing pure  $K^-\pi^-\pi^+$  and  $\pi^-\pi^-\pi^+$  pseudodata samples. We performed also a first  
 5332 set of systematic studies covering potential influences from the event selection, the PWD model,  
 5333 and the 10-wave RMF model. From these studies, we obtained lower bounds for systematic  
 5334 uncertainties, which are typically of comparable size as the statistical uncertainties.

5335 In summary, we performed the so-far most comprehensive analysis of the  $K^-\pi^-\pi^+$  final state.  
 5336 We determined the parameters of 7 strange mesons by simultaneously fitting the intensities  
 5337 and interference terms of 10 selected waves. The parameters of 6 further strange mesons were  
 5338 determined in dedicated studies. Finally, the  $\rho(770)$ ,  $K^*(892)$ , and  $K_2^*(1430)$  mesons appearing  
 5339 in the  $\pi^-\pi^+$  and  $K^-\pi^+$  subsystems were studied in freed-isobar analyses. In total, the extracted  
 5340 resonances cover almost all  $J^P$  sectors as shown in figure 9.1. This way we obtained the so-far  
 5341 most complete picture of the strange-meson spectrum coming from a single analysis.

5342 We observe signals of well-known strange mesons, such as the  $K_1(1270)$  and the  $K_J^*$  states, but  
 5343 also of states that need further confirmation, such as the  $K_2(2250)$ , in the partial-wave intensities  
 5344 and in the interference terms represented by the relative phases. Given the large size of our  
 5345  $K^-\pi^-\pi^+$  sample we could study small signals down to the per-mil level such as the  $K_4^*(2045)$ .  
 5346 By binning our data in  $t'$ , we also studied the  $t'$  dependencies of the extracted resonances,

<sup>[a]</sup> The  $K_1(1400)$  could not be studied, because it is only a very small signal in the analyzed  $1^+$  waves. We had to fix the parameters of the corresponding component to the PDG average values in the RMFs.



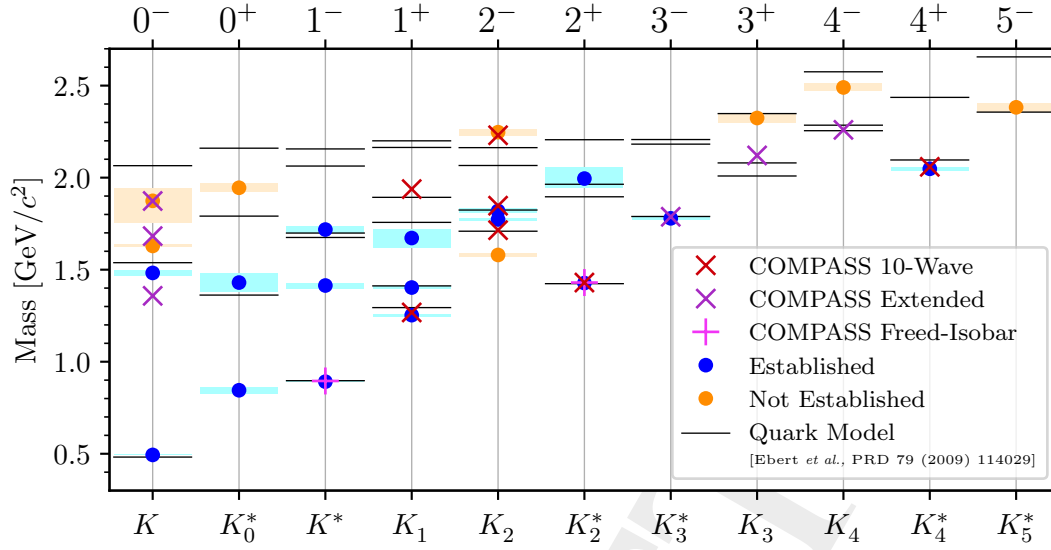


Figure 9.1: Spectrum of strange mesons, i.e. nominal masses of strange mesons grouped by their  $J^P$  quantum numbers. The crosses represented our measured mass values as obtained from the 10-wave RMF (red) or from the corresponding dedicated studies (violet) (see chapter 7). The magenta pluses represent our measured mass values as obtained from the freed-isobar analysis (see chapter 8). Analogously to figure 1.1, the blue data points show the masses of established states, the orange data points those of not established states as listed by the PDG [9]. The similarly colored boxes represent the corresponding uncertainties. The black horizontal lines show the masses of states as predicted by the quark-model calculation in ref. [10]. As we show only masses below  $2.7 \text{ GeV}/c^2$  for a better visualization, the not-established  $K(3100)$  is omitted here.

5347 which typically show the expected behavior. This supports the resonance nature of the observed  
 5348 signals. In most cases, our estimates for the masses and widths of the 14 studied strange mesons  
 5349 agree with previous measurements and with quark-model calculations (see figure 9.1). Our  
 5350 uncertainties for most of the measured masses and widths are competitive with the corresponding  
 5351 so far best measurements of these parameters. For the widths of the  $K_4^*(2045)$  and  $K_2(1820)$ , we  
 5352 obtained even the so far smallest uncertainties.<sup>[b]</sup>

5353 Our analysis not only provides a high-precision measurement of the masses and widths, but also  
 5354 adds complementary information. For example, we performed the first search<sup>[c]</sup> for the  $K_2(2250)$   
 5355 in final states other than  $\bar{\Lambda}^0 \bar{p}$ . In contrast to previous analyses of the  $J^P = 2^-$  sector [24, 30, 31,  
 5356 34–37, 152–155], we studied a wide mass range in a single self-consistent analysis by including  
 5357 three  $K_2$  states and by simultaneously fitting four  $2^-$  partial waves, which represent different  
 5358 decay modes. Similarly, we also studied the  $K_3(2320)$  and  $K_4(2500)$  for the first time in final  
 5359 states other than  $\bar{\Lambda}^0 \bar{p}$ .

<sup>[b]</sup> Disregarding measurements that were not included in the corresponding PDG average and measurements for which it is not clear whether their uncertainties include systematic uncertainties, we obtained in addition the so far smallest uncertainties for the masses of the  $K_1'$ ,  $K_2(1770)$ ,  $K_2(1820)$ , and  $K_4^*(2045)$ , and for the widths of the  $K_1'$  and  $K_2(1770)$ .

<sup>[c]</sup> According to the PDG listing [9].

5360 Furthermore, we performed a first study of excited pseudoscalar kaons over a wide mass range  
 5361 in a single analysis. We find indications for three excited pseudoscalar kaons; i.e. the  $K(1460)$ ,  
 5362 the  $K(1630)$ , and the  $K(1830)$ ; while quark-model calculations predict only two states in this  
 5363 mass region. Especially, the  $K(1630)$  signal is the clearest among these three signals and is least  
 5364 compatible with the two quark-model states (see figure 9.1). This suggests that the  $K(1630)$  is a  
 5365 supernumerary state and thus a candidate for a crypto-exotic state.

5366 Another way to represent our results is in the form of a Chew-Frautschi plot as shown in figure 9.2.  
 5367 As first discussed by Chew and Frautschi [45], mesons group into families, which lie on so-called  
 5368 Regge trajectories. It is a long-known experimental observation that these Regge trajectories  
 5369 correspond to approximately straight lines in the Chew-Frautschi plot [46].<sup>[d]</sup>

5370 Also, our measurements of strange mesons nicely group into three families in the Chew-Frautschi  
 5371 plot, i.e. the  $K_J^*$  ground states, the  $K_J$  ground states, and the  $K_J$  excited states. The members of  
 5372 these three families follow approximately linear Regge trajectories,

$$J(m_0) = \alpha_0 + \alpha' m_0^2, \quad (9.1)$$

5373 which are represented by the orange, green, and blue lines in figure 9.2.<sup>[e]</sup> Table 9.1 lists the  
 5374 parameters of all three Regge trajectories.<sup>[f]</sup> Our estimates for the parameters of the Regge  
 5375 trajectories are in agreement with those determined from a quark-model calculation in ref. [10]  
 5376 and with those determined from previous measurements in ref. [170], except for the trajectory of  
 5377 the  $K_J$  excited states, which has a slightly smaller slope value in our case and a larger intersect.<sup>[g]</sup>  
 5378 In summary, our analysis yields a Chew-Frautschi plot with three Regge trajectories up to high  
 5379 meson spins of  $J = 4$ , and gives a consistent picture of the strange-meson spectrum. This  
 5380 again demonstrates that we explored a large fraction of the known strange-meson spectrum at  
 5381 COMPASS using data from only a single reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ .

## 5382 9.1 Outlook and Further Prospects

5383 In this work, we performed a first set of systematic studies. In order to obtain estimates for  
 5384 the full systematic uncertainties, a complete set of systematic studies has to be performed in a  
 5385 further analysis. Obtaining such a complete set of systematic studies was not possible within the

<sup>[d]</sup> Also, QCD string models [168] and calculations using Salpeter equations [169] predict linear Regge trajectories. More detailed studies allow for a non-zero curvature of the Regge trajectories, from which conclusions on the “appropriate dynamic equation and potential to describe mesons” [170] can be drawn.

<sup>[e]</sup> Our estimate for the  $K_4(2500)$  mass (violet point for  $J = 4$ ) might be too low to fit onto the corresponding linear Regge trajectory (green line). This may indicate a non-zero curvature of the Regge trajectory as observed in e.g.ref. [170]. However, since we do not yet have systematic uncertainties for this mass estimate, we cannot make a clear statement on the curvature of the Regge trajectories here.

<sup>[f]</sup> See caption of figure 9.2 for details on the fitting of the three Regge trajectories.

<sup>[g]</sup> The smaller slope value for trajectory of the  $K_J$  excited states can partly be explained by our comparably low mass estimate for the  $K(1460)$ , for which we have, however, no systematic uncertainty. This may also explain the larger intersect.

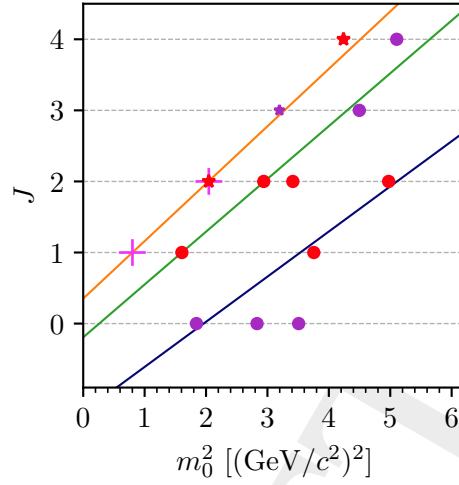


Figure 9.2: Chew-Frautschi plot of strange mesons, i.e. spin  $J$  of the state versus its nominal-mass squared as obtained from our analysis. The stars represent  $K_J^*$  ground states, the dots represent  $K_J$  states. The red stars and dots show the results obtained from the 10-wave RMF, the violet stars and dots show the results of the corresponding extended RMF. The magenta pluses show the results for the  $K^*(892)$  and  $K_2^*(1430)$  as obtained from the freed-isobar analyses. The orange, green, and blue lines represent fits of Regge trajectories to the  $K_J^*$  states,  $K_J$  ground states, and  $K_J$  excited states, respectively. The  $K_2(1820)$  is not considered for the green Regge trajectory of the  $K_J$  ground states. The  $K(1460)$  is considered for the blue Regge trajectory of the excited  $K_J$  states. The  $K(1630)$  and  $K(1830)$  were not considered for the fit, because they belong to higher excitations or are potential supernumerary states. In order to obtain the linear Regge trajectories, we performed  $\chi^2$  fits where we took into account only the statistical uncertainties of our mass estimates and where we neglected all correlations for simplicity.

Table 9.1: Intercepts  $\alpha_0$  and slopes  $\alpha'$  of the three Regge trajectories of the  $K_J^*$  ground states,  $K_J$  ground states, and  $K_J$  excited states ( $K_J'$ ). The first line lists our rough estimates for the parameters of the Regge trajectories, the second line lists the parameters as obtained from a quark-model calculation in ref. [10], the third line lists the parameters as obtained from previous measurements (prev. meas.) in ref. [170]. As we do not yet have systematic uncertainties for the parameter estimates from the extended RMFs and the freed-isobar analyses, we cannot give systematic uncertainties for our parameters of the Regge trajectories. Hence, we quote here only rough estimates without uncertainties. Also, in ref. [170] no uncertainties are quoted and we do not list the uncertainties from ref. [10] for a clear arrangement.

	$K_J^*$		$K_J$		$K_J'$	
	$\alpha_0$	$\alpha'$ [(GeV/c <sup>2</sup> ) <sup>-2</sup> ]	$\alpha_0$	$\alpha'$ [(GeV/c <sup>2</sup> ) <sup>-2</sup> ]	$\alpha_0$	$\alpha'$ [(GeV/c <sup>2</sup> ) <sup>-2</sup> ]
COMPASS	0.35	0.81	-0.19	0.74	-1.24	0.64
Quark model	0.318	0.839	-0.197	0.780	-2.240	0.964
Prev. meas.	0.25	0.89	-0.15	0.69	-2.1	0.97

5386 scope of this work. For example, systematic effects from the choice of partial waves and model  
 5387 components included in the RMFs have to be studied. Nonetheless, we expect our first estimates  
 5388 for the systematic uncertainties to not drastically underestimate the full systematic uncertainties.  
 5389 Also, systematic studies of the extended RMFs and the freed-isobar analyses still have to be  
 5390 performed.

5391 There are also aspects of our analysis that may be improved in the future in order to reduce  
 5392 systematic uncertainties. Furthermore, by comparing the results of improved analyses to our  
 5393 results, our results could be further scrutinize. While we used a rank=3 model in the final 238-  
 5394 wave PWD, we performed the wave-set selection using only a rank=1 model, because a wave-set  
 5395 selection using a rank=3 model is computationally and technically much more demanding. This  
 5396 in principle can lead to a too large wave set. However, we do not find artifacts that hint at a  
 5397 too large wave set in the results of the 238-wave PWD. In a future analysis, performing the  
 5398 wave-set selection using a rank=3 model could validate our results. Also, Breit-Wigner models  
 5399 as used in our RMFs are good approximations only in the case of narrow isolated resonances.  
 5400 In cases of overlapping resonances, such as the  $K_2(1770)$  and  $K_2(1820)$ , more elaborate models  
 5401 that incorporate constraints imposed by unitarity and analyticity may in principle improve the  
 5402 RMF results. In particular, such elaborate models would allow a future analysis to determine the  
 5403 pole parameters and couplings, which—in contrast to Breit-Wigner parameters and branching  
 5404 fractions—represent the actual, fundamental, and process-independent properties of a resonance.  
 5405 A step in this direction was achieved by the authors of ref. [134], who developed such a model  
 5406 for the  $\eta^{(\prime)}\pi$  final state. However, three-body final states, such as the  $K^-\pi^-\pi^+$  final state analyzed  
 5407 in our work, are much more complicated and there are no already applicable models for them  
 5408 available. Developing such models for three-body final states requires close collaboration  
 5409 between experimentalists and theorists.

5410 At COMPASS, the  $K^-\pi^-\pi^+$  final state is the flag-ship channel for strange-meson spectroscopy.  
 5411 The COMPASS samples for other charge combinations such as the  $K^-\pi^0\pi^0$  or the  $K_S^0\pi^-\pi^0$   
 5412 final states are expected to be significantly smaller due to the smaller experimental acceptance  
 5413 for detecting and reconstructing a  $\pi^0$ . However, as the  $\pi^0$  and the  $K_S^0$  are identified by their  
 5414 reconstruction, the charged particles in these final states do not need to be positively identified by  
 5415 the RICH. Thus, in contrast to our analysis, these two channels do not suffer from acceptance  
 5416 effects from the RICH particle identification. Therefore, the study of the  $K^-\pi^0\pi^0$  and  $K_S^0\pi^-\pi^0$   
 5417 final states may give complementary information to our analysis.

5418 While the  $K\pi\pi$  final state allows us to study in principle the full strange-meson spectrum,  
 5419 strange mesons can be studied at COMPASS also in other final states, which provide additional  
 5420 information on parts of the strange-meson spectrum. For example, an analysis of the  $K_S^0\pi^-\pi^0$  final  
 5421 state, in which  $K_j^*$  states can be studied with high precision, is currently ongoing [65, 171].<sup>[h]</sup>  
 5422 States at higher masses can be addressed in final states with heavier particles such as  $K^-\phi$ ,  $K^-\omega$ ,  
 5423 and  $\Lambda\bar{p}$ . At COMPASS, also these final states can in principle be studied. Hence, COMPASS  
 5424 will contribute further to improve our understanding of the strange-meson sector.

<sup>[h]</sup> Unfortunately,  $K_0^*$  states, i.e. the  $[K\pi]_S$  amplitude, cannot be studied in this final state, because states with  $J^P = 0^+$  cannot be produced in diffractive scattering of a kaon beam.

5425 Furthermore, strange mesons will be studied in the decays of heavy mesons and  $\tau$  leptons using  
 5426 upcoming high-precision data from currently running experiments such as Belle II, BES III,  
 5427 and LHCb. For example, strange mesons can be studied in the decay  $\tau^- \rightarrow K^- \pi^- \pi^+ \nu_\tau$ , for  
 5428 which Belle II will measure a large sample. However,  $\tau$  decays are dominated by only  $K_1$  states.  
 5429 Also, often only a limited mass range is accessible in the decays of heavy mesons and  $\tau$  leptons,  
 5430 as discussed, for example, in section 7.1.1 for the  $B^+ \rightarrow J/\psi \phi K^+$  decay studied by LHCb at  
 5431 CERN [34]. Still, with continuously growing data samples, we can expect more precise studies  
 5432 of the strange-meson sector from decays of heavy mesons or  $\tau$  leptons.

5433 Another laboratory to study strange mesons are photo-production reactions. There are plans [172,  
 5434 173] to study final states with strange mesons such as  $KK\pi\pi$  at the GlueX experiment at Jefferson  
 5435 Lab by employing an upgraded final-state particle identification based on a DIRC detector  
 5436 originally used by the BaBar experiment [25, 174]. This would allow GlueX to study strange  
 5437 mesons appearing in the  $K\pi\pi$  and  $K\pi$  subsystems using methods similar to our freed-isobar  
 5438 approach. Also at Jefferson Lab, a proposal for strange-hadron spectroscopy with a secondary  
 5439  $K_L^0$  beam using the GlueX spectrometer was recently approved [175]. The meson spectroscopy  
 5440 part of the physics program focuses mainly on the  $K\pi$  final state, with the goal to study  $K_J^*$  states  
 5441 with high precision.

5442 While the spectroscopy program of the PANDA experiment, which is currently under construction  
 5443 at GSI, focuses on mainly charm and hyperon physics, PANDA can in principle also study strange  
 5444 mesons in reactions such as  $\bar{p}p \rightarrow K^+ K^0 \pi^- \pi^+ \pi^-$  [176].

5445 Finally, there is a letter of intent for a new QCD facility at CERN's M2 beam line called  
 5446 AMBER [177]. A pilot run for the first phase of this experiment using the existing M2 beam  
 5447 line has already been approved by CERN [178]. The second phase of this experiment proposes  
 5448 to upgrade the M2 beam line in order to allow radio-frequency separation of the beam particles  
 5449 and thereby drastically increasing the antiproton and kaon fraction in the hadron beam. The  
 5450 very broad physics program of the second phase includes strange-meson spectroscopy. The goal  
 5451 is to collect a  $K^- \pi^- \pi^+$  sample of more than  $10 \times 10^6$  events, i.e. roughly 10 times larger than  
 5452 our existing COMPASS  $K^- \pi^- \pi^+$  sample. With such a data sample, AMBER could map out the  
 5453 strange-meson spectrum with unprecedented detail and precision, similar to what the analysis of  
 5454 the large COMPASS  $\pi^- \pi^- \pi^+$  sample did for the non-strange light-meson sector [39, 41]. With  
 5455 our work, we prepared the road map for such an analysis by applying sophisticated techniques  
 5456 such as the wave-set selection, the correction for the  $\pi^- \pi^- \pi^+$  background, and the freed-isobar  
 5457 analysis.

5458 In summary, with our results from the  $K^- \pi^- \pi^+$  final state at COMPASS and with many upcoming  
 5459 results from various experiments, strange-meson spectroscopy is entering a high-precision era.  
 5460 This will lead to a more precise and in particular a more complete picture of the excitation  
 5461 spectrum of strange mesons. It will deepen our understanding of the strong interaction, which  
 5462 forms these mesons, and it will also have an impact on other fields of physics, such as the search  
 5463 for  $CP$  violation in multi-body decays of heavy mesons, where these strange mesons appear as  
 5464 well.



# 5465 A Particle Identification

## 5466 A.1 Beam-Particle Identification

### 5467 A.1.1 Calibration Data Sample

5468 In section 3.1.4, we developed a method for beam-particle identification using the information  
5469 of both CEDAR detectors, based on a likelihood ansatz. The parameters of the corresponding  
5470 likelihood function in equation (3.13) can be determined by any calibration sample containing a  
5471 mixture of the different beam-particle species. The only requirement for this calibration samples  
5472 is that it needs to be sufficiently large to perform a time-dependent calibration.

### 5473 Preselection

5474 First, a preselection was performed, which is common to the calibration sample and the per-  
5475 formance validation samples discussed in appendix A.1.2. The following cuts were applied:

- 5476
- 5477 • DT0 trigger
- 5478 • Exactly one candidate for the interaction vertex of the beam particle was reconstructed
- 5479 • Beam track was measured with the silicon detectors of the beam telescope<sup>[a]</sup>
- 5480 • The beam track coincides with the event in time:  $|t_{\text{Beam}}| < 5 \text{ ns}$ <sup>[b]</sup>

### 5481 Final Selection

5482 To obtain a large calibration sample with good quality, we used an event sample with three  
5483 charged hadrons in the final state. In addition, this sample has a similar resolution of the measured  
5484 beam-particle inclination as the  $K^- \pi^- \pi^+$  sample, which important for the likelihood calibration  
5485 as discussed in section 3.1.4 of the main text. The following cuts were applied:

---

<sup>[a]</sup> This is done by requiring that the last measured  $z$  position of the beam track was at most 200 cm upstream of the target.

<sup>[b]</sup> The time of the event, i.e. the time of the trigger signal is by construction  $t_{\text{trigger}} = 0 \text{ ns}$ .

- 5486 • Preselection as discussed above
- 5487 • Three charged tracks leave the interaction vertex
- 5488 • Vertex  $z$  position in the target region:  $-65 \text{ cm} < z_{\text{PV}} < -30 \text{ cm}$
- 5489 • Exclusivity:  $|E_{\text{sum}} - 191 \text{ GeV}| < 8 \text{ GeV}$  with  $E_{\text{sum}} = \sum_{i=1}^3 E_{\text{track},i}$

5490 It is very important to use the DT0 trigger. Otherwise, the CEDAR trigger, which was tuned to  
 5491 trigger on events with incoming beam kaons, heavily biases the result of the calibration.

### 5492 A.1.2 Validation Data Samples

5493 To study the properties of the likelihood-based beam-particle identification and to determine its  
 5494 efficiency and impurity, clean pion-beam and kaon-beam samples are needed.

5495 A pion-beam sample with small kaon contribution was obtained by selecting events of the  
 5496 reaction  $\pi^- + p \rightarrow \pi^- \pi^0 \pi^0 + p$ . In this channel, the complete final state can be identified. The  $\pi^0$   
 5497 were identified via their decay  $\pi^0 \rightarrow \gamma\gamma$  using the ECALs and the  $\pi^-$  was identified using the  
 5498 RICH detector. The following selection cuts were applied to the events:

- 5499 • Preselection (see appendix A.1.1)
- 5500 • One charged track leaving the interaction vertex
- 5501 • Vertex  $z$  position in the target region:  $-65 \text{ cm} < z_{\text{PV}} < -30 \text{ cm}$
- 5502 • Exactly four ECAL clusters without associated charged track called neutral clusters with:  
 5503 (see ref. [179] for details)
  - 5504 \*  $E_{\text{Cluster}} > 0.6 \text{ GeV}$  for ECAL1 or  $E_{\text{Cluster}} > 1.2 \text{ GeV}$  for ECAL2
  - 5505 \*  $|t_{\text{Cluster}} - t_0(E_{\text{Cluster}})| < 3\sigma_{\text{ECAL}}(E_{\text{Cluster}})$ <sup>[c]</sup>
- 5506 • Exactly one combination of these four clusters to build two  $\pi^0$  candidates that each fulfills  
 5507  $|m_{\gamma_i\gamma_j} - 135 \text{ MeV}/c^2| < 11 \text{ MeV}/c^2$
- 5508 • Exclusivity:  $|E_{\pi^- \pi^0 \pi^0} - 191 \text{ GeV}| < 10 \text{ GeV}$
- 5509 • The charged outgoing particle was identified as a pion using the RICH detector
  - 5510 \* Particle momentum in the range  $10 \text{ GeV}/c < p_{\pi^-} < 30 \text{ GeV}/c$
  - 5511 \* RICH likelihood:  $\mathcal{L}^{\text{RICH}}(\pi) \geq 1.4\mathcal{L}^{\text{RICH}}(K)$  and  $\mathcal{L}^{\text{RICH}}(\pi) \geq 1.4\mathcal{L}^{\text{RICH}}(p)$

5512 Applying these cuts, we obtained pion-beam samples of 1 223 190 events for the 2008 and  
 5513 1 159 220 events for the 2009 diffraction data set, which are large enough to make reliable  
 5514 statements about efficiency and impurity. Figure A.1a shows the ratio of the distribution of the  
 5515 beam-particle inclinations for this pion-beam sample and the corresponding distribution of the  
 5516 three-hadron sample used to calibrate the likelihood parameterization (see section 3.1.4). Both  
 5517 distributions are normalized to their data set size. In the important central region, the ratio is

<sup>[c]</sup> This cut was applied only to the 2008 diffraction data set, because there is no calibration of the time resolution available for the 2009 diffraction data set.



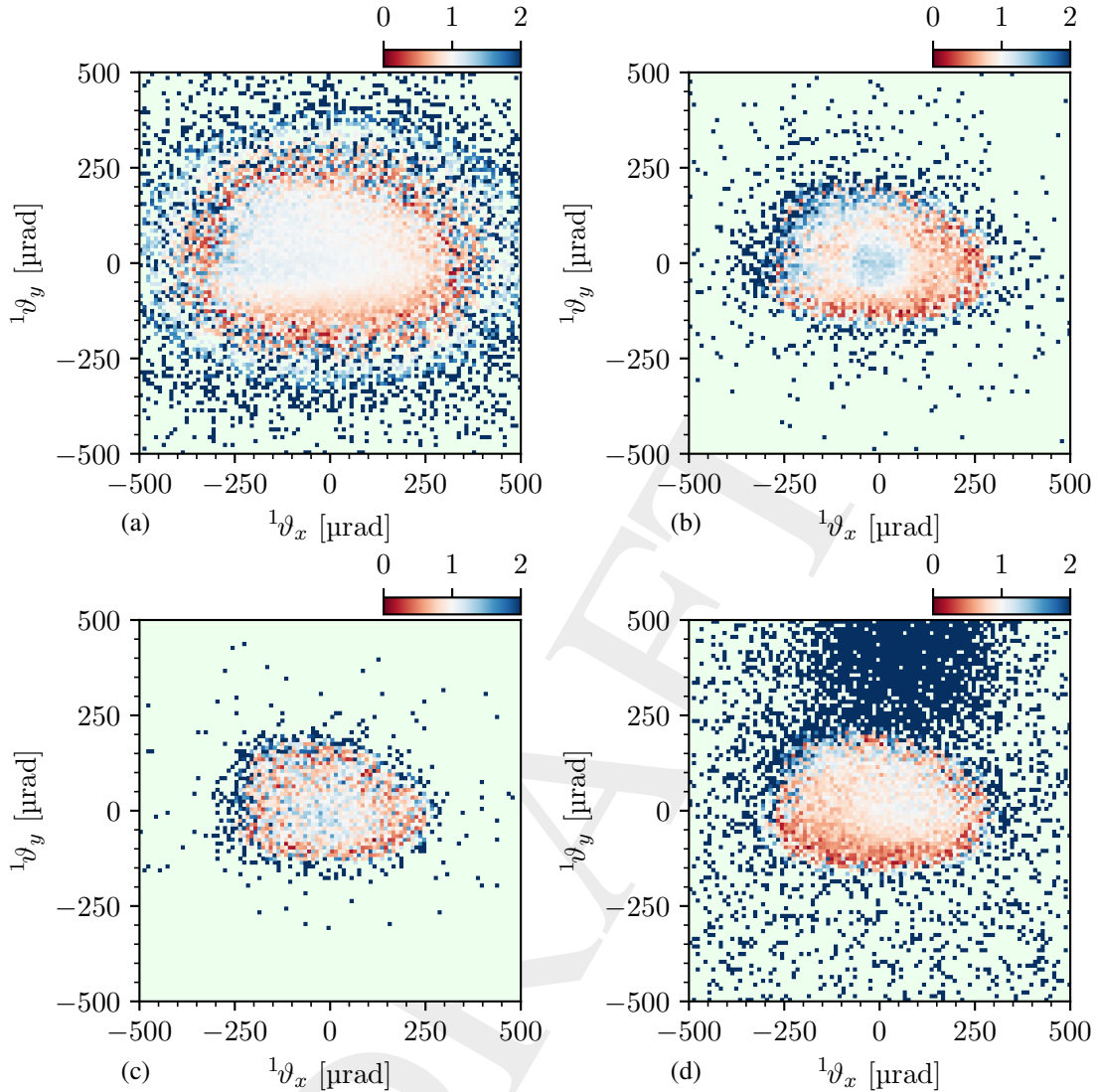


Figure A.1: Ratios of the beam inclination distribution for the various validation samples and the three-hadron sample used for calibration. Before calculating the ratio, each distribution was normalized to the number of events in the corresponding data sample. (a) shows the pion-beam sample and (b), (c), and (d) show the kaon-beam samples from the  $K^- \rightarrow \mu^- \bar{\nu}_\mu$ ,  $\pi^- \pi^- \pi^+$ , and  $\pi^- \pi^0$  decays, respectively.

5518 around one, which means that the pion-beam sample illuminates the CEDARs in a similar way  
 5519 as the three-hadron sample. Therefore, the efficiency and impurity values we obtained from the  
 5520 pion-beam sample are expected to be comparable to the ones for the three-hadron sample and  
 5521 thus to the ones for the  $K^- \pi^- \pi^+$  data.

5522 We obtained a clean kaon-beam sample by selecting decays of beam kaons into various final  
 5523 states. The first kaon-beam sample is based on the decay  $K^- \rightarrow \mu^- \bar{\nu}_\mu$ , where the following cuts  
 5524 were applied:

- 5525 • Preselection (see appendix A.1.1)
- 5526 • One charged track leaving the reconstructed vertex
- 5527 • Vertex  $z$  position upstream of the target:  $-270 \text{ cm} < z_{\text{PV}} < -70 \text{ cm}$
- 5528 • Sum of energies deposited into both ECALs  $< 5 \text{ GeV}$
- 5529 • Outgoing track is identified as a muon: Track traversed  $> 60$  radiation lengths
- 5530 • Momentum of the outgoing muon track  $p_{\mu} < 180 \text{ GeV}/c$
- 5531 • Reconstructed beam-particle mass  $|m_{\mu\bar{\nu}} - 493.677 \text{ MeV}/c^2| < 42 \text{ MeV}/c^2$ <sup>[d]</sup>
- 5532 (see figure A.2b)

5533 Applying the above cuts, we obtained a  $K^{-} \rightarrow \mu^{-}\bar{\nu}_{\mu}$  sample of 84 313 events for the 2008 and  
 5534 71 274 events for the 2009 diffraction data set. In contrast to the pion-beam sample, the beam  
 5535 inclination distribution of the  $K^{-} \rightarrow \mu^{-}\bar{\nu}_{\mu}$  sample has relatively more events in the center as  
 5536 compared to the three-hadron sample (see figure A.1b). This may slightly bias the efficiency  
 5537 towards larger values as the efficiency for kaon identification is higher for kaons traversing the  
 5538 CEDARs parallel to their optical axes. Similarly, also the impurity value determined from this  
 5539 sample may be slightly biased.

5540 To overcome this problem and to get an estimate for the systematic uncertainty of the efficiency  
 5541 and impurity values, two further kaon-beam samples were used. The second kaon-beam sample  
 5542 is based on the kaon decay  $K^{-} \rightarrow \pi^{-}\pi^{-}\pi^{+}$ . The following cuts were applied:

- 5543 • Preselection (see appendix A.1.1)
- 5544 • Three charged tracks leaving the interaction vertex
- 5545 • Vertex  $z$  position upstream of the target:  $-270 \text{ cm} < z_{\text{PV}} < -70 \text{ cm}$
- 5546 • Exclusivity:  $|E_{\pi^{-}\pi^{-}\pi^{+}} - 191 \text{ GeV}| < 8 \text{ GeV}$
- 5547 • Reconstructed mass  $|m_{\pi^{-}\pi^{-}\pi^{+}} - 493.677 \text{ MeV}/c^2| < 14 \text{ MeV}/c^2$  (see figure A.2a)

5548 With only 15 212 events for the 2008 and 14 969 events for the 2009 diffraction data set, this  
 5549 kaon-beam sample is significantly smaller than the  $K^{-} \rightarrow \mu^{-}\bar{\nu}_{\mu}$  sample. This is mainly due to  
 5550 the smaller branching fraction of the  $K^{-} \rightarrow \pi^{-}\pi^{-}\pi^{+}$  decay. The beam inclination distribution  
 5551 is not in perfect agreement with the one of the three-hadron sample, but more similar than the  
 5552  $K^{-} \rightarrow \mu^{-}\bar{\nu}_{\mu}$  sample (see figure A.1c). Thus, this kaon-beam sample can be used to obtain a  
 5553 better estimated for the efficiency and impurity values.

5554 The third kaon-beam sample is based on the kaon decay  $K^{-} \rightarrow \pi^{-}\pi^{0}$ . The following cuts were  
 5555 applied:

- 5556 • Preselection (see appendix A.1.1)
- 5557 • One charged tracks leaving the reconstructed vertex
- 5558 • Vertex  $z$  position upstream of the target:  $-270 \text{ cm} < z_{\text{PV}} < -70 \text{ cm}$

<sup>[d]</sup> The neutrino momentum is given by  $\vec{p}_{\bar{\nu}} = \vec{p}_{\text{beam}} - \vec{p}_{\mu}$ , where  $\vec{p}_{\text{beam}} = 190 \text{ GeV}/c \cdot (dx/dz, dy/dz, 1)$  using the measured beam inclination and an average beam momentum of approximately  $190 \text{ GeV}/c$ . The neutrino energy is  $E_{\bar{\nu}} = |\vec{p}_{\bar{\nu}}|c$ .

- 5559 • Neutral ECAL cluster with the largest energy must have an energy of at least 10 GeV
- 5560 • Exactly one combination of the highest-energy neutral ECAL cluster with another neutral
- 5561 ECAL cluster, where
  - 5562 \* Energy of the second neutral ECAL cluster was larger than 2 GeV
  - 5563 \*  $|m_{\gamma_i\gamma_j} - 135 \text{ MeV}/c^2| < 10 \text{ MeV}/c^2$
- 5564 • Energy of the second neutral ECAL cluster with lower energy larger than 8 GeV<sup>[e]</sup>
- 5565 • Exclusivity:  $|E_{\pi^-\pi^0} - 191 \text{ GeV}| < 8 \text{ GeV}$

5566 Applying the above cuts we obtained 94 890 events for the 2008 and 93 639 events for the 2009  
 5567 diffraction data set. However, in the kaon peak, we find only approximately 7500 events in  
 5568 the 2008 and 6300 events in the 2009 diffraction data set (see figure A.2c). Therefore, the  
 5569  $K^- \rightarrow \pi^-\pi^0$  sample is the smallest of all validation samples. Compared to the three-hadron  
 5570 sample, the beam inclination distribution exhibits an increased number of events above the main  
 5571 beam spot for  $^1\vartheta_y > 200 \mu\text{rad}$  and therefore a reduced number of events for  $^1\vartheta_y \lesssim 0 \mu\text{rad}$  (see  
 5572 figure A.1d). The reason for this could be the comparably large background below the kaon peak  
 5573 (see figure A.2c). Also, the distribution within the main beam spot is different from that of the  
 5574 three-hadron sample.

5575 Each of the kaon-beam samples has some caveats. However, comparing the results from all three  
 5576 samples provides a handle on the systematic uncertainties of the efficiency and impurity values  
 5577 and yields more reliable results.

### 5578 A.1.3 Determination of Efficiency and Purity

5579 To determine the efficiency  $P_{\text{ID}}(K \rightarrow K)$  for kaon identification, we applied the CEDAR  
 5580 particle identification cut for kaons, i.e. the log-likelihood different smaller than  $\mathcal{T}_C(K)$  [see  
 5581 equation (3.15)], to all three kaon-beam samples. We estimated the efficiency as the ratio of  
 5582 the event numbers before and after applying the CEDAR particle identification cut. Due to  
 5583 the pion contamination of the kaon-beam sample, this approach only gives a lower limit for  
 5584 the efficiency. For the  $K^- \rightarrow \pi^-\pi^0$  and  $K^- \rightarrow \mu^-\bar{\nu}_\mu$  validation samples, the kaon peak sits on a  
 5585 considerable background (see figures A.2b and A.2c). To extract the efficiency also from these  
 5586 samples, we fitted a Gaussian signal function plus a second-order background polynomial to the  
 5587  $\pi^-\pi^0$  and  $\mu^-\bar{\nu}_\mu$  mass spectra. Then, we calculated the efficiency as the ratio of the integrals of  
 5588 the Gaussian signal functions before (figure A.2c) and after (figure A.2d) applying the CEDAR  
 5589 particle identification cut for kaons. Similarly, the efficiency for pion identification is the ratio  
 5590 of the pion-beam sample before and after applying the CEDAR particle identification cut for  
 5591 pions.

<sup>[e]</sup> First, we applied the more relaxed constrained of a cluster energy larger than 2 GeV in order to allow for more combinations of neutral clusters in one event. Then we required that exactly one of these combinations exist. This reduced combinatorial background.

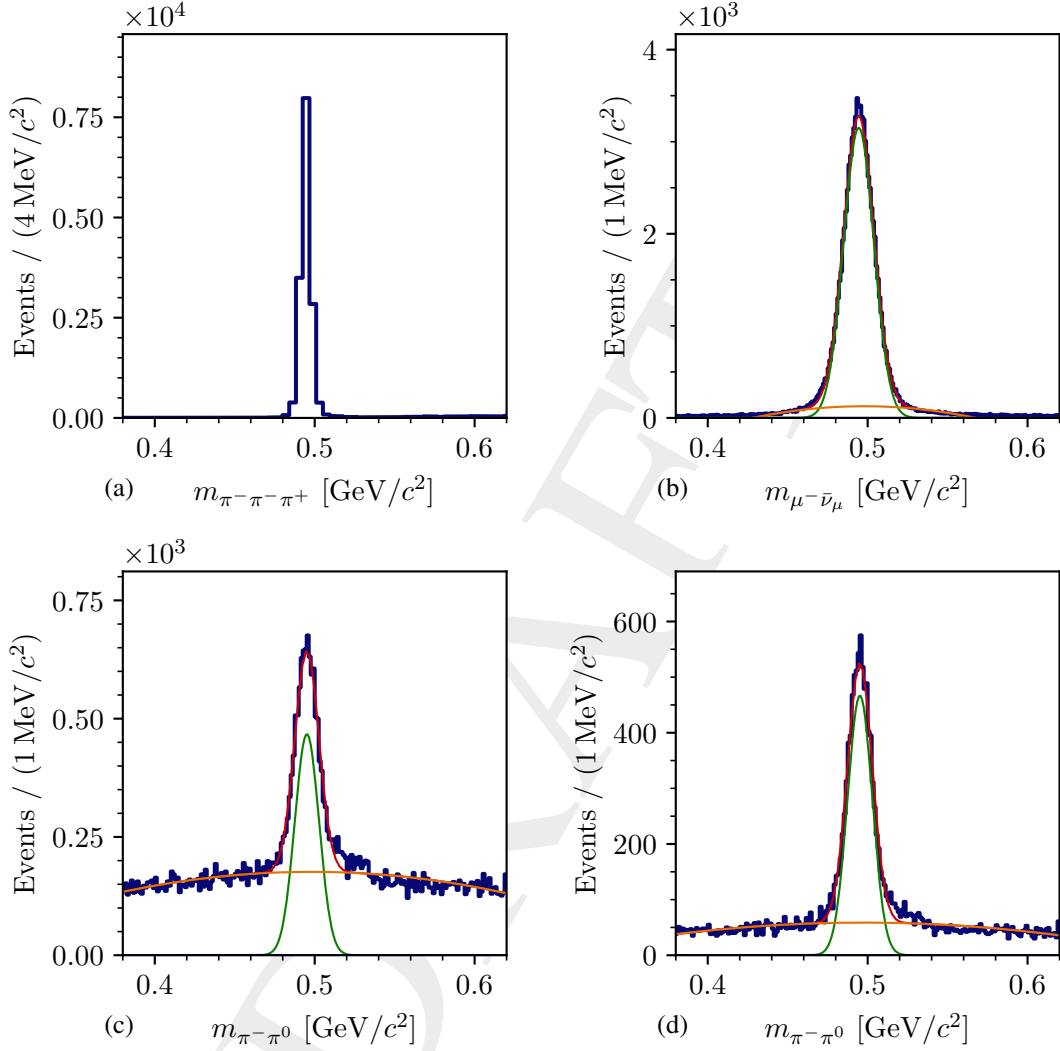


Figure A.2: Kaon peak in the invariant mass spectra of the kaon-beam samples. (a)  $\pi^- \pi^- \pi^+$  invariant mass spectrum of the  $K^- \rightarrow \pi^- \pi^- \pi^+$  sample, (b)  $\mu^- \bar{\nu}_\mu$  invariant mass spectrum of the  $K^- \rightarrow \mu^- \bar{\nu}_\mu$  sample, and (c)  $\pi^- \pi^0$  invariant mass spectrum of the  $K^- \rightarrow \pi^- \pi^0$  sample before applying the CEDAR particle identification cut for kaons. (d)  $\pi^- \pi^0$  invariant mass spectrum of the  $K^- \rightarrow \pi^- \pi^0$  sample after applying the CEDAR particle identification cut for kaons. The dark blue histogram represents the data. In (b)-(d), the red curve is the result of a fit with a the Gaussian signal function plus a second-order background polynomial. The green curve is the Gaussian signal function, and the orange curve is the background polynomial. The sample of the decay  $K^- \rightarrow \pi^- \pi^- \pi^+$  shown in (a) is background free. Therefore, we did not perform a fit to extract the number of kaon decays, but we directly used the number of selected events.

5592 To estimate the probability  $P_{\text{ID}}(\pi \rightarrow K)$  to misidentify a pion as a kaon, we applied the CEDAR  
5593 particle identification cut for kaons on the pion-beam sample and calculated the ratio of the  
5594 remaining events and the total number of events of the pion-beam sample. Similarly, the  
5595 probability to misidentify a kaon as a pion was obtained from each kaon-beam sample by  
5596 applying the cut on the CEDAR particle identification for a pion.

5597 To determine the purity of the identified-kaon sample, the impurity from pions, muons, electrons,  
5598 and antiprotons in the beam had to be determined. The total impurity is dominated by the  
5599 impurity from misidentified pions in the identified-kaon sample, which was calculated in the  
5600 following way

$$\text{Impurity}(K) = \frac{N_{K \rightarrow \pi}}{N_{K \rightarrow K} + N_{\pi \rightarrow K}} = \frac{P_{\text{ID}}(\pi \rightarrow K) \cdot R_{\pi K}}{P_{\text{ID}}(K \rightarrow K) + P_{\text{ID}}(\pi \rightarrow K) \cdot R_{\pi K}}, \quad (\text{A.1})$$

5601 taking into account the number ratio of pions to kaons  $R_{\pi K} = 35.9 \pm 1.0$  in the beam [63]. The  
5602 impurity of an identified-pion sample from misidentified kaons was calculated in an analogous  
5603 way.

## 5604 A.2 Final-State Particle Identification

### 5605 A.2.1 The Likelihood Approach

5606 The likelihood for a given particle-species hypothesis  $S$  for a final-state particle is formulated  
5607 in terms of the probability of the observed hit pattern of individual Cherenkov photons,  $j$ , in  
5608 the RICH. The distribution of measured Cherenkov angle  $\theta_j$  of a single photon is modeled  
5609 by a Gaussian function with width  $\sigma_\theta$ . A uniform distribution of emitted Cherenkov photons  
5610 is assumed in the azimuthal angle  $\varphi_j$  around the direction of the particle. Finally, the total  
5611 probability to observe a photon in the RICH detector under the Cherenkov angle  $\theta_j$  is modeled in  
5612 ref. [64] as:

$$f(\theta_j, \varphi_j | S) = \frac{A}{\sqrt{2\pi}\sigma_\theta} \exp\left[-\frac{(\theta_j - \theta_{\text{Ch}}^S)^2}{2\sigma_\theta^2}\right] \epsilon(\theta_j, \varphi_j) + b(\theta_j, \varphi_j). \quad (\text{A.2})$$

5613 Here,  $A = A_0 \sin^2 \theta_{\text{Ch}}^S$  is the expected number of Cherenkov photons,  $\epsilon(\theta_j, \varphi_j)$  the probability  
5614 that a photon emitted with the angles  $(\theta_j, \varphi_j)$  reaches the photon detector and is detected, and  
5615  $b(\theta_j, \varphi_j)$  is the strength of background contributions<sup>[f]</sup> that are uncorrelated with the final-state  
5616 particle.

---

<sup>[f]</sup> The strength of the background can be computed as a function of the photon position in the photon-detector plane as explained in ref. [64].

5617 The information from all  $N$  measured photons is combined in one extended likelihood:<sup>[g]</sup>

$$\tilde{\mathcal{L}}(S) = e^{-F(S)} \prod_{j=1}^N f(\theta_j, \varphi_j; S). \quad (\text{A.3})$$

5618 Here,  $F(S)$  is the expected number of photons. It is calculated by integrating  $f(\theta_j, \varphi_j; S)$  over  
5619 the  $(\theta_j, \varphi_j)$  reference region defined by the RICH acceptance (see ref. [64]).

5620 The likelihood is normalized to the number of photons:

$$\mathcal{L}(S) = \sqrt[N]{\tilde{\mathcal{L}}(S)}. \quad (\text{A.4})$$

5621 This allows to consistently tune the likelihood-ratio threshold for particles with different number  
5622 of photons.

## 5623 A.2.2 Validation Samples

5624 In order to estimate the performance of the RICH particle identification; i.e. the efficiency  
5625  $P(S \rightarrow S)$  to identify a particle and the misidentification probability  $P(S \rightarrow S')$  to assign the  
5626 wrong particle hypothesis  $S'$ , validation samples of final-state particles are required. These  
5627 samples need to contain particles that were identified without using the RICH information. We  
5628 determined efficiency and misidentification probability separately for  $\pi^+$ ,  $K^+$ ,  $p$  and  $\pi^-$ ,  $K^-$ ,  $\bar{p}$ .  
5629 We also treated the 2008 and 2009 diffraction data sets individually.

### 5630 Kaon Validation Sample

5631 We used  $\phi(1020) \rightarrow K^- K^+$  decays as source of kaons. As the  $\phi(1020)$  is very short-lived, we  
5632 cannot separate its decay vertex from the interaction vertex where the  $\phi(1020)$  was produced,  
5633 which is the point of interaction of the beam particle with the target. Therefore, we considered  
5634 only events where the interaction vertex is within the region of the target, i.e.  $-65 \leq Z_{\text{Vtx}} < -30$  cm. For all events with at least two charged particles leaving the interaction vertex, we  
5635 considered all possible combinations of two oppositely charged particle pairs. Assuming the  
5636 kaon hypothesis, we calculated the mass of the  $K^- K^+$  system and required that it is around the  
5637  $\phi(1020)$  mass, i.e.  $0.98 \leq m_{KK} < 1.07 \text{ GeV}/c^2$ .<sup>[h]</sup> To keep the signal-to-background ratio of the  
5638  $\phi(1020)$  signal sufficiently large, we required that one of the two kaons was identified by the RICH.  
5639

<sup>[g]</sup> For each final-state particle, all photons with  $\theta_j < 70$  mrad were considered in equation (A.3). This threshold of 70 mrad is larger than the maximum possible Cherenkov angle. For final states with more than one particle, there can be ambiguities in the association of Cherenkov photons to particles. This combinatorial background was accounted for by  $b(\theta_j, \varphi_j)$ .

<sup>[h]</sup> We estimated the combinatorial background below the  $\phi(1020)$  peak. For about 5% of all  $K^- K^+$  combinations whose invariant mass lies within five standard deviations around the  $\phi(1020)$  peak, one of the two kaons was used multiple times also in other combinations.

Thus, when selecting the  $K^+$  validation sample, we identified the  $K^-$  via the RICH information using a likelihood-ratio threshold of  $\mathcal{T}_R = 1$  and vice versa.<sup>[i]</sup> For the 2008 diffraction data set, we obtained 44 059 131 events for the  $K^-$  and 40 828 357 events for the  $K^+$  validation sample. For the 2009 diffraction data set, we obtained 35 105 832 events for the  $K^-$  and 31 887 217 events for the  $K^+$  validation sample. However, only 3.6 % of these events come from  $\phi(1020) \rightarrow K^- K^+$  decays.

From these data samples, we can determine the probability that a particle hypothesis  $S$  is assigned to a kaon by the RICH:

$$P(K \rightarrow S) = \frac{N_{K \rightarrow S}}{N_{\text{tot}}}, \quad (\text{A.5})$$

where  $N_{\text{tot}}$  is the total number of kaons in the validation sample and  $N_{K \rightarrow S}$  is the number of kaons that were identified as species  $S$ . The probability  $P(K \rightarrow K)$  is the kaon identification efficiency and  $P(K \rightarrow S)$  with  $S \neq K$  are the misidentification probabilities.

Figure A.3a shows the invariant mass spectrum of the  $K^- K^+$  system for the  $K^-$  validation sample, i.e. when identifying the  $K^+$ . It exhibits a clear peak at about  $1.02 \text{ GeV}/c^2$  from the decay  $\phi(1020) \rightarrow K^- K^+$ . However, the  $\phi(1020)$  peak sits on a large background. Thus, in equation (A.5) we could not directly use the numbers of particles in the data sample, but we had to determine the number of  $\phi(1020)$  decays in the peak. Therefore, we modeled the  $m_{KK}$  distribution as a sum of signal functions for the  $\phi(1020)$  decays and a smooth background component, which was modeled by a second-order polynomial in  $m_{KK}$ . The measurement resolution in  $m_{KK}$  of about  $1.5 \text{ MeV}/c^2$  is at the same order of magnitude as the total decay width of the  $\phi(1020)$  of  $4.249 \text{ MeV}/c^2$  [9]. Therefore, we used a Voigt function [180], which is a convolution of a non-relativistic Breit-Wigner shape with FWHM  $\Gamma$  and a Gaussian function with standard deviation  $\sigma$  to parameterize the signal component. In total, our model function is given by

$$\frac{dN}{dm_{KK}} = A \text{Voigt}(m_{KK} - m_0; \sigma, \Gamma) + a + b(m_{KK} - m_0) + c(m_{KK} - m_0)^2. \quad (\text{A.6})$$

Here;  $A$ ,  $m_0$ ,  $\sigma$ ,  $a$ ,  $b$ , and  $c$  are free parameters that were determined by a fit to the data. We fixed the width,  $\Gamma$ , of the Breit-Wigner term to its know value from ref. [9]. We determined the number of  $\phi(1020)$  decays by integrating the signal function over the range  $1.0 \leq m_{KK} < 1.05 \text{ GeV}/c^2$ .<sup>[j]</sup> By performing this fit individually for the total data sample and for the subsamples where the kaon was assigned the hypothesis  $S$ , we can determine  $N_{\text{tot}}$  and  $N_{K \rightarrow S}$ , respectively.<sup>[k]</sup> The results are discussed in appendix A.2.3. Figure A.3b shows exemplarily the  $m_{KK}$  distribution in a selected ( $|\vec{p}_R|$ ,  $\sqrt{\theta_R}$ ) cell. The red curve represents a fit of the model function in equation (A.6) to the distribution. It reproduces well the data with a  $p$ -value of 0.73.

<sup>[i]</sup> The identification of both particles is independent. Thus, identifying one kaon using the RICH does not bias the identification probabilities of the other one. However, the kinematic range of the other particle might be limited.

<sup>[j]</sup> In practice we, calculated the integral of the histogram and the integral of the background function, because this method has proven to be more robust with respect to systematic effects.

<sup>[k]</sup> As  $m_0$  and  $\sigma$  should be the same for the subsamples, we fixed these parameters in the fits to the subsamples to the values obtained in the fit to the full sample. This improved the fit stability and thereby reduced systematic effects.

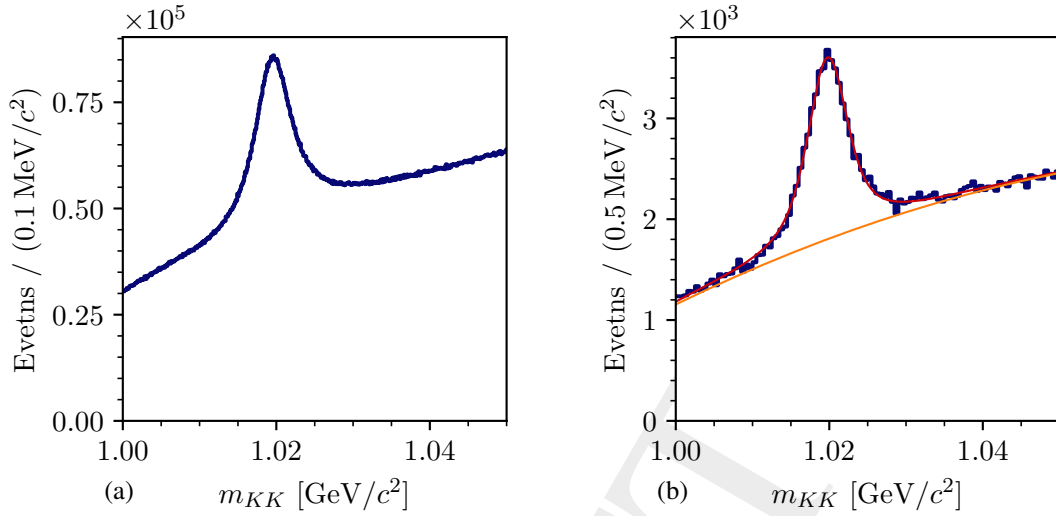


Figure A.3: Invariant mass spectrum of the  $K^- K^+$  system in the 2008  $K^-$  validation sample, i.e. after identifying the positive particle as a  $K^+$  (see text). (a) shows the complete data set. (b) shows a subset of the data in a  $(|\vec{p}_R|, \sqrt{\theta_R})$  cell around  $(18.75 \text{ GeV}/c, 0.19 \sqrt{\text{rad}})$ . The blue histograms represents the data. The red curve in (b) represents the result of a fit of equation (A.6) to the data. The orange curve shows the background component in equation (A.6).

### 5671 Preselection for Pion and Proton Validation Samples

5672 We used  $K_S^0 \rightarrow \pi^- \pi^+$ ,  $\Lambda \rightarrow \pi^- p$ , and  $\bar{\Lambda} \rightarrow \pi^+ \bar{p}$  decays as a sources of pions and (anti)protons.  
5673 As the decay of these neutral particles, which are commonly called  $V^0$  particles, proceeds via the  
5674 weak interaction, the  $V^0$  particles have long lifetimes. Thus, their decay vertex is displaced from  
5675 the interaction vertex where they were produced. These displaced vertices of  $V^0$  decays were  
5676 reconstructed from the two measured charged daughter particles.

5677 We considered all displaced decay vertices with two oppositely charged tracks leaving the vertex  
5678 within the region  $-28 \leq Z_{\text{ddv}} < 150 \text{ cm}$  after the target.<sup>[1]</sup> We required that the decaying  $V^0$   
5679 particle was produced in a interaction vertex. To do so, we reconstructed the direction of the  $V^0$   
5680 particle by summing the measured momenta of the two daughter particles. We required, that  
5681 the distance of closest approach between the direction of the reconstructed  $V^0$  track and the  
5682 interaction vertex that is closest to this track is smaller than 3 mm. Finally, we ensured that none  
5683 of the two daughter tracks was associated with this closest interaction vertex.

5684 This sample contains contributions from two-body decays of  $K_S^0$ ,  $\Lambda$ , and  $\bar{\Lambda}$ ; which appear as arks  
5685 with only little background in the Armenteros plot in figure A.4.<sup>[m]</sup>

[1] We excluded the target region to exclude vertices from beam interactions that were erroneously reconstructed as displaced decay vertices.

[m] The Armenteros plot shows the momentum component,  $p_T$ , of one of the daughter particles that is transversal to the  $V^0$  momentum,  $p_T$ , versus the asymmetry of the longitudinal momentum components,  $p_L^+$ , of the positive and negative daughter particles. By construction,  $p_T$  is the same for both daughter particles.



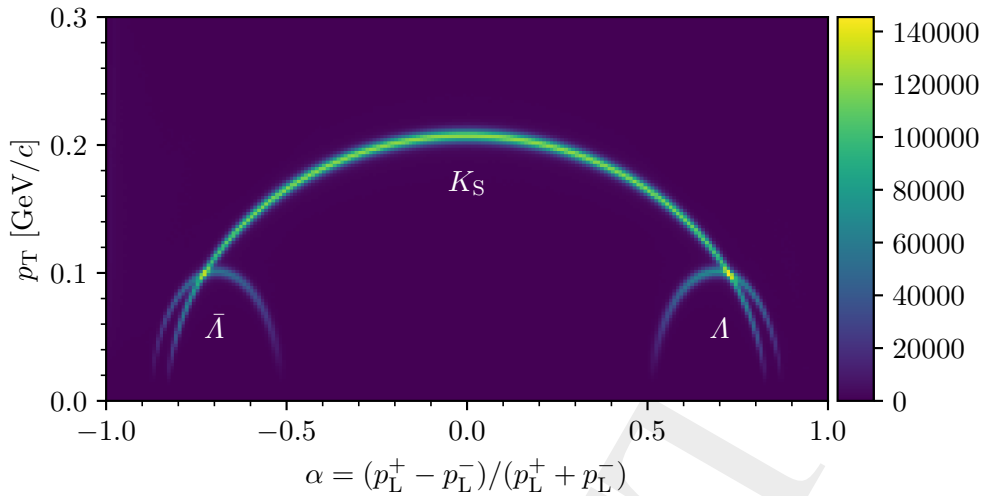


Figure A.4: Armenteros plot<sup>[m]</sup> of the  $V^0$  data sample of the 2008 diffraction data set.

#### 5686 Pion Validation Sample

5687 In order to obtain a clean pion sample from  $K_S^0 \rightarrow \pi^- \pi^+$  decays, we needed to reject background  
5688 contributions from  $\Lambda$  and  $\bar{\Lambda}$  decays from the  $V^0$  sample. Therefore, we calculated the invariant  
5689 pion-proton mass and rejected events in the range within  $\pm 7 \text{ MeV}/c^2$  around the peak position of  
5690  $1116.1 \text{ GeV}/c^2$ , which is consistent with the nominal  $\Lambda$  mass [9].<sup>[n]</sup> For the 2008 diffraction data  
5691 set, we obtained 72 608 756  $K_S^0$  decay candidates (see figure A.5). For the 2009 diffraction data  
5692 set, we obtained 60 865 406  $K_S^0$  decay candidates.

5693 The  $K_S^0$  sample exhibits only little background in the signal region of the  $m_{\pi^- \pi^+}$  spectrum, in  
5694 contrast to the kaon validation sample discussed above. Therefore, we performed only a side-  
5695 band subtraction to account for the background when determining the number of  $K_S^0$  decays.  
5696 We used a signal region of  $450 \leq m_{\pi\pi} < 550 \text{ MeV}/c^2$  and sideband regions of  $420 \leq m_{\pi\pi}$   
5697  $< 450 \text{ MeV}/c^2$  and  $550 \leq m_{\pi\pi} < 580 \text{ MeV}/c^2$ .

5698 Using this sample, we determined efficiency and misidentification probability for negative and  
5699 positive pions using equation (A.5) in the same way as discussed for negative and positive  
5700 kaons.

<sup>[n]</sup> The peak position was determined from a fit of a sum of two Gaussian and a second-order polynomial to the mass spectrum.

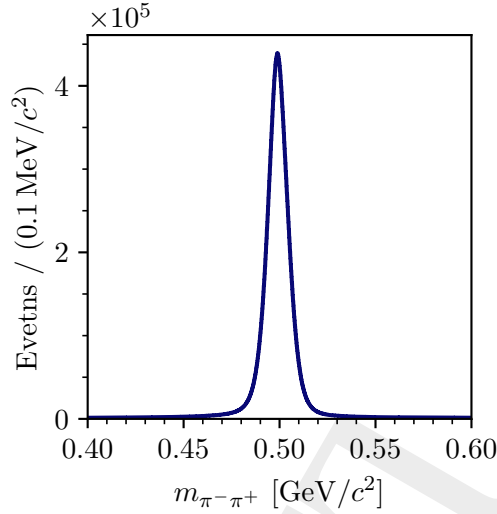


Figure A.5: Invariant mass distribution of the  $\pi^- \pi^+$  system for the  $V^0$  sample from the 2008 diffraction data set.

### 5701 Proton Validation Sample

5702 We used the decays  $\Lambda \rightarrow \pi^- p$  and  $\bar{\Lambda} \rightarrow \pi^+ \bar{p}$  as sources of protons and antiprotons. To reject  
5703 the  $K_S^0$  background contribution in the  $V^0$  sample, we rejected events where the invariant  $\pi^- \pi^+$   
5704 mass,  $m_{\pi^- \pi^+}$ , is within  $20 \text{ MeV}/c^2$  around the  $K_S^0$  peak at  $499 \text{ MeV}/c^2$ , which is consistent with  
5705 the nominal  $K_S^0$  mass [9].<sup>[n]</sup>

5706  $\Lambda$  decays are well separated from  $\bar{\Lambda}$  decays in the Armenteros plot (see figure A.4). In order  
5707 to obtain a clean proton sample from  $\Lambda$  decays and a clean antiproton sample from  $\bar{\Lambda}$  decays,  
5708 we selected events with  $\alpha > 0$  and  $\alpha < 0$ , respectively. For the 2008 diffraction data set, we  
5709 obtained 10 930 951  $\Lambda$  decay candidates (see figure A.6a) and 11 825 422  $\bar{\Lambda}$  decay candidates  
5710 (see figure A.6b). For the 2009 diffraction data set, we obtained 10 038 288  $\Lambda$  decay candidates  
5711 and 11 256 626  $\bar{\Lambda}$  decay candidates. Analogous to the pion validation sample, we determine  
5712 the number of  $\Lambda$  and  $\bar{\Lambda}$  decays from a side-band subtraction of the  $m_{\pi^- p}$  and  $m_{\pi^+ \bar{p}}$  spectra,  
5713 respectively. The signal region is  $1100 \leq m_{\pi^\pm \bar{p}} < 1130 \text{ MeV}/c^2$ . The sideband regions are  
5714  $1080 \leq m_{\pi^\pm \bar{p}} < 1100 \text{ MeV}/c^2$  and  $1130 \leq m_{\pi^\pm \bar{p}} < 1150 \text{ MeV}/c^2$ .

5715 Using this sample, we determined efficiency and misidentification probability for protons and  
5716 antiprotons using equation (A.5) in the same way as discussed for negative and positive kaons.

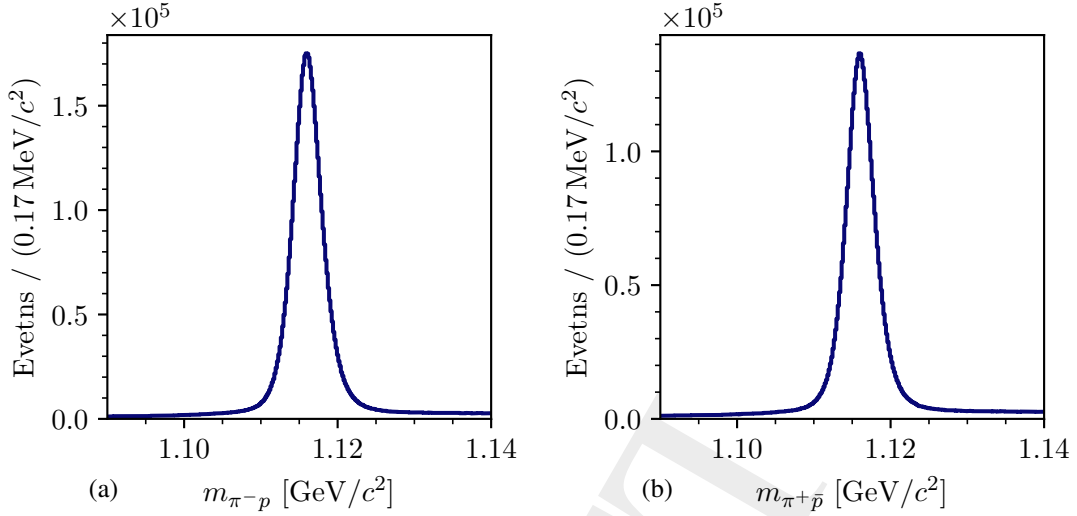


Figure A.6: Invariant mass distribution of the pion-proton system. (a) shows the  $m_{\pi^- p}$  distribution for the  $\Lambda$  decay assumption. (b) shows the  $m_{\pi^+ \bar{p}}$  distribution for the  $\bar{\Lambda}$  decay assumption. Both plots show the 2008 diffraction data set.

### 5717 A.2.3 RICH Particle-Identification Performance

5718 In this section, we present the results of the RICH performance studies, i.e. the efficiency and  
5719 misidentification probabilities shown in figures A.7 to A.9 for the 2008 diffraction data set and a  
5720 threshold of  $\mathcal{T}_R = 1.15$  of the RICH likelihood ratio in equation (3.19). The same threshold value  
5721 was used for the event selection of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  discussed in section 4.1.  
5722 Here, we will discuss technical aspects of the RICH performance matrices. The main aspects of  
5723 the RICH performance are discussed in the main text in section 3.2.2.

5724 Figure A.7 shows the efficiency and misidentification probabilities for negative kaons. Fig-  
5725 ure A.7a shows the sum over all probabilities in each  $(|\vec{p}_R|, \sqrt{\theta_R})$  cell. It is in good agreement  
5726 with one, except at the kinematic borders of the kaon validation sample, where the number of  
5727 events becomes small. It is not exactly one as we estimated  $N_{K \rightarrow S}$  and  $N_{\text{tot}}$  in equation (A.5)  
5728 from independent fits. The overall good agreement with one proves, that we are able to reliably  
5729 estimate efficiencies and impurities from fits to the  $m_{KK}$  spectrum.

5730 Figure A.8 shows the efficiency and misidentification probabilities for negative pions. Since the  
5731 pion validation sample is much larger than the kaon validation sample, we used a finer binning in  
5732  $(|\vec{p}_R|, \sqrt{\theta_R})$ . Also here, sum over all probabilities is in good agreement with one, showing that  
5733 the side-band subtraction approach introduces only small systematic effects.

5734 Figure A.9 shows the efficiency and misidentification probabilities for antiprotons. As for the  
5735 pion validation sample, the sum over all probabilities is in good agreement with one. Due to  
5736 the higher antiproton mass, we can identify antiprotons only above about 18 GeV/c. The upper

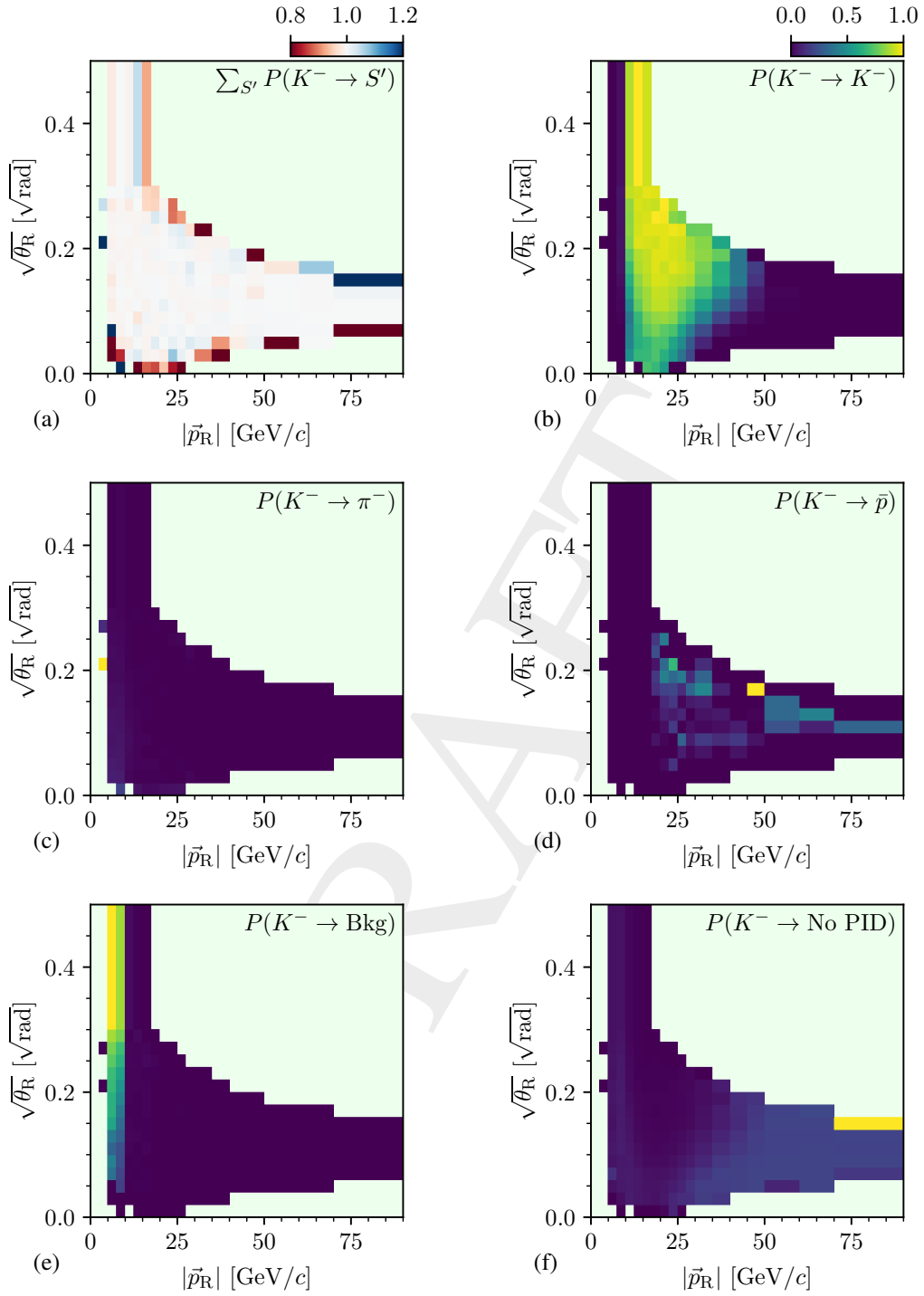


Figure A.7: RICH efficiency and misidentification probability for negative kaons in cells of the particle momentum  $|\vec{p}_R|$  and the square-root of the track angle  $\theta_R$  at the RICH position for the 2008 diffraction data set using a likelihood-ratio threshold of  $\mathcal{T}_R = 1.15$ . (b) shows the identification efficiency. (c) to (e) show the probability to misidentify the kaon as a pion, antiproton, or as background, respectively. (f) shows the probability to not identify a kaon. (a) shows the sum over (b) to (f). (b) to (f) have the same color scale. Regions without calibration data are drawn in light green.

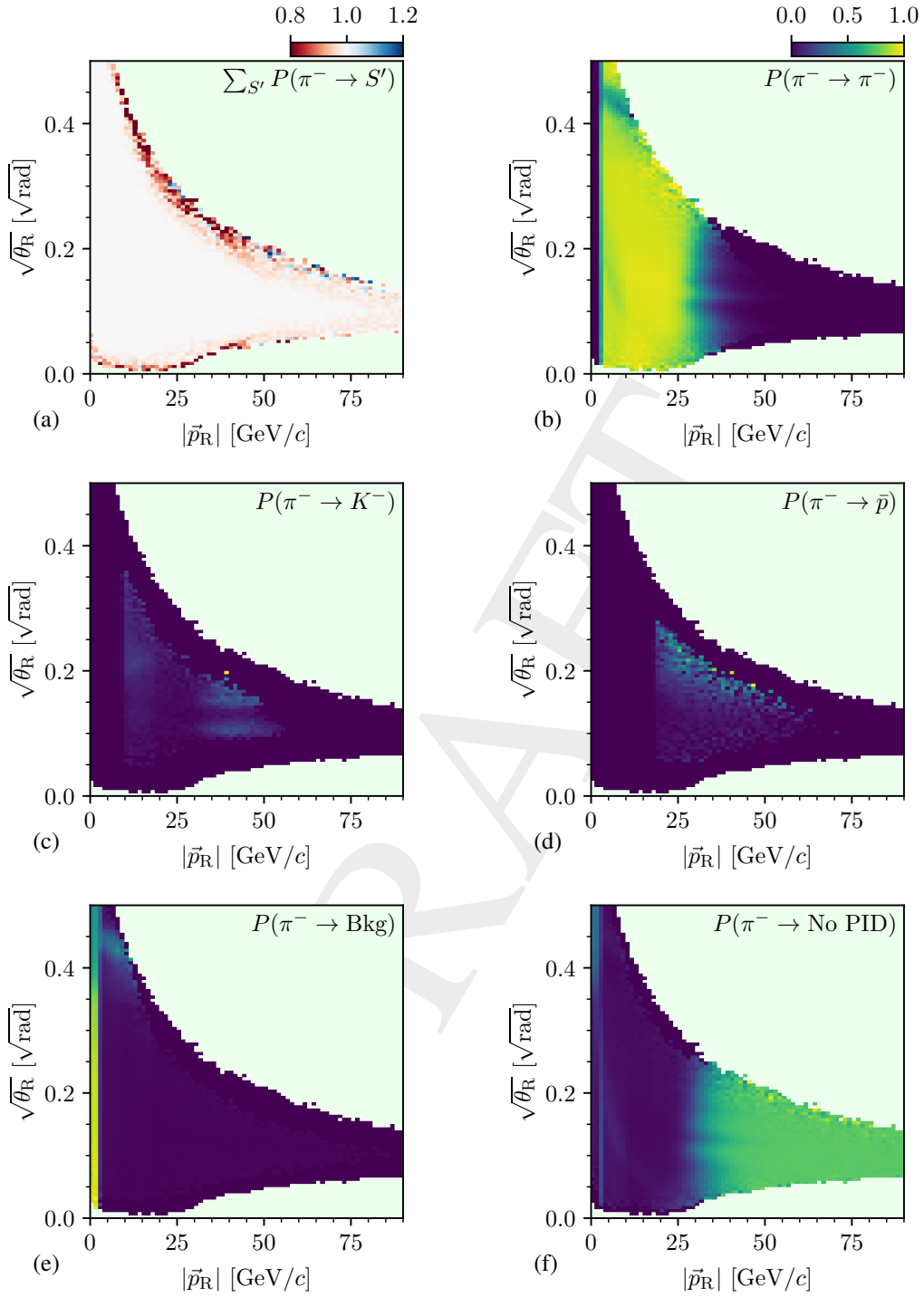


Figure A.8: RICH efficiency and misidentification probability for negative pions in cells of the particle momentum  $|\vec{p}_R|$  and the square-root of the track angle  $\theta_R$  at the RICH position for the 2008 diffraction data set using a likelihood-ratio threshold of  $\mathcal{T}_R = 1.15$ . (b) shows the identification efficiency. (c) to (e) show the probability to misidentify the pion as a kaon, antiproton, or as background, respectively. (f) shows the probability to not identify a pion. (a) shows the sum over (b) to (f). (b) to (f) have the same color scale. Regions without calibration data are drawn in light green.

5737 momentum limit depends on the track angle and reaches up to 75 GeV/c. In the center of the  
5738 distribution, we achieve a high antiproton identification efficiency of about 86 %.

5739 The RICH efficiencies and misidentification probabilities for positive kaons, pions, and protons  
5740 are in good agreement with those for the corresponding negative particle species discussed above,  
5741 except for small differences between the efficiency of negative and positive pions at the kinematic  
5742 borders of the validation sample. As those differences are the borders, they are not important  
5743 here.

5744 The RICH performance studies for the 2009 diffraction data set yielded similar results as those  
5745 for the 2008 diffraction data set. Figure A.10 shows as an example the efficiencies for negative  
5746 pions and kaons. Nonetheless, we still treat the RICH performance separately for both years as  
5747 the experimental setup for both years was slightly different.

#### 5748 **A.2.4 RICH Threshold Tuning for the $K^-\pi^-\pi^+$ Final State**

5749 We estimated the efficiency to identify the  $K^-\pi^-\pi^+$  final state for a given  $\mathcal{T}_R$  by comparing the  
5750 number of events that pass the  $K^-\pi^-\pi^+$  event selection described in section 4.1, relative to the  
5751 number of selected  $K^-\pi^-\pi^+$  events for  $\mathcal{T}_R = 1.00$ . The blue curve in figure 3.14 shows the  
5752 efficiency determined from the 2008 diffraction data set.

5753 The purity (orange curve in figure 3.14) is the fraction of events where the  $K^-$  and  $\pi^-$  hypotheses  
5754 were correctly attribute to the final-state particles. As the determination of the purity requires  
5755 knowledge about the true particle species, we used a pseudodata sample of  $K^-\pi^-\pi^+$  events that  
5756 is uniformly distributed in the  $K^-\pi^-\pi^+$  phase space to estimate the purity. The Monte Carlo  
5757 method used to obtain such a pseudodata sample is described in appendix C. This estimate may  
5758 be biased, because in the measured data  $K^-\pi^-\pi^+$  events are not uniformly distributed in phase  
5759 space. However, at this stage of the analysis, i.e. before the partial-wave decomposition, this was  
5760 the best approximation which could be employed. Furthermore, here we are not interested in  
5761 the absolute value of the purity, but we are mainly interested in its  $\mathcal{T}_R$  dependence, which is less  
5762 sensitive to the distribution of the final-state particles.

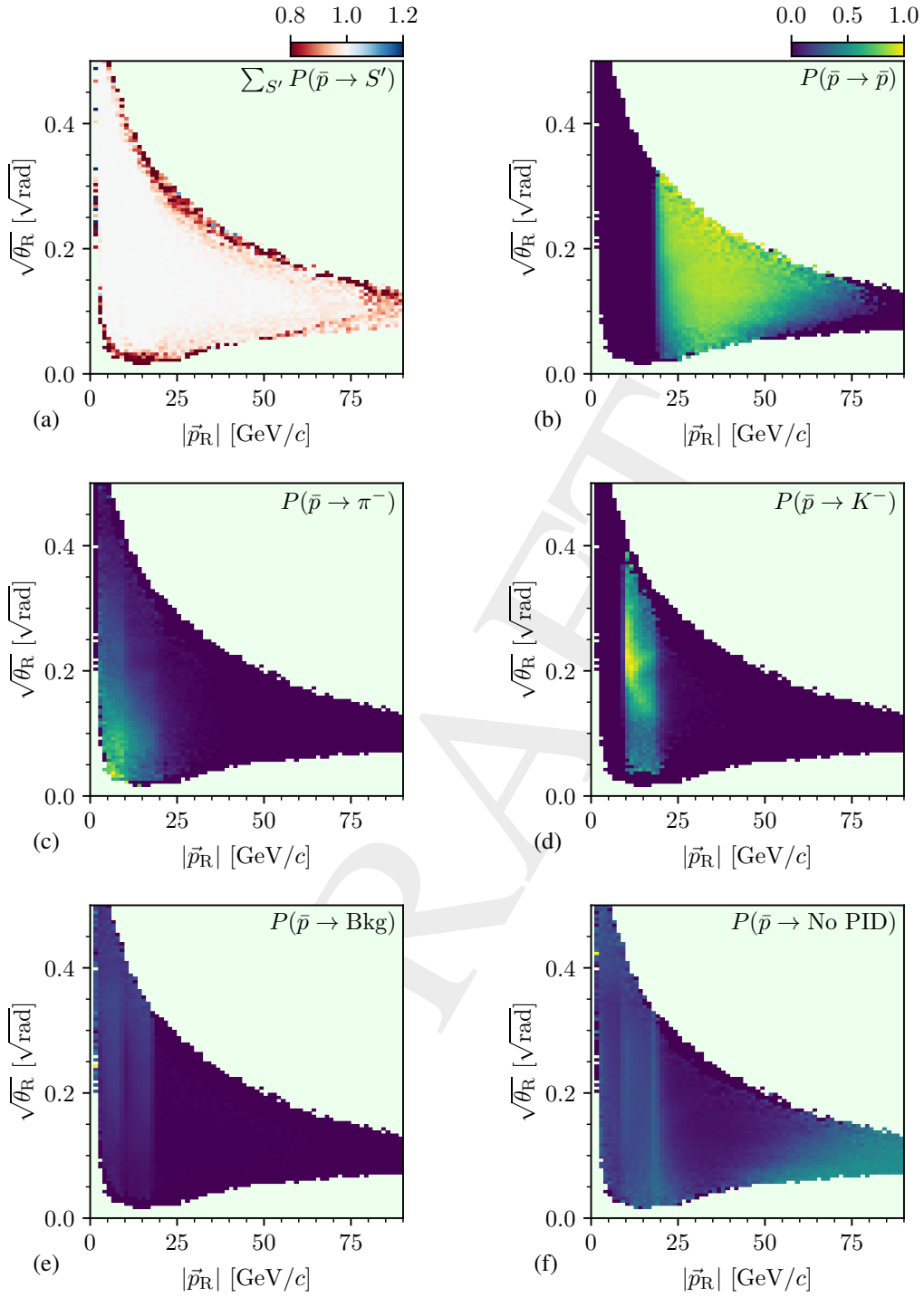


Figure A.9: RICH efficiency and misidentification probability for antiprotons in cells of the particle momentum  $|\vec{p}_R|$  and the square-root of the track angle  $\theta_R$  at the RICH position for the 2008 diffraction data set using a likelihood-ratio threshold of  $\mathcal{T}_R = 1.15$ . (b) shows the identification efficiency. (c) to (e) show the probability to misidentify the antiproton as a pion, kaon, or as background, respectively. (f) shows the probability to not identify a antiproton. (a) shows the sum over (b) to (f). (b) to (f) have the same color scale. Regions without calibration data are drawn in light green.

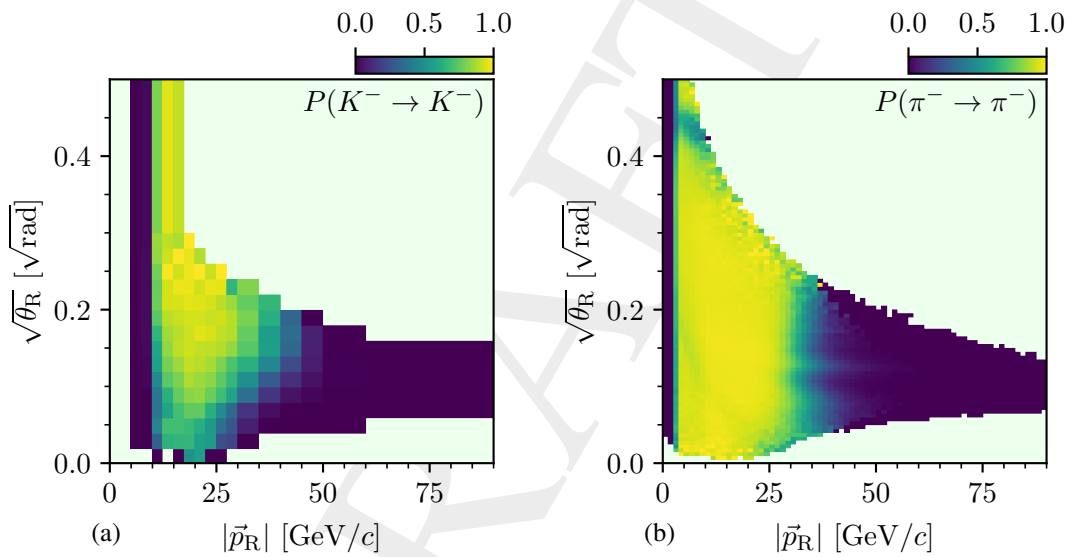


Figure A.10: RICH efficiency for (a) kaons and (b) pions in cells of the particle momentum  $|\vec{p}_R|$  and the square-root of the track angle  $\theta_R$  at the RICH position for the 2009 diffraction data set using a likelihood-ratio threshold of  $\mathcal{T}_R = 1.15$ . Compare figures A.7b and A.8b, respectively.



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## B Event Selection

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### B.1 Reconstruction of Beam Energy

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At COMPASS, the energy of the beam particle was not directly measured by the experimental setup. However, we reconstructed it from the measured three-momenta of the  $K^- \pi^- \pi^+$  final-state particles and the measured inclination of the beam particle track; assuming an exclusive event, assuming the target particle to be a proton, and assigning the beam and final-state particle masses according to the CEDAR and RICH information, respectively. The energy of the beam particle reconstructed in this way is an important quantity to ensure the exclusivity of an event. It was used to suppress background events where not all final-state particles were detected.

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To calculate the energy  $E_{\text{beam}}$  of the beam kaon we used the following approach. First, we determine the magnitude  $|\vec{p}_{\text{beam}}|$  of its three-momentum. From the four-momenta  $p_i$  of the final-state particles we calculate the total four-momentum,

$$p_X = (E_X, \vec{p}_X) = \sum_{i=1}^3 p_i, \quad (\text{B.1})$$

5775

of the final-state system  $X$ .

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The Mandelstam variable  $t$  can be calculated in two different ways (see figure B.1): (i) from the kinematics of the beam vertex in the laboratory frame, i.e.

$$t = (p_{\text{beam}} - p_X)^2 = m_{\text{beam}}^2 + m_X^2 - 2(E_{\text{beam}}E_X - |\vec{p}_{\text{beam}}| |\vec{p}_X| \cos \theta), \quad (\text{B.2})$$

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where  $\theta$  is the scattering angle, i.e. the angle between the momentum of the  $X$ -system and of the beam particle. It is calculated from  $\vec{p}_X$  in equation (B.1) and the measured beam-particle inclination; (ii) from the kinematics of the target vertex, i.e.

$$t = (p_{\text{target}} - p_{\text{recoil}})^2 = 2m_{\text{target}}(m_{\text{target}} - E_{\text{recoil}}) = 2m_{\text{target}}(E_X - E_{\text{beam}}), \quad (\text{B.3})$$

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where we use that the target proton is at rest in the laboratory frame and where we assume that the target proton stays intact in the scattering reaction. Therefore, the energy transferred between the upper and lower vertex is  $(m_{\text{target}} - E_{\text{recoil}}) = (E_X - E_{\text{beam}})$ .

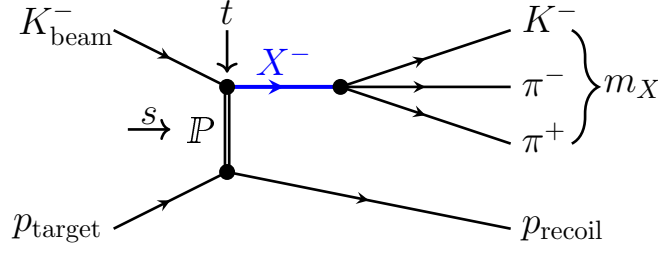


Figure B.1: Schematic view of the diffractive scattering reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  with the kinematic variables of interest.  $s$  is the total center-of-momentum energy of the  $K_{\text{beam}}^- p_{\text{target}}$  system;  $t$  is the squared four-momentum transferred between the beam kaon and the target proton; and  $m_X$  is the invariant mass of the  $K^- \pi^- \pi^+$  final state.

5784 Combining equations (B.2) and (B.3)

$$m_{\text{beam}}^2 + m_X^2 - 2(E_{\text{beam}} E_X - |\vec{p}_{\text{beam}}| |\vec{p}_X| \cos \theta) = 2m_{\text{target}}(E_X - E_{\text{beam}}) \quad (\text{B.4})$$

5785 and substituting the beam energy by the beam momentum via  $E_{\text{beam}} = \sqrt{m_{\text{beam}}^2 + |\vec{p}_{\text{beam}}|^2}$  yields

$$m_{\text{beam}}^2 + m_X^2 - 2(E_{\text{beam}} E_X - |\vec{p}_{\text{beam}}| |\vec{p}_X| \cos \theta) = 2m_{\text{target}}(E_X - E_{\text{beam}}) \quad (\text{B.5})$$

$$2m_{\text{target}} E_X - m_{\text{beam}}^2 - m_X^2 - 2|\vec{p}_{\text{beam}}| |\vec{p}_X| \cos \theta = -2(E_X - m_{\text{target}}) \sqrt{m_{\text{beam}}^2 + |\vec{p}_{\text{beam}}|^2}. \quad (\text{B.6})$$

5786 By taking the square of equation (B.6) and sorting the result by powers of  $|\vec{p}_{\text{beam}}|$ , we obtain a  
5787 quadratic equation in  $|\vec{p}_{\text{beam}}|$ :

$$\begin{aligned} 0 &= \overbrace{\left[ 4(|\vec{p}_X| \cos \theta)^2 - 4(E_X - m_{\text{target}})^2 \right]}^{\equiv a} |\vec{p}_{\text{beam}}|^2 \\ &+ \overbrace{\left[ 4(m_{\text{beam}}^2 + m_X^2 - 2m_{\text{target}} E_X) |\vec{p}_X| \cos \theta \right]}^{\equiv b} |\vec{p}_{\text{beam}}| \\ &+ \overbrace{\left[ (m_{\text{beam}}^2 + m_X^2 - 2m_{\text{target}} E_X)^2 - 4(E_X - m_{\text{target}})^2 m_{\text{beam}}^2 \right]}^{\equiv c} \end{aligned} \quad (\text{B.7})$$

5788 Solving equation (B.7) allows to calculate the beam momentum from measured quantities:<sup>[a]</sup>

$$|\vec{p}_{\text{beam}}| = \frac{-b + \sqrt{b^2 - 4ac}}{2a}. \quad (\text{B.8})$$

<sup>[a]</sup> Only one of the two solutions of the quadratic equation in equation (B.7) is physical, i.e. yields a positive momentum.

5789 Finally, the beam energy is calculated from the beam momentum via

$$E_{\text{beam}} = \sqrt{m_{\text{beam}}^2 + |\vec{p}_{\text{beam}}|^2}. \quad (\text{B.9})$$

## 5790 B.2 Estimation of the Non-Exclusive Background

5791 In order to estimate the non-exclusive background in the final  $K^-\pi^-\pi^+$  sample, we needed to  
5792 separate exclusive from non-exclusive contributions in the distribution of the reconstructed beam  
5793 energy  $E_{\text{beam}}$  shown in figure B.2.

5794 The finite width of the peak in the beam-energy distribution of exclusive events arises from  
5795 the intrinsic energy spread of the resolution of the apparatus. As a rough approximation, we  
5796 parameterized the peak by a sum of two Gaussian functions  $\mathcal{N}$  with different means  $\mu_i$  and widths  
5797  $\sigma_i$ .

5798 As there are many possible sources for non-exclusive events contributing to our data, there  
5799 is no physics model for their  $E_{\text{beam}}$  distribution. We assumed that the  $E_{\text{beam}}$  distribution of  
5800 non-exclusive events has a non-peaking shape in the energy region around the nominal beam  
5801 energy and that it vanishes above this region, because the total energy in any reaction is limited  
5802 by the beam energy. We parameterize the non-exclusive contributions by an arcus-tangents  
5803 function, which models the vanishing background above the peak region, multiplied by a fourth  
5804 order polynomial in the beam energy. The full model reads:

$$f(E_{\text{beam}}) = \mathcal{N}(E_{\text{beam}}, \mu_1, \sigma_1) + \mathcal{N}(E_{\text{beam}}, \mu_2, \sigma_2) + \underbrace{\left[ \sum_{i=0}^4 a_i (E_{\text{beam}} - \mu_1 - \Delta E)^i \right] \cdot \left[ \frac{\pi}{2} - \arctan \{ b (E - \mu_1 - \Delta E) \} \right]}_{\text{BG}(E_{\text{beam}})}, \quad (\text{B.10})$$

5805 where  $\mu_i, \sigma_i, a_i, b, \Delta E$  are the free parameter, which we fit to the data.

5806 Figure B.2 shows the result of a fit<sup>[b]</sup> of equation (B.10) to the distribution after applying all cuts,  
5807 except for the cut on  $E_{\text{beam}}$ . The non-exclusive contribution,  $\text{BG}(E_{\text{beam}})$  shown by the orange  
5808 curve, drops quickly above the nominal beam energy of about 191 GeV.

5809 Using this fit result we estimated the total number of events and the number of non-exclusive  
5810 events in our selected data sample by integrating the red and orange curves over the selected  $E_{\text{beam}}$   
5811 range. We obtained 402 051 events for the total number of events, which deviates only slightly  
5812 from the measured number of 397 701 events in this energy region. This shows, that the model

<sup>[b]</sup> We performed a binned maximum-likelihood fit using a Poisson assumption for the distribution of the number of events in each bin. We fit a wide energy region from 155 to 221 GeV, to determine the parameters especially of the non-exclusive background term.

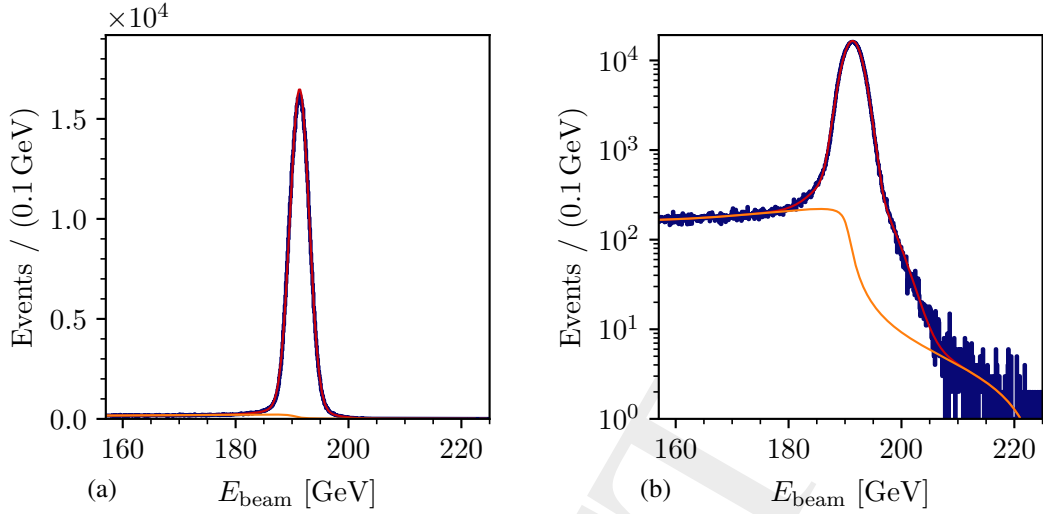


Figure B.2: Distribution of the reconstructed beam energy of the  $K^- \pi^- \pi^+$  sample (blue histogram) after applying all cuts, except for the cut on  $E_{\text{beam}}$ , (a) in linear scale and (b) in logarithmic scale. The red curves show the fit of equation (B.10) to the distribution. The orange curves show the non-exclusive contributions  $\text{BG}(E_{\text{beam}})$  [see equation (B.10)].

5813 describes the data well. Given the ad-hoc nature of our parameterization  $\text{BG}(E_{\text{beam}})$  for the non-  
 5814 exclusive contributions, the result may depend on this choice. To investigate this, we performed  
 5815 systematic studies where we reduced and increased the order of the background polynomial  
 5816 in equation (B.10). We also tested other fit ranges. Finally, we estimated a contribution of  
 5817 non-exclusive events to our data sample of  $(2 \pm 1 \text{ (sys.)}) \%$ .

### 5818 B.3 Fit of $t'$ Spectra

5819 In section 4.2, we qualitatively discuss the  $t'$  distribution. In this section, we parameterize the  
 5820 shape of the  $t'$  distribution and determine its parameters and its  $m_{K\pi\pi}$  dependence. The shape of  
 5821 the  $t'$  distribution is also required as input to generate pseudodata (see appendix C). Since this is  
 5822 done independently for the years 2008 and 2009, we studied the  $t'$  distribution independently for  
 5823 both years. Here, we discuss only the results for 2008. The results for 2009 are similar.

5824 The slope of the  $t'$  spectrum is steeper in the low- than in the high- $t'$  region. In order to  
 5825 describe the full  $t'$  spectrum with one parameterization, we modeled it by a double-exponential  
 5826 distribution

$$\frac{d\widehat{N}_{\text{ev}}(t'; m_{K\pi\pi})}{dt'} = A(m_{K\pi\pi}) \left[ e^{-b_1(m_{K\pi\pi})t'} + R(m_{K\pi\pi}) e^{-b_2(m_{K\pi\pi})t'} \right], \quad (\text{B.11})$$

5827 where  $b_i(m_{K\pi\pi})$  are the slope parameters and  $R$  is the ratio between the strength of second and  
 5828 first exponential contribution.  $b_1$ ,  $b_2$ ,  $A$ , and  $R$  depend on  $m_{K\pi\pi}$ .

5829 The measured  $t'$  spectrum is distorted by acceptance effects caused by the experimental setup.  
 5830 In order to take these effects into account, we approximated the acceptance in two-dimensional  
 5831 cells of  $m_{K\pi\pi}$  and  $t'$  based on a Monte Carlo sample that is uniformly distributed in the phase  
 5832 space (see appendix C for details).<sup>[c]</sup> We parameterized the  $t'$  dependence of the acceptance  $\eta$  in  
 5833 a given  $m_{K\pi\pi}$  bin by

$$\eta(t'; m_{K\pi\pi}) = \eta_0 + \frac{1}{(t' - t'_0)^\alpha} [a + bt' + ct'^2], \quad (\text{B.12})$$

5834 where  $\eta_0$ ,  $t'_0$ ,  $\alpha$ ,  $a$ ,  $b$ , and  $c$  are free parameters. These free parameters are determined from a fit of  
 5835 equation (B.12) to the acceptance obtained from the Monte Carlo sample. The fit was performed  
 5836 in the  $t'$  range  $0.08 \leq t' < 2.0$  (GeV/c)<sup>2</sup>. Figure B.3a shows the result of such a fit in the range  
 5837  $1.2 \leq m_{K\pi\pi} < 1.4$  GeV/c<sup>2</sup>. In the shown and in all other  $m_{K\pi\pi}$  ranges, the used parameterization  
 5838 describes the acceptance well.

5839 Finally, we modeled the measured  $t'$  spectrum as

$$\begin{aligned} \frac{d\widehat{N}_{\text{ev}}(t'; m_{K\pi\pi})}{dt'} &= \eta(t'; m_{K\pi\pi}) \cdot \frac{d\widehat{N}_{\text{ev}}(t'; m_{K\pi\pi})}{dt'} \\ &= \eta(t'; m_{K\pi\pi}) \cdot A(m_{K\pi\pi}) \left[ e^{-b_1(m_{K\pi\pi}) t'} + R(m_{K\pi\pi}) e^{-b_2(m_{K\pi\pi}) t'} \right]. \end{aligned} \quad (\text{B.13})$$

5840 We fitted equation (B.13) to the  $t'$  spectrum in the range  $0.1 \leq t' < 2.0$  (GeV/c)<sup>2</sup> independently  
 5841 in 400 MeV/c<sup>2</sup> wide bins of  $m_{K\pi\pi}$  to determine the  $m_{K\pi\pi}$  dependence of the free parameters  $b_i$ ,  $A$ ,  
 5842 and  $R$ .<sup>[d]</sup> Figure B.3b shows, for example, the  $t'$  spectrum in the range  $1.2 \leq m_{K\pi\pi} < 1.6$  GeV/c<sup>2</sup>.  
 5843 Our model (red curve) reproduces the measured  $t'$  spectrum well. This also holds for all other  
 5844  $m_{K\pi\pi}$  ranges.

5845 Figure B.4a shows the slope parameters as a function of  $m_{K\pi\pi}$ . The first exponential term  
 5846 exhibits a steeper slope, i.e. a larger slope parameter, than the second exponential by construction  
 5847 of the fitting procedure. The steeper exponential becomes shallower with increasing  $m_{K\pi\pi}$ ,  
 5848 while the slope of the shallower exponential stays almost constant with a maximum at about  
 5849  $m_{K\pi\pi} \approx 2$  GeV/c<sup>2</sup>. The low- $m_{K\pi\pi}$  region is dominated by the steeper exponential as shown by  
 5850 the ratio of their strength in figure B.4b. In the high- $m_{K\pi\pi}$  region at about 3 GeV/c<sup>2</sup> the shallower  
 5851 exponential becomes more significant, but its contribution stays below about 11 %. We observed  
 5852 qualitatively similar features in the COMPASS data of the reaction  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  [39].

## 5853 B.4 Time Stability

5854 In order to reject data where some of the detectors were malfunctioning, we tested the time  
 5855 stability of the data taking. Therefore, we studied the change of various kinematic distributions  
 5856 with time for the reactions  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  and  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  [43]. We mainly

<sup>[c]</sup> Doing so, we neglected the non-uniform distribution of the measured events in the phase space. However, this has only a minor effect on the acceptance in  $t'$  and hence, it does not strongly influence the extracted slope parameters.

<sup>[d]</sup> We performed a binned maximum-likelihood assuming a Poisson distribution for the number of events in each bin.

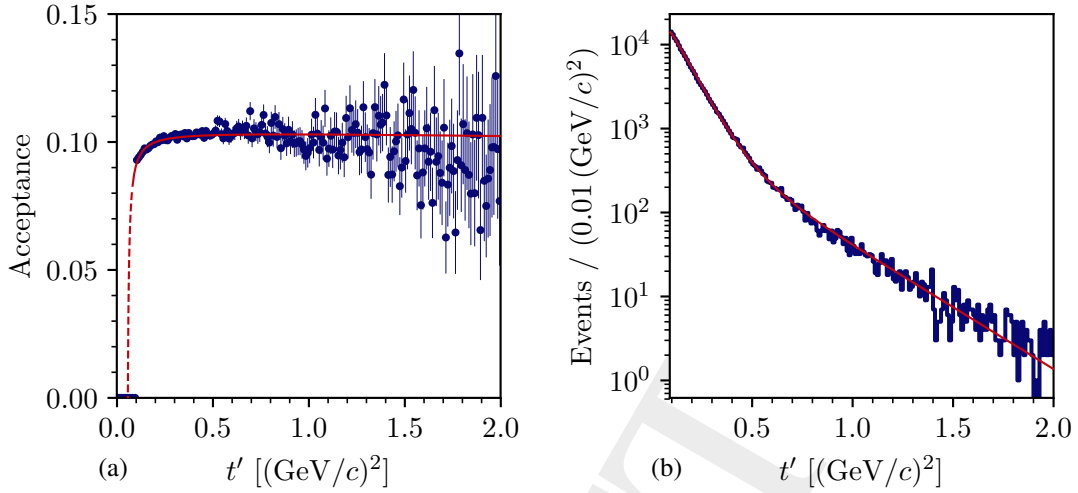


Figure B.3: Result of fits to extract the  $t'$  slope parameters from the 2008 diffraction data set. (a) shows the experimental acceptance as a function of  $t'$  in the range  $1.2 \leq m_{K\pi\pi} < 1.4 \text{ GeV}/c^2$  (blue points) together with a fit of equation (B.12) (solid red curve). The dashed red curve shows the extrapolation beyond the fitted  $t'$  range. (b) shows the measured  $t'$  spectrum in the range  $1.2 \leq m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$  (blue histogram) together with a fit of equation (B.13) (red curve).

5857 studied distributions in final-state kinematic variables, which are analyzed in the partial-wave  
 5858 decomposition (see section 5.1). As a simple test to check for changes in the distributions, we  
 5859 determined the moments of the distributions as a function of time and check for deviations from  
 5860 the average value of the corresponding moment.

5861 Figure B.5 shows the mean value, i.e. first moment, of the  $m_{K\pi\pi}$  distribution as a function of  
 5862 time represented by the run number. Outliers, i.e. data points that significantly deviate from the  
 5863 average value, in this or one of the other studied kinematic distributions that could be correlated  
 5864 to problems in the experimental setup were removed from the final data sample (see section 4.1).  
 5865 These data are shown as gray points. The remaining data, shown as blue points, exhibit no  
 5866 significant time dependence. Using a  $\chi^2$  test,<sup>[e]</sup> for example the time dependence of the mean  
 5867 value of  $m_{K\pi\pi}$  is consistent with a constant with a  $p$ -value of 0.7. With this approach, we were  
 5868 able to clean up our data sample from artifacts caused by problems during the data taking.

<sup>[e]</sup> See sections 4.5 and 4.7 in ref. [119] for details on the  $\chi^2$  test.

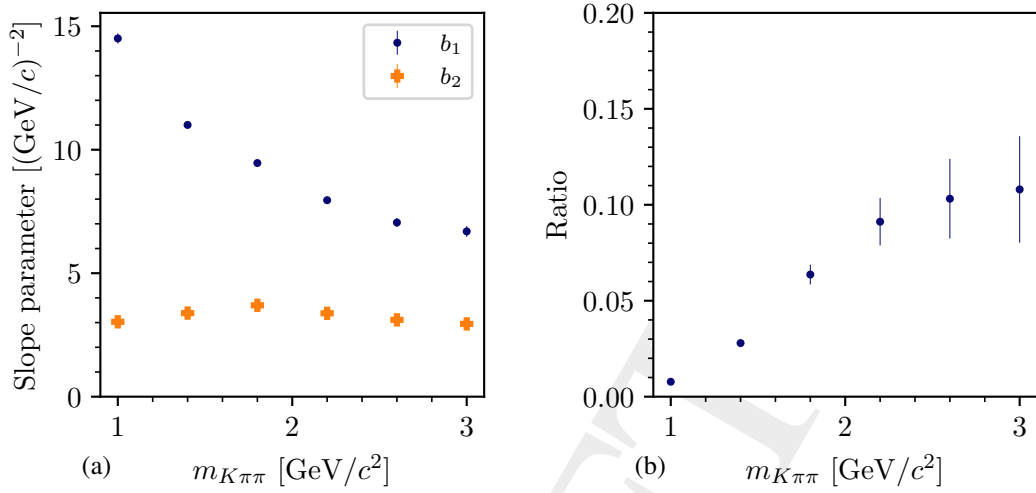


Figure B.4: Results of fitting equation (B.13) to the measured  $t'$  spectra in bins of  $m_{K\pi\pi}$  as obtained from the 2008 diffraction data set. (a) shows the slope parameters of the first (blue) and second (orange) exponential. (b) shows the ratio of the strength of the second and the first exponential term in equation (B.13). The uncertainties are smaller than the marker size for most of the data points.

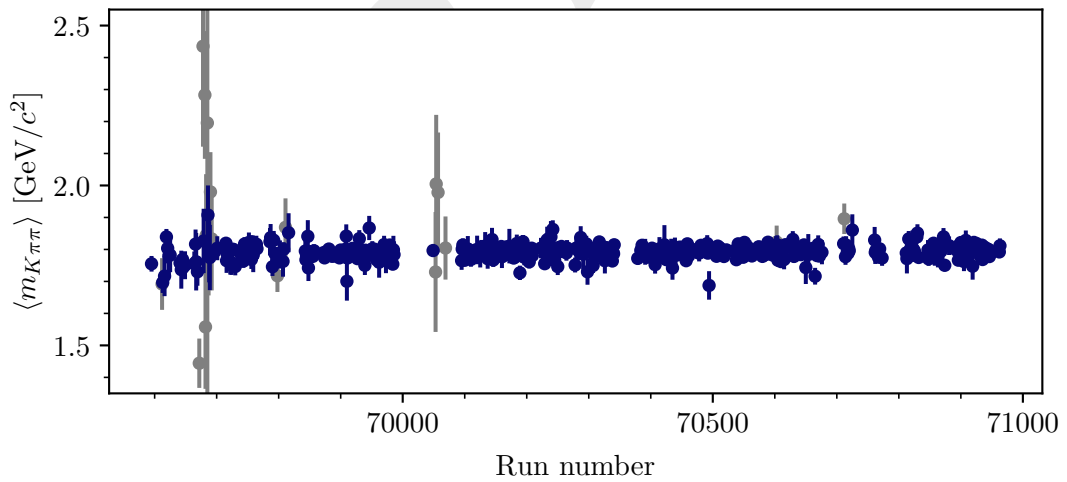


Figure B.5: Time stability of the  $m_{K\pi\pi}$  distribution. The mean mass  $\langle m_{K\pi\pi} \rangle$  per chunk of data in time, called run, is shown, versus the number of the run ordered in time. The blue points show the selected data, the gray points show the rejected data. The errors bars represent the statistical uncertainty of the mean values.





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## C Monte Carlo Simulation

5870 Monte Carlo simulations are an important tool in partial-wave analyses. They allow us to verify  
5871 the applied analysis methods or to trace the origin of some systematic effects. In addition, they are  
5872 necessary to study effects caused by the finite probability to experimentally observe a produced  
5873 event, i.e. by the acceptance.

5874 We performed Monte Carlo simulations by generating so-called produced pseudodata samples  
5875 of events that are randomly distributed according to a certain model input. We used different  
5876 physics models or generated samples that are uniformly distributed in the phase-space variables.  
5877 The procedure is described in appendix C.1.

5878 To study the experimental acceptance and resolution and to take the effects they cause into  
5879 account when comparing models to measured data, we applied both to the produced pseudo-  
5880 data samples. The procedure is described in appendix C.2. Thereby, we obtained so-called  
5881 reconstructed pseudodata samples.

5882 The distributions of the reconstructed pseudodata, called reconstructed distributions, mimic the  
5883 measured distributions of data recorded by the experiment, which we refer to as measured data  
5884 in the following. The distributions of produced pseudodata events, called produced distributions,  
5885 are the “true” distribution of the underlying physics process, i.e. without acceptance and res-  
5886 olution effects. We also call the “true” distributions of the underlying physics process of  
5887 measured data produced distributions of produced events. Finally, the reconstructed values of  
5888 kinematic variables of reconstructed pseudodata mimic measured values of measured data and  
5889 the produced values are the true values of the kinematic variable with which the event was  
5890 produced.

5891 As the measurement effects induced by the apparatus can be different for the diffraction data  
5892 taking campaigns in 2008 and 2009, we treated both years separately. In this chapter, we discuss  
5893 the main features of the measurement effects exemplarily for the 2008 setup. The measurement  
5894 effects of the 2009 setup show similar features.

## 5895 C.1 Generating Pseudodata of Diffractive Scattering Reactions

5896 In this section, we will briefly summarize how to generate pseudodata samples of diffractive  
 5897 scattering reactions. The generic topology of these reactions is depicted in figure C.1. An  
 5898 example of such a reaction is the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  analyzed in this work.

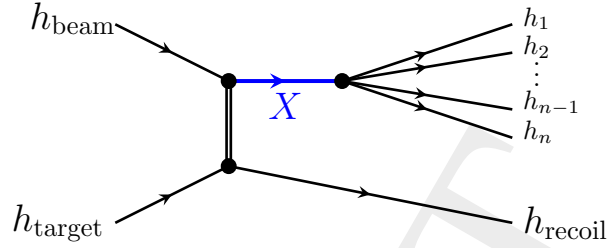


Figure C.1: Schematic view of diffractive scattering of a high-energy hadronic beam particle  $h_{\text{Beam}}$  off some hadronic target particle  $h_{\text{target}}$ . In this process, the target particle scatters elastically and the beam particle gets excited into some intermediate state  $X$ , which further decays into a hadronic  $n$ -body final state.

5899 As we analyzed our data independently in kinematic cells of the invariant mass  $m_X$  of the  $X$   
 5900 system and of the reduced four-momentum transfer squared  $t'$ , we generate pseudodata samples  
 5901 independently in  $(m_X, t')$  cells. For fixed  $m_X$  and  $t'$ , the probability of an event is proportional  
 5902 to the decay rate of the intermediate state  $X$  to the  $n$ -body final state, which is proportional to  
 5903 two factors (see equation (43.10) in ref. [9]): (i) the matrix element squared  $|\mathcal{M}|^2$  and (ii) the  
 5904 differential  $n$ -body phase-space volume  $d\Phi_n$ . The first one encodes the properties of the physical  
 5905 process, the latter one is a purely kinematic factor.

5906 In order to generate events that are distributed according to their reaction cross-section, we first  
 5907 generated a sample of events that is uniformly distributed in the  $n$ -body phase space, i.e. the  
 5908 probability to produce an event is proportional only to  $d\Phi_n$ .

5909 Second, we obtained a produced pseudodata sample of a given model for  $|\mathcal{M}|^2$  by randomly  
 5910 accepting events from the phase-space distributed sample according to their probability, which  
 5911 is proportional to  $|\mathcal{M}|^2$ .<sup>[a]</sup> For example, when generating a pseudodata sample from the results  
 5912 of a partial-wave decomposition, i.e. from the modeled intensity distribution  $\mathcal{I}(\tau, m_{K\pi\pi}, t')$  [see  
 5913 equation (5.16)], we used  $|\mathcal{M}(\tau, m_{K\pi\pi}, t')|^2 \propto \mathcal{I}(\tau, m_{K\pi\pi}, t')$ . The  $m_X$  and  $t'$  dependence is  
 5914 accounted for by generating a number of events in each  $(m_X, t')$  cell that is proportional to the  
 5915 number of events predicted by the model.

5916 A special case are pseudodata samples that are distributed uniformly in the  $n$ -body phase space  
 5917 of the final-state particles, i.e.  $|\mathcal{M}|^2 = 1$ . For example, such so-called phase-space pseudodata  
 5918 samples were used to accounting for acceptance effects in the partial-wave decomposition. For  
 5919 these samples, we drew  $m_X$  uniformly in the analyzed mass range and  $t'$  according to the  $t'$

<sup>[a]</sup> See [181, 182] for details on this accept-reject method.

5920 spectra we observed in the corresponding measured sample (see appendix B.3 for the  $t'$  spectra  
5921 of the  $K^- \pi^- \pi^+$  sample).

## 5922 C.2 Monte Carlo Simulation of the Experimental Setup

5923 Although, the COMPASS experimental setup covers a wide kinematic range, its acceptance and  
5924 measurement resolution are finite. These measurement effects distort the distribution of produced  
5925 events. Thus, they have to be taken into account when comparing measured distributions to, e.g.  
5926 model expectations. The dominant effect for the  $K^- \pi^- \pi^+$  final state is the limited momentum  
5927 range of the final-state particle identification.

5928 In order to obtain a reconstructed pseudodata sample that incorporates acceptance and reso-  
5929 lutions effects, we processed the events of the produced pseudodata sample through a Monte  
5930 Carlo simulation of the full COMPASS setup. Then, we applied the same event reconstruction  
5931 algorithm [53] to the simulated detector responses, as applied to measured data. Finally, only  
5932 those events entered the reconstructed pseudodata sample that survived the same event-selection  
5933 criteria as applied to measured data. Following this approach, a reconstructed pseudodata sample  
5934 is distributed as if it had been measured by the experimental apparatus.

5935 The Monte Carlo simulation of the COMPASS setup is described in section 10 of ref. [49]. In the  
5936 following, we describe aspects of the Monte Carlo simulation that were improved in this analysis  
5937 (appendix C.2.1) or that are particular to this analysis (appendices C.2.2 and C.2.3).

### 5938 C.2.1 Simulation of the Beam and Vertex Distribution

5939 In order to simulate the experimental setup, we transformed the event kinematics from the center-  
5940 of-momentum system of the reaction to the laboratory frame. This required the distribution of  
5941 beam particle momentum to be known. In addition, the interaction vertex had to be placed within  
5942 the target volume. The spatial distribution of the interaction vertices is given by the distribution  
5943 of the beam particles in the plane transverse to the beam direction and by the target material  
5944 (see figure 4.2). In total, the six-dimensional beam-particle distribution is required to generate  
5945 pseudodata, i.e. the vertex position  $(X_{\text{Vtx}}, Y_{\text{Vtx}}, Z_{\text{Vtx}})$  and the beam momentum. The latter one  
5946 is expressed in terms of the beam energy  $E_{\text{beam}}$  and in terms of the inclinations  $\frac{p_x}{|\vec{p}|}$  and  $\frac{p_y}{|\vec{p}|}$  of  
5947 the beam track in horizontal and vertical direction, respectively. The orientation angle of the  
5948 production plane of the reaction (see section 5.1.1) around the direction of the beam particle is  
5949 uniformly distributed, due to rasion symmetry.

5950 The beam-particle distribution is high-dimensional, complicatedly correlated, and thus hard to  
5951 model. Therefore, we generated the beam-particle distribution of pseudodata events by using the  
5952 beam-particle kinematics from randomly chosen events of a measured beam sample.

5953 In total, we generated about 200 times more pseudodata events than measured events, which  
 5954 required a large beam sample. In order to obtain a beam sample, we selected events with three  
 5955 charged particles in the final state, because measuring three charged tracks allows for a precise  
 5956 reconstruction of the interaction vertex, which reduces systematic effects from the beam sample.  
 5957 Simulating resolution effects at the borders of the kinematic regions that were selected for the  
 5958 measured  $K^- \pi^- \pi^+$  sample requires generating pseudodata events also outside these regions.  
 5959 Therefore, the cuts to select the beam sample were chosen to be wider compared to the ones for  
 5960 the measured  $K^- \pi^- \pi^+$  sample. Starting from the same preselection as for the  $K^- \pi^- \pi^+$  final state  
 5961 (see section 4.1 for details), we applied the following additional cuts:

- 5962 • Signal from the diffraction trigger DT0
- 5963 • Interaction vertex position along the beam direction:  $-70 \leq Z_{\text{Vtx}} < -27$  cm
- 5964 • Interaction vertex position in the plane transverse to the beam direction:  
 5965  $\sqrt{X_{\text{Vtx}}^2 + Y_{\text{Vtx}}^2} < 1.9$  cm
- 5966 • Momentum conservation in  $\Delta\phi_{\text{recoil}}$  using the measured recoil proton (see section 4.1)
- 5967 • Reconstructed beam-particle energy  $|E_{\text{beam}} - 191.35 \text{ GeV}| < 17.95 \text{ GeV}$
- 5968 • Uncertainty in the reconstructed beam energy<sup>[b]</sup> is less than 20 GeV

5969 The kinematic distributions of this beam sample are distorted by acceptance and resolution  
 5970 effects. However, the physical distributions are needed as input to the Monte Carlo simulation.  
 5971 Therefore, we had to correct the beam sample for these effects.

5972 The strongest acceptance effect is in the  $Z_{\text{Vtx}}$  distribution. Final-state particles produced in  
 5973 reactions at the upstream end of the target have to fly a long path through the target and thereby  
 5974 undergo multiple scattering.<sup>[c]</sup> Thus, the acceptance is lower for events with an interaction  
 5975 vertex located at the upstream end of the target. In the other variables of the beam sample the  
 5976 acceptance is approximately uniform in the range of interest. To correct for the acceptance in  
 5977  $Z_{\text{Vtx}}$ , we determined the acceptance in bins of  $Z_{\text{Vtx}}$  from a reconstructed phase-space pseudodata  
 5978 sample of the reaction  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$ , which is the dominant contribution to the beam  
 5979 sample. Then, the acceptance was parameterized by a third-order polynomial in  $Z_{\text{Vtx}}$ :

$$\eta(Z_{\text{Vtx}}) = A \left[ 1 + a(Z_{\text{Vtx}} + 50 \text{ cm}) + b(Z_{\text{Vtx}} + 50 \text{ cm})^2 + c(Z_{\text{Vtx}} + 50 \text{ cm})^3 \right], \quad (\text{C.1})$$

5980 where  $A$ ,  $a$ ,  $b$ , and  $c$  are free parameters we fitted to the acceptance in bins of  $Z_{\text{Vtx}}$ . Using the  
 5981 parameterization in equation (C.1), we corrected the beam sample for acceptance effects in the

<sup>[b]</sup> We calculated the uncertainty in  $E_{\text{beam}}$  using linear error propagation of equation (B.9). We used the uncertainties of the measured momenta of the final-state particles and of the measured beam-particle inclination. We also took into account the correlations between these measured quantities from the event-reconstruction fit [53].

<sup>[c]</sup> The material thickness of the liquid-hydrogen target along the beam axis corresponds to 4.5 % of a radiation length and 5.5 % of a nuclear interaction length [49].

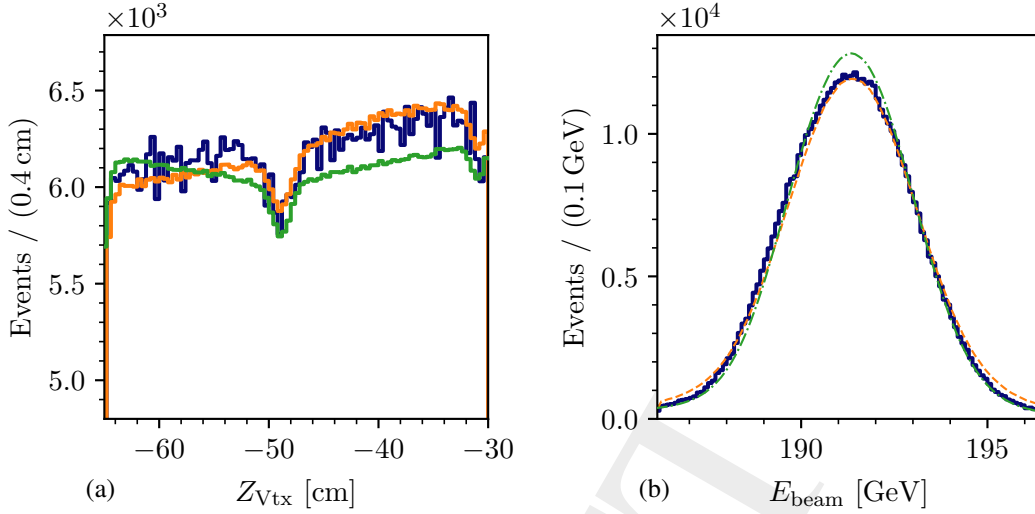


Figure C.2: (a) Interaction vertex position along the beam axis and (b) beam energy of a reconstructed  $K^- \pi^- \pi^+$  phase-space pseudodata sample for the 2008 diffraction data taking (orange histograms). The blue histograms show the corresponding measured distributions of the  $K^- \pi^- \pi^+$  sample from the 2008 diffraction data set. The green histograms show the distributions of the beam sample extracted from the 2008 diffraction data set corrected for the dominant acceptance and resolution effects (see text). The corrected beam sample is used as input to the Monte Carlo simulation. The histograms are normalized to the same integral as the measured  $K^- \pi^- \pi^+$  data histograms in the shown ranges.

5982  $Z_{Vtx}$  distribution by randomly accepting events with a probability proportional to the weight<sup>[d]</sup>

$$w(Z_{Vtx}) = \frac{1}{1 + a(Z_{Vtx} + 50 \text{ cm}) + b(Z_{Vtx} + 50 \text{ cm})^2 + c(Z_{Vtx} + 50 \text{ cm})^3}. \quad (\text{C.2})$$

5983 Thereby, we accepted a large fraction of the beam sample of about 94 %.

5984 Figure C.2a shows the  $Z_{Vtx}$  distribution of the beam sample after this acceptance correction  
 5985 (green histogram). It disagrees with the measured  $Z_{Vtx}$  distribution of the  $K^- \pi^- \pi^+$  sample  
 5986 (blue histogram) due to the acceptance effects. The orange histogram shows the reconstructed  
 5987  $Z_{Vtx}$  distribution of a reconstructed  $K^- \pi^- \pi^+$  phase-space pseudodata sample. This sample  
 5988 was generated using the acceptance-corrected beam sample as input. Then, it was processed  
 5989 through the detector Monte Carlo simulation. Thereby, acceptance effects were applied to this  
 5990 reconstructed  $K^- \pi^- \pi^+$  phase-space pseudodata sample. It is in fair agreement with the measured  
 5991  $K^- \pi^- \pi^+$  distribution, which demonstrates that our acceptance correction of the beam sample  
 5992 works. Using the  $Z_{Vtx}$  distribution from the beam sample to generate events allows us to take  
 5993 into account effects that are not modeled in the detector Monte Carlo simulation. For example,  
 5994 the dip in the  $Z_{Vtx}$  distribution at about -48 cm, which is caused by inefficient areas of the RPD  
 5995 scintillator slabs due to connectors for the calibration laser [183].

<sup>[d]</sup> As we were interested only in the deviation from a flat acceptance and not in an absolute normalization, we dropped the  $A$  parameter here, which is the acceptance at  $Z_{Vtx} = -50$  cm. As  $A \approx 0.5$ , this drastically improved the efficiency of the acceptance correction.

5996 The strongest resolution effect is in the measured beam-particle energy  $E_{\text{beam}}$ . As for the  
 5997 acceptance effects in  $Z_{\text{Vtx}}$ , we needed to correct the beam sample for this resolution effect in  
 5998 order to use it as input to the Monte Carlo simulation. Using Bayes' formula, the probability that  
 5999 the beam particle was produced with energy  $\tilde{E}_{\text{beam}}$  given that we measured  $E_{\text{beam}}$  is

$$P(\tilde{E}_{\text{beam}}|E_{\text{beam}}) = \frac{P(E_{\text{beam}}|\tilde{E}_{\text{beam}})P(\tilde{E}_{\text{beam}})}{P(E_{\text{beam}})}. \quad (\text{C.3})$$

6000 Here,  $P(E_{\text{beam}})$  is the probability distribution of the measured energy,  $P(\tilde{E}_{\text{beam}})$  is the probability  
 6001 distribution of the produced beam energy, i.e. without resolution effects, and  $P(E_{\text{beam}}|\tilde{E}_{\text{beam}})$  is  
 6002 the probability to measure an energy  $E_{\text{beam}}$  if the event was produced with an energy  $\tilde{E}_{\text{beam}}$ , i.e.  
 6003 it encodes the smearing effect due to the resolution.

6004 We modeled the resolution function,  $P(E_{\text{beam}}|\tilde{E}_{\text{beam}})$ , by a Gaussian function centered around  
 6005 zero with standard deviation  $\sigma_{\text{R}}$ .<sup>[e]</sup> We approximated the distribution  $P(\tilde{E}_{\text{beam}})$  of the produced  
 6006 energy of the beam particle also by a Gaussian function with mean  $\tilde{\mu}$  and standard deviation  
 6007  $\tilde{\sigma}$ . This is only a rough approximation, e.g. it neglects the weak correlation between the beam-  
 6008 particle energy and other kinematic variables of the beam particle introduced by the beam-line  
 6009 optics.

6010 The energy resolution  $\sigma_{\text{R}} = 0.78 \text{ GeV}$ <sup>[f]</sup> was taken from the detector Monte Carlo simulation.<sup>[g]</sup>  
 6011 The mean and standard deviation of the produced-energy distribution  $P(\tilde{E}_{\text{beam}})$  were calculated  
 6012 from the measured energy distribution  $P(E_{\text{beam}})$  of the beam sample. Under the assumptions  
 6013 made here,  $P(E_{\text{beam}})$  is a Gaussian distribution with standard deviation  $\sigma = \sqrt{\tilde{\sigma}^2 + \sigma_{\text{R}}^2}$  and mean  
 6014  $\mu = \tilde{\mu}$ . We determined  $\sigma = 1.82 \text{ GeV}$  and  $\mu = 191.35 \text{ GeV}$ <sup>[f]</sup> by fitting a Gaussian function plus  
 6015 a second-order background polynomial to the  $E_{\text{beam}}$  distribution of the beam sample.

6016 Using the assumptions made above and equation (C.3),  $P(\tilde{E}_{\text{beam}}|E_{\text{beam}})$  becomes a Gaussian  
 6017 shape with mean and standard deviation of

$$\hat{\mu} = \frac{\tilde{\sigma}^2}{\sigma_{\text{R}}^2 + \tilde{\sigma}^2} E_{\text{beam}} + \frac{\sigma_{\text{R}}^2}{\sigma_{\text{R}}^2 + \tilde{\sigma}^2} \tilde{\mu} \quad \text{and} \quad \hat{\sigma} = \sqrt{\frac{1}{\frac{1}{\sigma_{\text{R}}^2} + \frac{1}{\tilde{\sigma}^2}}}. \quad (\text{C.4})$$

6018 In order to correct for the  $E_{\text{beam}}$  resolution when generating a pseudodata event from the  
 6019 beam sample, we randomly drew the energy  $\tilde{E}_{\text{beam}}$  of the pseudo beam particle according  
 6020 to  $P(\tilde{E}_{\text{beam}}|E_{\text{beam}})$  using the measured energy  $E_{\text{beam}}$  of a randomly chosen event from the beam  
 6021 sample.<sup>[h]</sup>

<sup>[e]</sup> Thereby, we neglected a potential energy dependence of the energy resolution.

<sup>[f]</sup> Here, we give the values for the 2008 setup. The values for the 2009 setup are similar.

<sup>[g]</sup> We fit a Gaussian function with standard deviation  $\sigma_{\text{R}}$  to the distribution of the differences between the physical and the reconstructed energy of beam particles from the reconstructed phase-space pseudodata sample of the reaction  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$  discussed above.

<sup>[h]</sup> Note that we used  $E_{\text{beam}}$  from the beam sample, and we used  $P(\tilde{E}_{\text{beam}}|E_{\text{beam}})$  only to correct for the energy resolution. The reason for this is, that  $E_{\text{beam}}$  from the beam sample is distributed according to the physical distribution, which

6022 The green histogram in figure C.2b shows the distribution of the resolution-corrected beam-  
 6023 particle energy  $\tilde{E}_{\text{beam}}$  of the beam sample. It is narrower than the measured  $E_{\text{beam}}$  distribution of  
 6024 the  $K^-\pi^-\pi^+$  sample shown by the blue histogram. The orange histogram shows the reconstructed  
 6025 beam-particle energy from a reconstructed  $K^-\pi^-\pi^+$  phase-space pseudodata sample, which was  
 6026 generated using the resolution-corrected beam sample as input. It is in good agreement with  
 6027 the measured  $K^-\pi^-\pi^+$  data in the peak region. This shows, that the correction of the resolution  
 6028 effects works well. Only in the tails of the distribution, where the Gaussian assumption is not a  
 6029 good approximation anymore, the reconstructed  $K^-\pi^-\pi^+$  phase-space pseudodata sample slightly  
 6030 deviates from the measured sample.

### 6031 C.2.2 Modeling the CEDAR Acceptance

6032 The likelihood approach discussed in section 3.1 is able to identify the beam particles in a wide  
 6033 kinematic range. Figure C.3a shows that the acceptance, i.e. the efficiency to identify a beam  
 6034 kaon, is above about 95 % for small beam-particle inclinations. However, it drops to about 60 %  
 6035 for inclination angles above about 100 mrad.

6036 A full simulation of the CEDAR response in the detector Monte Carlo simulation is not feasible  
 6037 as it is computationally too expensive.<sup>[i]</sup> Therefore, we incorporated the CEDAR acceptance  
 6038 effect in the detector Monte Carlo simulation in an approximate way by randomly accepting  
 6039 a pseudodata event with beam-particle inclination  $(^1\vartheta_x, ^1\vartheta_y)$  with the probability given by the  
 6040 acceptance as shown in figure C.3a.<sup>[j]</sup> When simulating events with beam pions, but still applying  
 6041 an event selection for beam kaons as done in section 5.10, we randomly accepted pseudodata  
 6042 events with beam-particle inclination  $(^1\vartheta_x, ^1\vartheta_y)$  with the misidentification probability as shown  
 6043 in figure C.3b.<sup>[j]</sup>

### 6044 C.2.3 Modeling the RICH Acceptance

6045 A full simulation of the RICH response in the detector Monte Carlo simulation is not feasible  
 6046 for the same reasons as for the CEDAR response. Following ref. [49], we inferred the RICH  
 6047 response from data. As shown in section 3.2.2, we determined for a given RICH likelihood-ratio  
 6048 threshold  $\mathcal{T}_R$  the final-state particle identification probabilities  $P(X \rightarrow S)$  independently in

is only roughly approximated by a Gaussian function and which includes all correlations with other kinematic variables. In our approach, the Gaussian approximation is used only for the resolution correction, while generating events directly according to  $P(\tilde{E}_{\text{beam}})$  would imply a Gaussian approximation for the energy distribution.

<sup>[i]</sup> A full simulation of the CEDAR response would require to simulate each single Cherenkov photon including its path through the CEDAR optics and its detection in the PMTs. This is difficult to implement and computationally very expensive. As we do not expect large influence of the CEDAR acceptance on the kinematic distribution of the final-state particles, which is studied in the partial-wave decomposition, a full simulation of the CEDAR response would be inadequately time-consuming.

<sup>[j]</sup> Doing so, we linearly interpolated between the  $(^1\vartheta_x, ^1\vartheta_y)$  cells. In the green regions in figure C.3 without calibration data, we never identified the beam kaon. However, only a negligible fraction of pseudodata events has beam-particle inclinations in these regions.

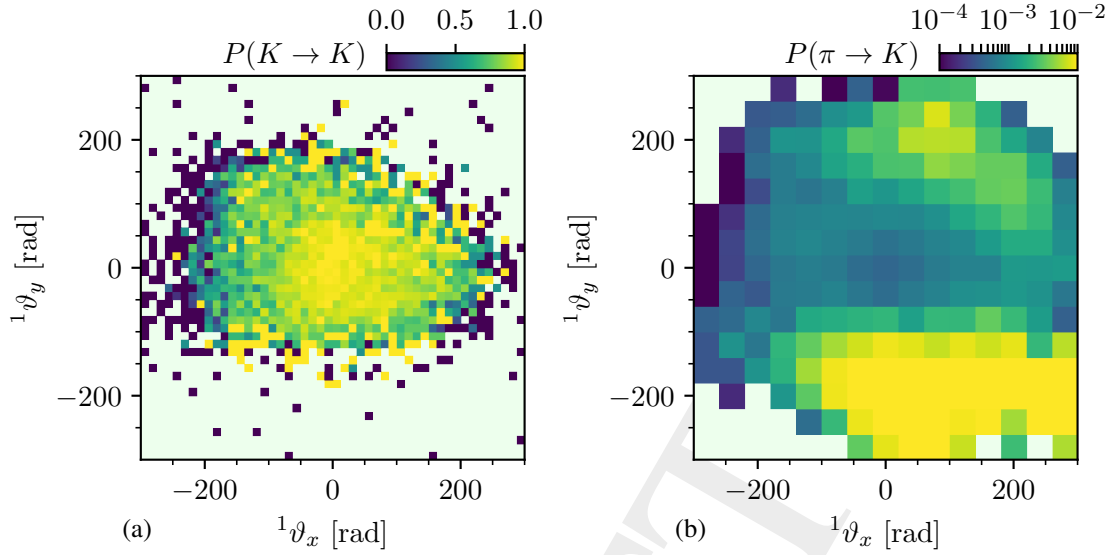


Figure C.3: (a) acceptance for the identification of beam kaons and (b) misidentification probability to identify a beam pion as a kaon by the CEDAR detectors as a function of the inclination of the beam-particle track with respect to the optical axis of CEDAR1. The acceptance was determined from the  $K \rightarrow \pi^- \pi^- \pi^+$  validation sample of the 2008 diffraction data set and the misidentification probability was determined from the pion-beam validation sample of the 2008 diffraction data set (see appendix A.1.2). Given the small fraction of misidentified beam pions, we chose a more coarse binning in (b). We chose the reference system of CEDAR1 for the beam-particle inclination. Regions without calibration data are drawn in light green.

6049 cells of the particle momentum  $|\vec{p}_R|$  and the square-root of its track angle  $\theta_R$  with respect to the  
 6050 nominal beam axis, both defined at the RICH position, for the different particle species  $X$  and for  
 6051 the different particle-species hypotheses  $S$ . Using these probabilities, we simulated the RICH  
 6052 response to a particle of species  $X$  by randomly drawing a particle-species assignment  $S$  by the  
 6053 RICH according to  $P(X \rightarrow S)$ .<sup>[k]</sup> As muons and pions are very close in mass, we approximated  
 6054 the probability to identify a muon as particle species  $S$  using the pion validation sample, i.e. we  
 6055 assumed  $P(\mu \rightarrow S) \approx P(\pi \rightarrow S)$ .<sup>[l]</sup>

### 6056 C.3 Predictions for Kinematic Distributions from the 6057 Partial-Wave Decomposition

6058 In order to study kinematic distributions as predicted by some model for  $|\mathcal{M}|^2$ , e.g. for the  
 6059 comparison of the PWD result with measured data discussed in section 5.6, we generated phase-  
 6060 space pseudodata samples and assigned a weight  $w_i$  to each event that is proportional to  $|\mathcal{M}|^2$

<sup>[k]</sup> Doing so, we linearly interpolated between the  $(|\vec{p}_R|, \sqrt{\theta_R})$  cells and normalized the sum over all probabilities to be one.

<sup>[l]</sup> Muons can appear in the simulation, e.g. from decays of final-state kaons. However, these contributions are negligible for the reactions simulated in this work.



6061 of the event (cf. appendix C.1).<sup>[m]</sup> When weights are assigned to a reconstructed phase-space  
 6062 pseudodata sample, the obtained distribution resembles the distribution of measured events. When  
 6063 weights are assigned to a produced phase-space pseudodata sample, the obtained distribution  
 6064 resembles true physical distribution. We chose the normalization of the weights such that the  
 6065 sum over all weights is the model prediction for the total number of events. This means that

$$\sum_i w_i \equiv \widehat{N}_{\text{ev}} \quad \text{or} \quad \sum_i w_i \equiv \widehat{N}_{\text{ev}} \quad (\text{C.5})$$

6066 for the distribution of reconstructed or produced events, respectively. Thus, histograms filled  
 6067 with these weights of reconstructed pseudodata events can be directly compared to histograms  
 6068 from measured data.

6069 When predicting distributions of a data sample that consists of different sub-samples,<sup>[n]</sup> we first  
 6070 obtained the distributions for the individual sub-samples following the approach described in the  
 6071 previous paragraph. As these distributions are normalized to the expected number of events in  
 6072 each sub-sample according to equation (C.5), we simply added them to obtain the distributions  
 6073 of the total sample.

6074 When predicting distributions based on the result of a PWD fit, we used  $|\mathcal{M}(\tau, m_{K\pi\pi}, t')|^2 \propto$   
 6075  $\mathcal{I}(\tau, m_{K\pi\pi}, t')$ , where  $\mathcal{I}(\tau, m_{K\pi\pi}, t')$  is the model intensity [see equation (5.16)] evaluated using  
 6076 the maximum-likelihood estimates of the transition amplitudes and data-set fraction parameters  
 6077 from the fit.

6078 When predicting distributions based on the results of a Bootstrapping of the PWD, as done in  
 6079 section 5.6, we used  $|\mathcal{M}(\tau, m_{K\pi\pi}, t')|^2 \propto \mathcal{I}(\tau, m_{K\pi\pi}, t')$ , where we evaluated the model intensity  
 6080 using the Bootstrapping estimates for the spin-density matrix elements and data-set fraction  
 6081 parameters. To this end, we used the formulation of  $\mathcal{I}(\tau, m_{K\pi\pi}, t')$  in terms of spin-density matrix  
 6082 elements as given in equation (5.19).<sup>[o]</sup>

<sup>[m]</sup> For the same number of generated phase-space events, using weights leads to a slightly reduced variance from the Monte Carlo sampling of the predicted quantities, compared to the accept-reject algorithm described in appendix C.1.

<sup>[n]</sup> For example, the  $K^-\pi^-\pi^+$  sample consists of three sub-samples from the 2008, the 2009W2X, and the 2009W35 diffraction data taking campaigns with slightly different acceptances.

<sup>[o]</sup> In ROOTPWA, which is our PWD software framework,  $\mathcal{I}(\tau, m_{K\pi\pi}, t')$  is implemented in terms of transition amplitudes as input parameters. Thus, in order to use the Bootstrapping estimates for the spin-density matrix elements, the corresponding spin-density matrix has to be decomposed into a set of transition amplitudes. Although we used a rank=3 spin-density matrix in the PWD model, the spin-density matrix obtained from Bootstrapping has maximum rank. This is because its elements are calculated individually by calculating the mean values of the corresponding estimates from the independent Bootstrapping fits. These mean values do not have the constraint of a rank=3 matrix implemented. In principle, a Cholesky decomposition of the spin-density matrix obtained from Bootstrapping could be used, which would yield a set of transition amplitudes that is similar to the Chung and Trueman parameterization [73]. However, the Cholesky decomposition yielded numerically unstable result. Thus, we used an eigenvalue decomposition, which yielded a set of transition amplitudes that given the same  $\mathcal{I}(\tau, m_{K\pi\pi}, t')$  as directly using the Bootstrapping estimates for the spin-density matrix elements in equation (5.19).

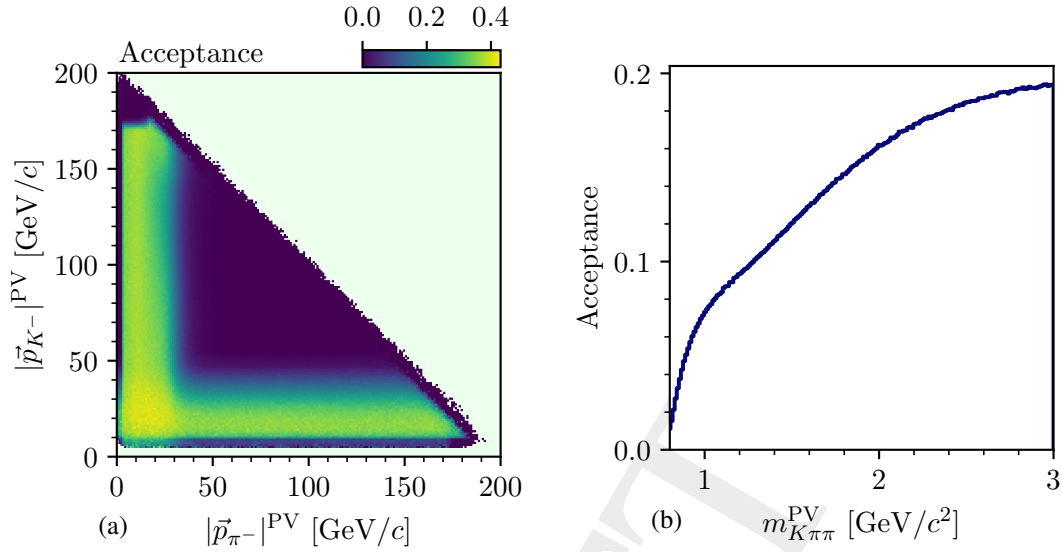


Figure C.4: Acceptance of the 2008 experimental setup as determined from a reconstructed  $K^- \pi^- \pi^+$  phase-space pseudodata sample as a function of (a) the momenta of the two identified negative final-state particles and (b) the invariant mass of the  $K^- \pi^- \pi^+$  system. The physical values (PV) of the kinematic variables with which the event was produced are shown, which do not involve smearing due to the detector resolution or misidentification of the final-stat particle species. Both figures show the acceptance for events that were produced uniformly in the  $K^- \pi^- \pi^+$  phase space, which is different from the distribution with which the measured events were produced.

#### 6083 C.4 Acceptance and Resolution for the $K^- \pi^- \pi^+$ Sample

6084 Using the approach discussed in appendices C.1 and C.2, we generated a reconstructed phase-space  
 6085 pseudodata sample of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . Based on this sample, we  
 6086 performed first studies of acceptance and resolution effects on different kinematic variables. One  
 6087 should keep in mind, that considering individual variables implies a marginalization over all  
 6088 other kinematic variables. Here, we marginalized using a sample that was generated uniformly  
 6089 in phase space. The events produced in the physical reaction follow a different distribution,  
 6090 which can be taken into account only using the model from the partial-wave decomposition (see  
 6091 section 5.6).

6092 The strongest acceptance effects originate from the limited momentum range of the RICH final-  
 6093 state particle identification (see section 3.2.2). The acceptance of the reconstructed phase-space  
 6094 pseudodata shows the same bands in the momentum distribution of the two identified negative  
 6095 final-state particles as the measured distribution (cf. figures 4.3 and C.4a). The acceptance is  
 6096 vanishing in the inner triangular region where both momenta are above about 50 GeV/c. This  
 6097 supports the statements about the experimental acceptance in section 4.1.

6098 The above discussed acceptance effects lead to a non-uniform acceptance also in other kinematic  
 6099 variables. For example, the acceptance as a function of  $m_{K\pi\pi}$  drops towards lower masses as

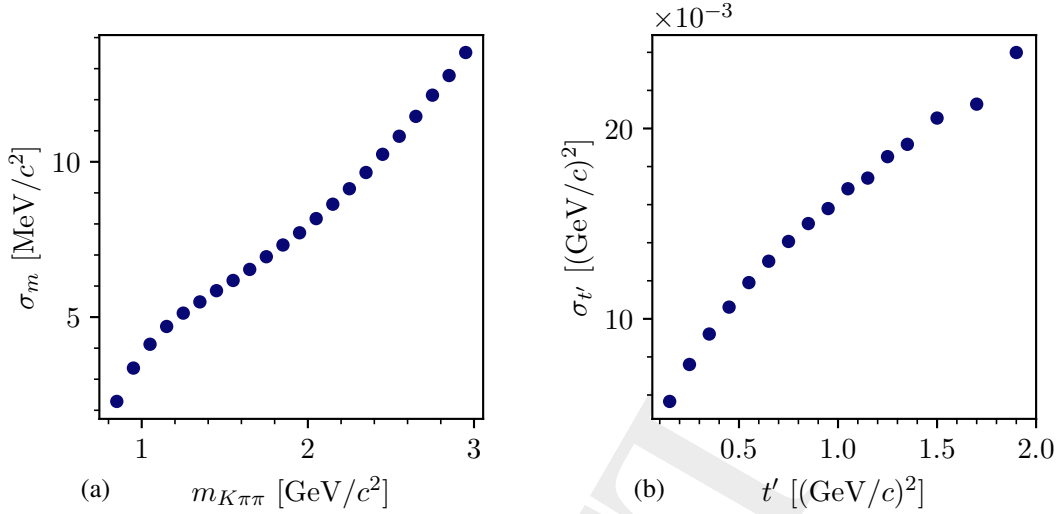


Figure C.5: Resolution of the 2008 experimental setup as determined from a reconstructed  $K^-\pi^-\pi^+$  phase-space pseudodata sample. (a) shows the resolution  $\sigma_m$  in the invariant mass of the  $K^-\pi^-\pi^+$  system as a function of  $m_{K\pi\pi}$ . (b) shows the resolution  $\sigma_{t'}$  in  $t'$  as a function of  $t'$ . We determined the resolution from a fit of a Gaussian function plus a constant background to the distribution of the differences between the reconstructed and the produced value. As the pseudodata falls exponentially with  $t'$ , we used a coarser binning at high- $t'$  to compensate for the smaller amount of data.

6100 shown in figure C.4b for the phase-space pseudodata sample. This demonstrates how crucial  
 6101 an accurate treatment of the acceptance is. Fortunately, the acceptance exhibits no peaking  
 6102 structures in  $m_{K\pi\pi}$ . Therefore, the structures observed in the measured  $m_{K\pi\pi}$  distribution shown  
 6103 in figure 4.6a can still be interpreted on a qualitative level.

6104 The reconstructed phase-space pseudodata sample also allows us to determine the experimental  
 6105 resolution of the detector setup. The resolution in  $m_{K\pi\pi}$  worsens continuously with increasing  
 6106  $m_{K\pi\pi}$  from about  $3 \text{ MeV}/c^2$  at  $m_{K\pi\pi} = 0.8 \text{ GeV}/c^2$  to about  $14 \text{ MeV}/c^2$  as  $m_{K\pi\pi} = 3 \text{ GeV}/c^2$   
 6107 (see figure C.5a). However, as most of the strange-meson resonances have widths of above  
 6108  $100 \text{ MeV}/c^2$ , the resolution in  $m_{K\pi\pi}$  will have a negligible influence on the width measurement  
 6109 of resonances.

6110 Also, the resolution in  $t'$  worsens from about  $6 \times 10^{-3} (\text{GeV}/c)^2$  at  $t' = 0.1 (\text{GeV}/c)^2$  to about  
 6111  $24 \times 10^{-3} (\text{GeV}/c)^2$  at  $t' = 2 (\text{GeV}/c)^2$  as shown in figure C.5b. The resolution in  $t'$  is sufficiently  
 6112 high to perform a partial-wave analysis in narrow  $t'$  bins. In this analysis, the narrowest  $t'$  bin  
 6113 at  $t' = 0.125 (\text{GeV}/c)^2$  has a width of  $50 \times 10^{-3} (\text{GeV}/c)^2$ , which is much larger than the  
 6114 resolution.



## D Partial-Wave Decomposition

### D.1 Wave-Set Selection

#### D.1.1 Determination of Intensity Thresholds

In order to determine the intensity threshold above which waves were included in the wave set, we studied the partial-waves intensities obtained from the wave-set selection fits in individual  $(m_{K\pi\pi}, t')$  cells. Figure D.1a exemplarily shows the partial waves ordered by intensity, i.e. the so-called ordered-intensity distribution. As discussed in section 5.2.5, ordered-intensity distributions exhibit jumps. The intensities at which those jumps appear determine the thresholds above which waves were selected for the wave set. In order to automatically determine the threshold for each  $(m_{K\pi\pi}, t')$  cell, we searched for all jumps in the ordered-intensity distribution of the  $(m_{K\pi\pi}, t')$  cell. We defined a jump as a discontinuity where the intensity changes by more than a factor eight, i.e. where the intensity of a wave is smaller than 1/8 of the intensity of the next larger wave.<sup>[a]</sup> If we found no discontinuity by at least a factor eight, the position where the relative change of wave intensities in the ordered-intensity distribution is largest was used as jump, exemplarily shown in figure D.1b where the change in intensity was smaller than a factor eight everywhere. The threshold (black horizontal lines in figure D.1) was given by the intensity at the position of the jump. If there were multiple jumps, we used the jump in the region of the highest intensity to define the threshold, i.e. the leftmost jump found in the ordered-intensity distribution. In order to avoid too small or too large wave sets, we did not consider jumps at the position of the two waves with the largest intensity and the ten waves with the smallest intensity. For example, jumps at waves with large intensity may be physical, as individual partial waves may dominate the physical distribution of the data.

Figure D.2 shows the thresholds for all 300  $(m_{K\pi\pi}, t')$  cells that were determined as explained above. For 129 cells, the threshold determination yielded thresholds in the reasonable range between about 1 and 20. In the remaining cells, the automatic threshold determination failed. The obtained thresholds were either too low, i.e. below 1, leading to a too large wave set, or too large, i.e. above 20, leading to a too small wave set. Additionally, we considered the threshold determination to be failed if the number of waves selected by the automatically determined threshold was larger than 150 or, for cells with  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$ ,<sup>[b]</sup> smaller than 5. For these

<sup>[a]</sup> We chose the minimal required intensity change to be a factor eight in order to be much larger than the average intensity fraction of subsequent waves in the ordered-intensity distribution.

<sup>[b]</sup> For  $m_{K\pi\pi} \leq 2 \text{ GeV}/c^2$ , we allowed wave sets with less than 5 waves, e.g. in the lowest  $m_{K\pi\pi}$  bins.

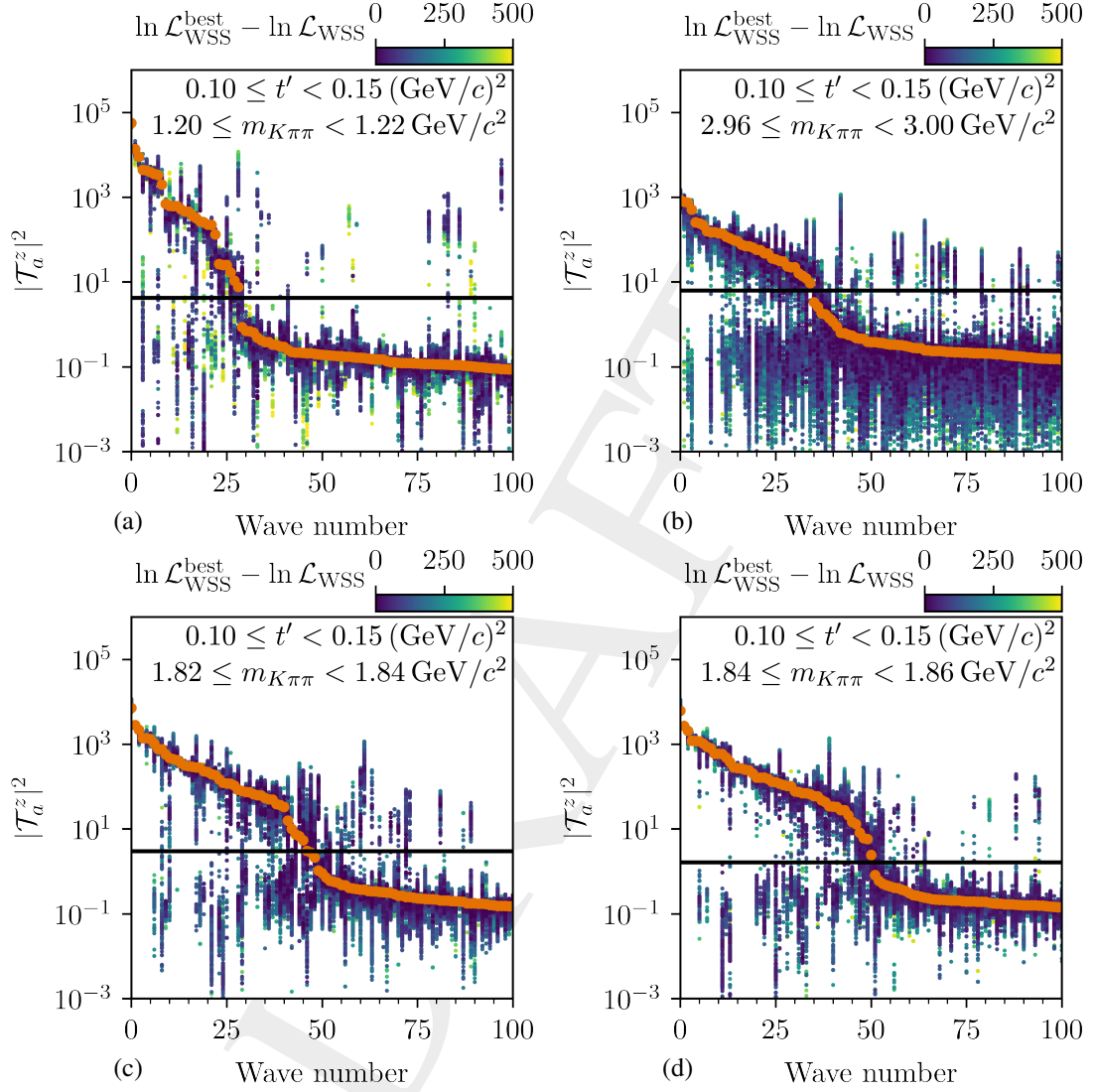


Figure D.1: Partial waves ordered by their intensity in the lowest  $t'$  bin in four different  $m_{K\pi\pi}$  bins. The waves are ordered by intensity as obtained from the best result in each cell and numbered accordingly. The orange points show the best result out of 700 fit attempts. The other colored points show the results from the other fit attempts. Their color represents  $\ln \mathcal{L}_{\text{WSS}}^{\text{best}} - \ln \mathcal{L}_{\text{WSS}}$ . Only results where this difference is smaller than 500 units are plotted. Only the 100 waves with the largest intensity are shown. The black horizontal line marks the threshold, above which waves were selected for the wave set (see text). (b) are the same as figures 5.9a and 5.9b in the main text, respectively.

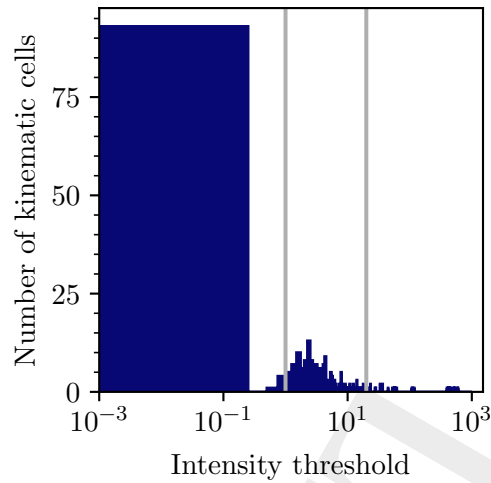


Figure D.2: Distribution of the automatically determined thresholds for all 300  $(m_{K\pi\pi}, t')$  cells. Only thresholds within the vertical gray lines are used to define the wave set.

6144 cells, we fixed the threshold to a value of 3, which corresponds to the peak in the distribution  
 6145 of thresholds from cells where the automatic threshold determination worked (see figure D.2).  
 6146 Figure D.1c shows the partial waves ordered by intensity in a  $(m_{K\pi\pi}, t')$  cell where the automatic  
 6147 threshold determination failed, because the distribution exhibits a smooth transition from waves  
 6148 with large to waves with low intensities instead of a sudden jump.<sup>[c]</sup> Still the manually defined  
 6149 threshold of 3 agrees with the distribution. In the neighboring  $(m_{K\pi\pi}, t')$  cell shown in figure D.1d,  
 6150 the intensity distribution showed again a clear jump and the threshold could be determined  
 6151 automatically.

<sup>[c]</sup> We observed such a “smearing” of the jump in a few cells. This behavior seems to be caused by slightly different jump positions in neighboring  $m_{K\pi\pi}$  cells via the continuity term in equation (5.57).

6152 **D.1.2 Manually Selected Waves**

Table D.1: Waves that were included in the wave sets over the corresponding  $m_{K\pi\pi}$  range given below independent of the result of the wave-set selection fits (see section 5.2.6). Waves and mass ranges were chosen that show interesting signals worth being studied in the resonance-model fit (see chapters 6 and 7). These waves were already selected in most  $(m_{K\pi\pi}, t')$  cells in the given  $m_{K\pi\pi}$  range by the wave-set selection fits. We only ensured that these waves are included in the waves sets in all  $(m_{K\pi\pi}, t')$  cells in the given  $m_{K\pi\pi}$  range.

Wave	$m_{K\pi\pi}$ Range	
	Start [GeV/ $c^2$ ]	End [GeV/ $c^2$ ]
$0^- 0^+ [K\pi]_S^{K\pi} \pi S$	1.6	2.4
$0^- 0^+ \rho(770) K P$	1.0	2.4
$1^+ 0^+ K^*(892) \pi S$	1.0	2.5
$1^+ 0^+ \rho(770) K S$	1.0	2.5
$1^+ 1^+ \rho(770) K S$	1.0	2.5
$2^+ 1^+ K^*(892) \pi D$	1.0	2.0
$2^+ 1^+ \rho(770) K D$	1.0	2.0
$2^- 0^+ K^*(892) \pi F$	1.5	3.0
$2^- 0^+ K_2^*(1430) \pi S$	1.4	3.0
$2^- 0^+ \rho(770) K F$	1.5	3.0
$2^- 0^+ f_0(980) K D$	1.5	3.0
$2^- 0^+ f_2(1270) K S$	1.5	3.0
$2^- 1^+ K_2^*(1430) \pi S$	1.5	2.5
$3^+ 0^+ K_3^*(1780) \pi S$	2.0	2.5
$3^+ 1^+ K_2^*(1430) \pi P$	2.0	2.5
$3^- 1^+ K^*(892) \pi F$	1.5	2.2
$3^- 1^+ \rho(770) \pi F$	1.6	2.5
$4^+ 1^+ K^*(892) \pi G$	1.6	3.0
$4^+ 1^+ \rho(770) K D$	1.6	3.0
$4^- 0^+ K^*(892) \pi F$	1.8	3.0
$4^- 0^+ K_2^*(1430) \pi D$	2.0	3.0
$4^- 0^+ \rho(770) K F$	1.8	3.0
$4^- 1^+ K^*(892) \pi F$	1.5	3.0



## 6153 D.1.3 The 238-Wave Set

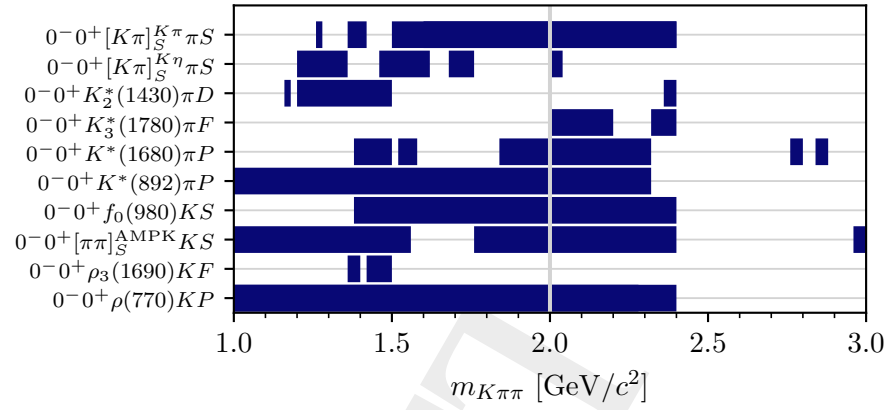


Figure D.3: Mass ranges of selected waves with  $J = 0$  in the range  $0.10 \leq t' < 0.15$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

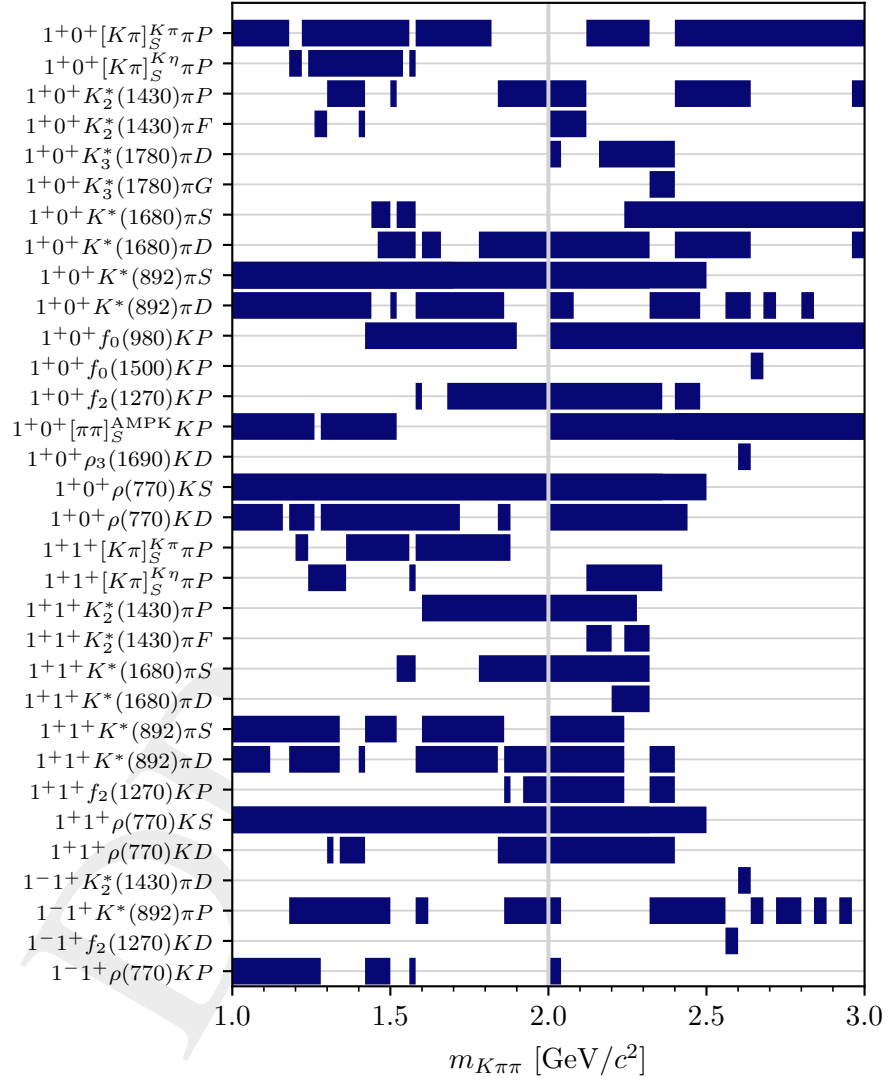


Figure D.4: Mass ranges of selected waves with  $J = 1$  in the range  $0.10 \leq t' < 0.15$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

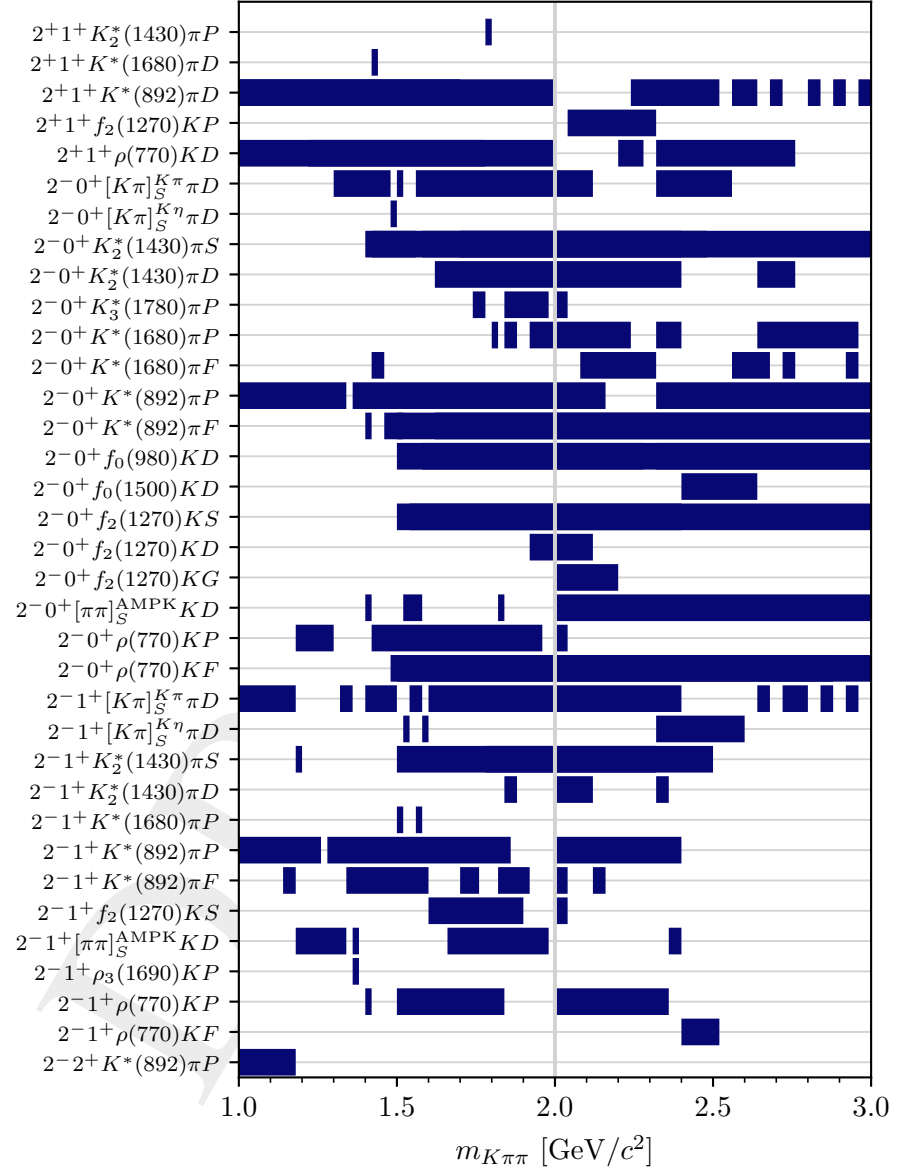


Figure D.5: Mass ranges of selected waves with  $J = 2$  in the range  $0.10 \leq t' < 0.15$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

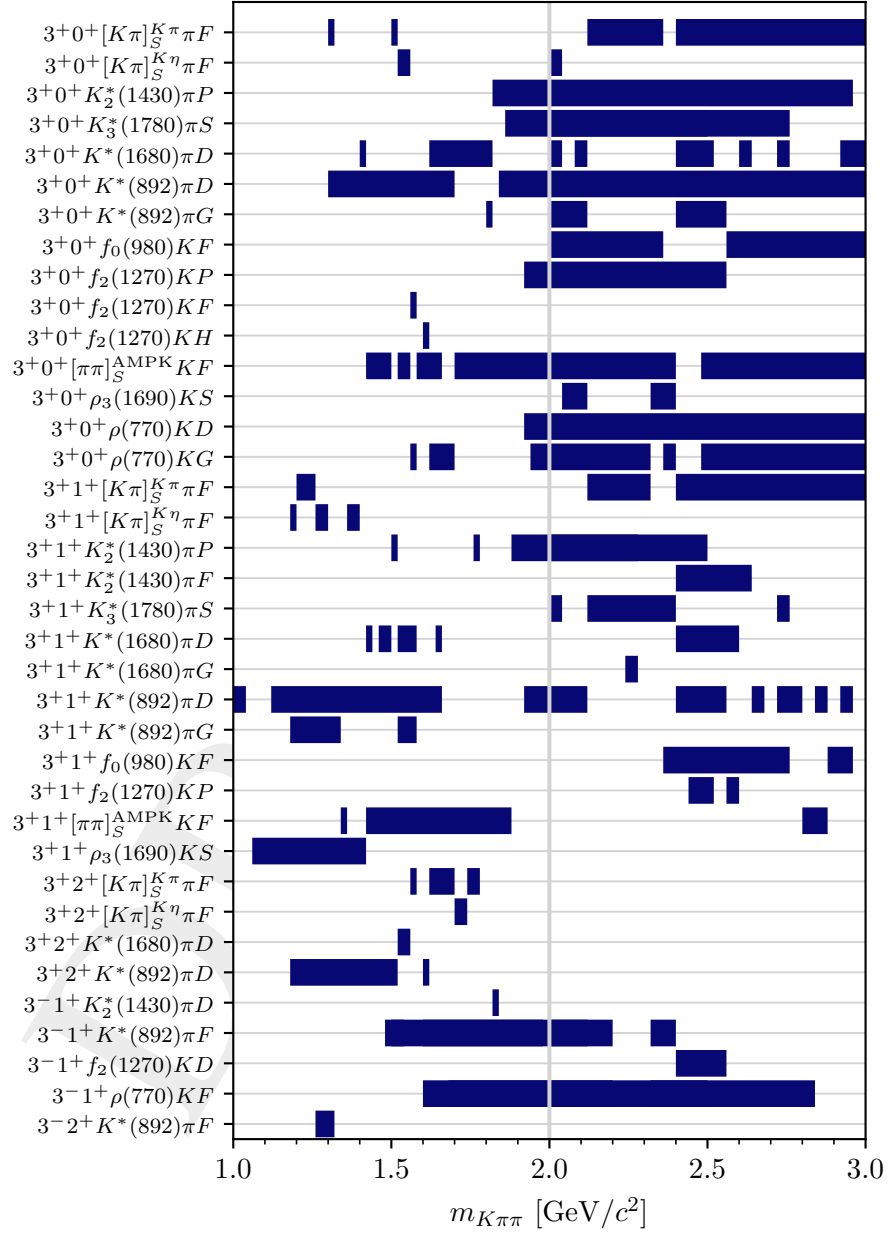


Figure D.6: Mass ranges of selected waves with  $J = 3$  in the range  $0.10 \leq t' < 0.15$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

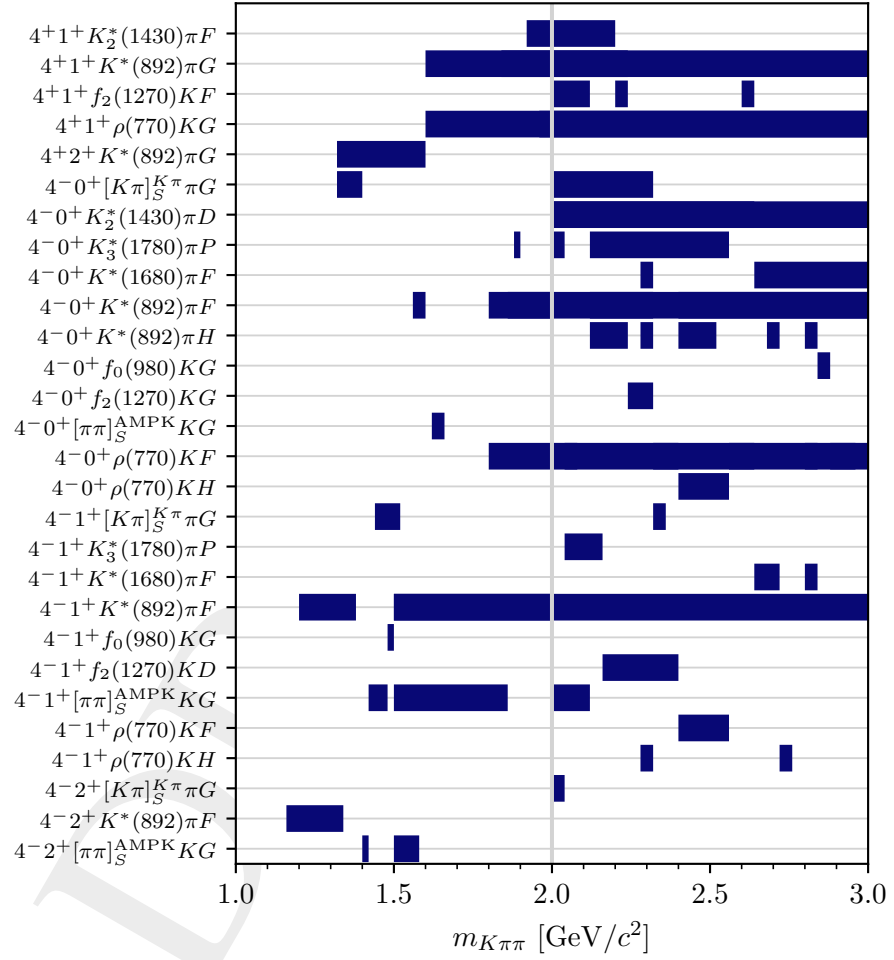


Figure D.7: Mass ranges of selected waves with  $J = 4$  in the range  $0.10 \leq t' < 0.15 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

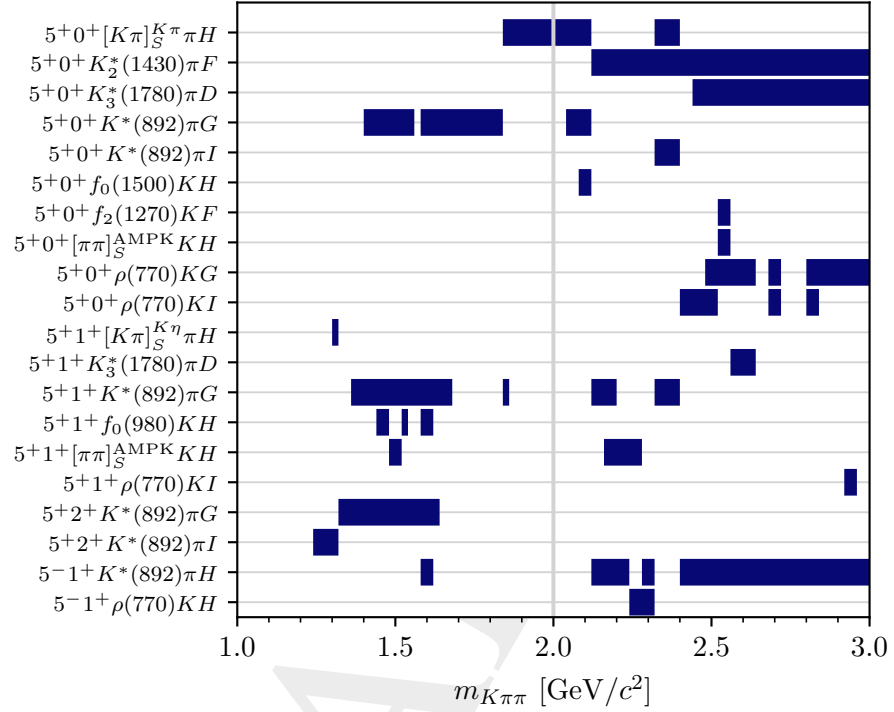


Figure D.8: Mass ranges of selected waves with  $J = 5$  in the range  $0.10 \leq t' < 0.15 \text{ (GeV}/c^2)$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

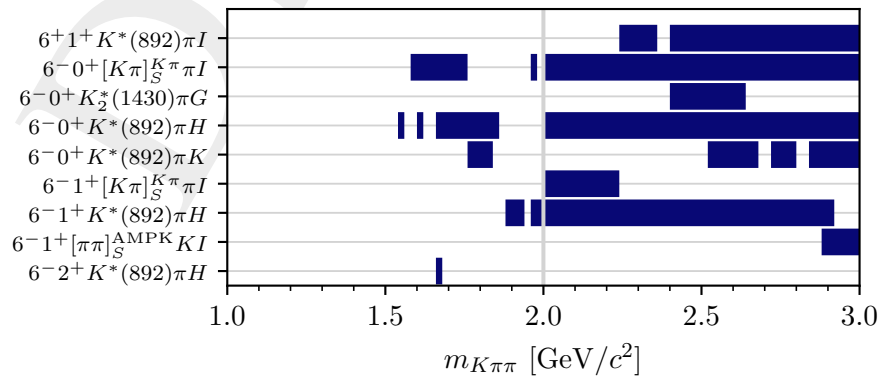


Figure D.9: Mass ranges of selected waves with  $J = 6$  in the range  $0.10 \leq t' < 0.15 \text{ (GeV}/c^2)$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

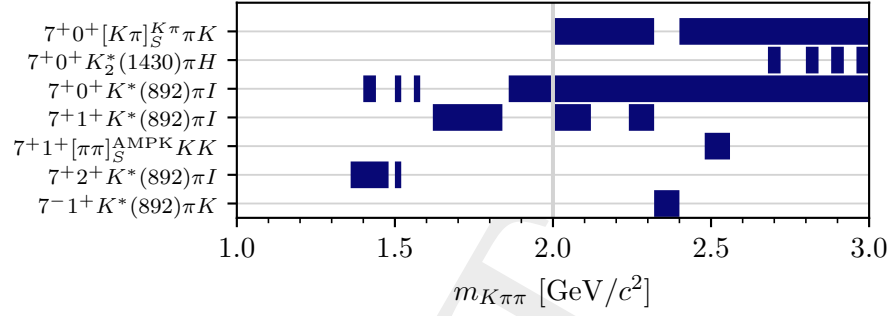


Figure D.10: Mass ranges of selected waves with  $J = 7$  in the range  $0.10 \leq t' < 0.15$  ( $\text{GeV}/c^2$ )<sup>2</sup>. The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from 20  $\text{MeV}/c^2$  to 40  $\text{MeV}/c^2$  wide bins.

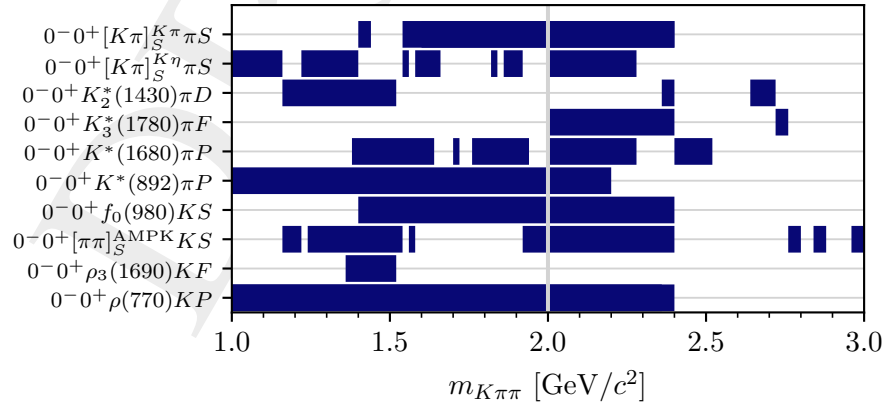


Figure D.11: Mass ranges of selected waves with  $J = 0$  in the range  $0.15 \leq t' < 0.24$  ( $\text{GeV}/c^2$ )<sup>2</sup>. The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from 20  $\text{MeV}/c^2$  to 40  $\text{MeV}/c^2$  wide bins.

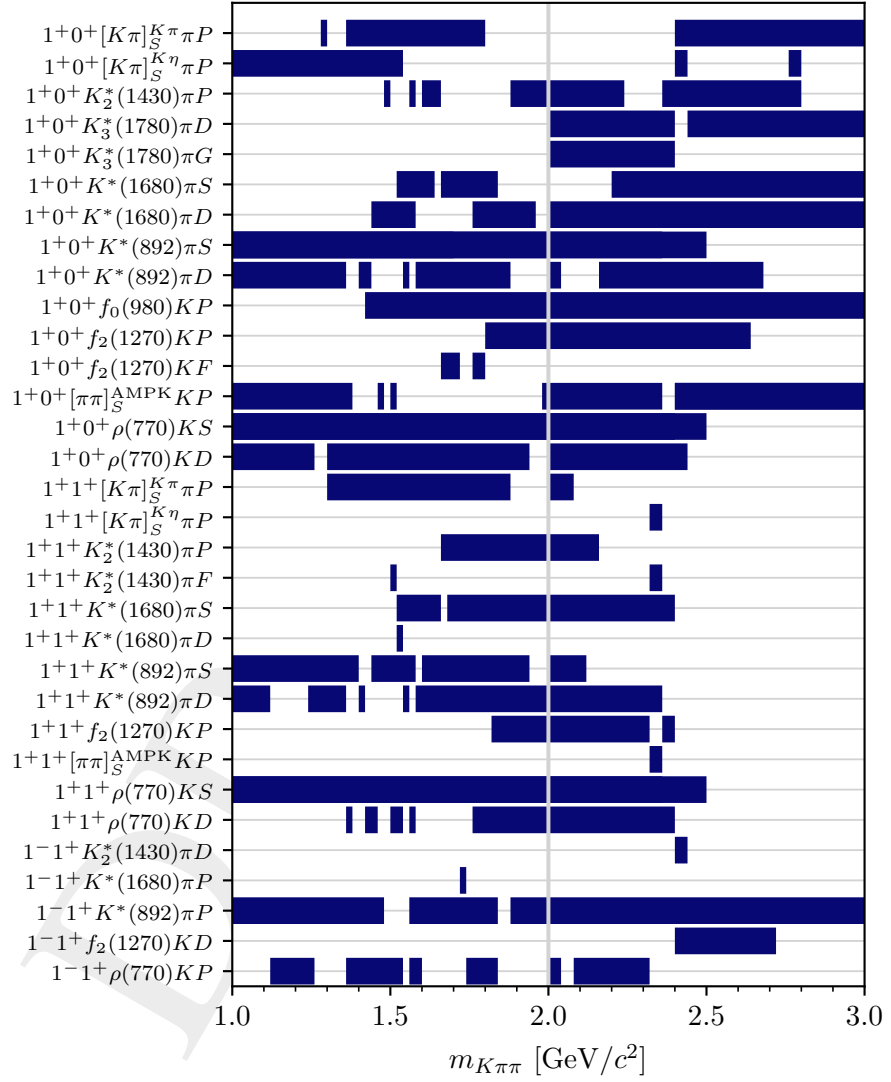


Figure D.12: Mass ranges of selected waves with  $J = 1$  in the range  $0.15 \leq t' < 0.24 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.



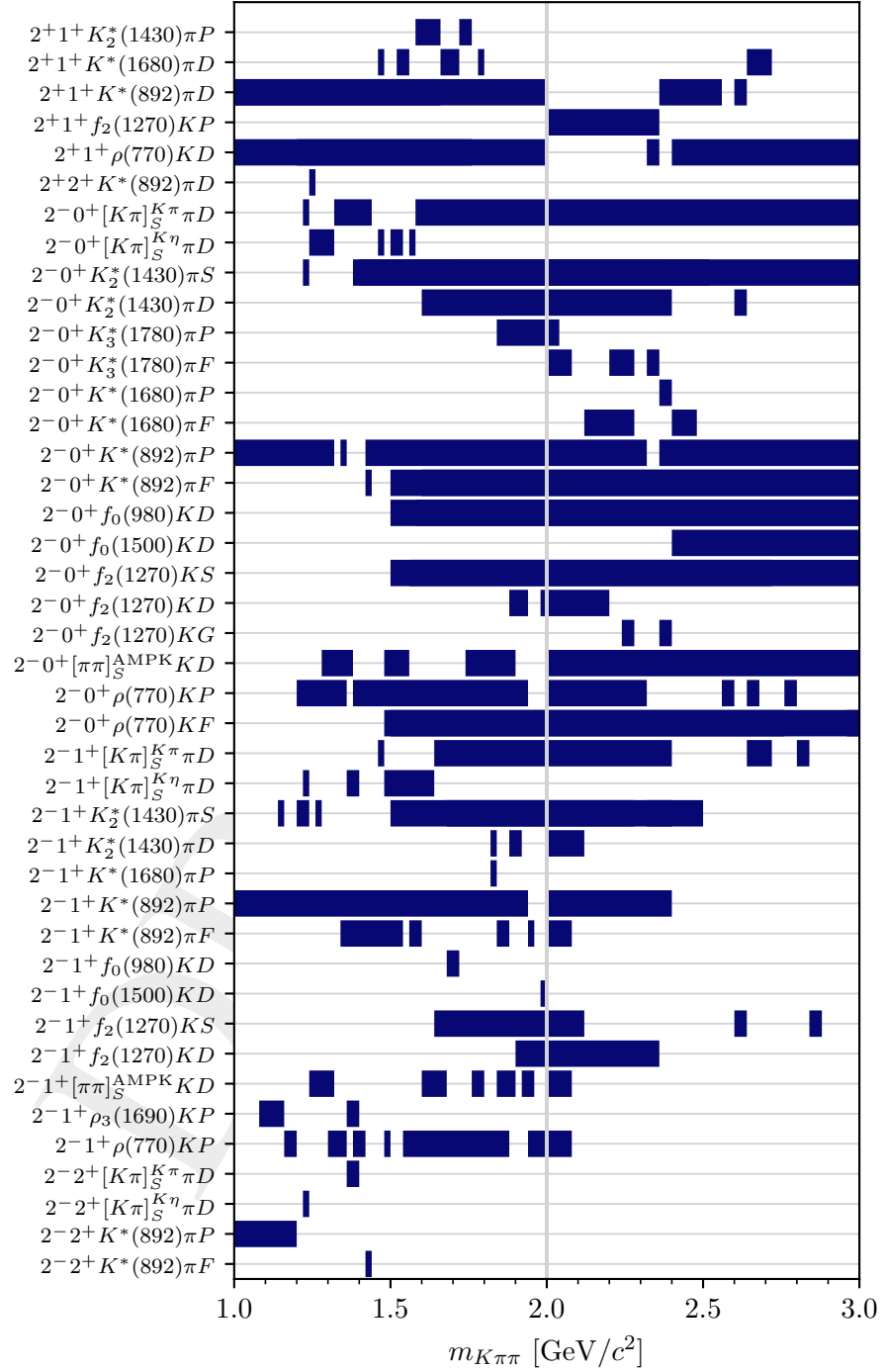


Figure D.13: Mass ranges of selected waves with  $J = 2$  in the range  $0.15 \leq t' < 0.24$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

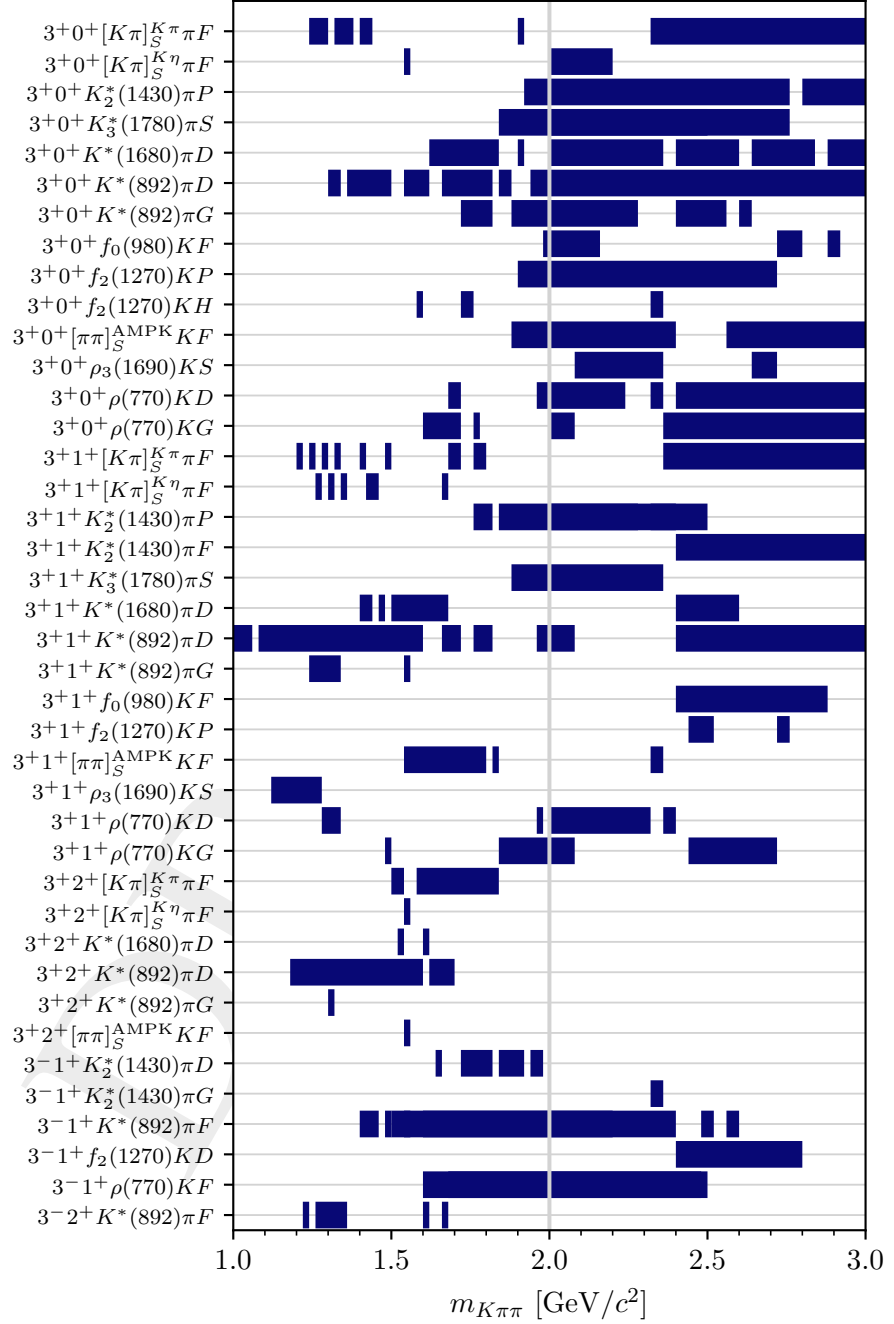


Figure D.14: Mass ranges of selected waves with  $J = 3$  in the range  $0.15 \leq t' < 0.24$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

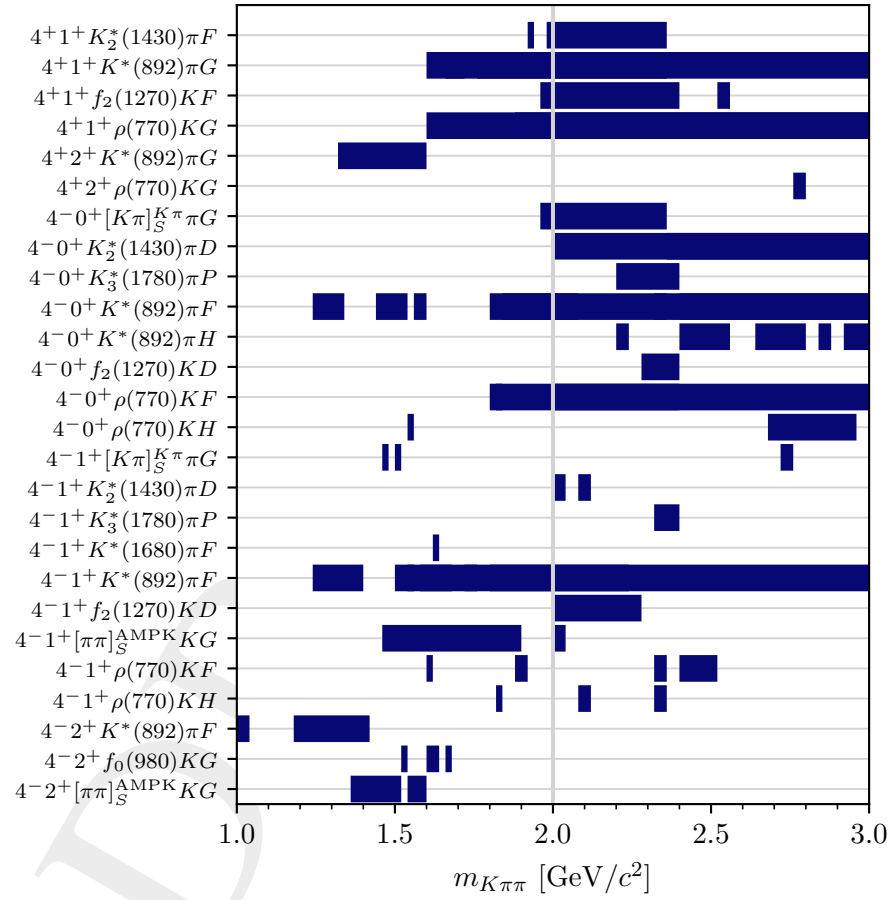


Figure D.15: Mass ranges of selected waves with  $J = 4$  in the range  $0.15 \leq t' < 0.24$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

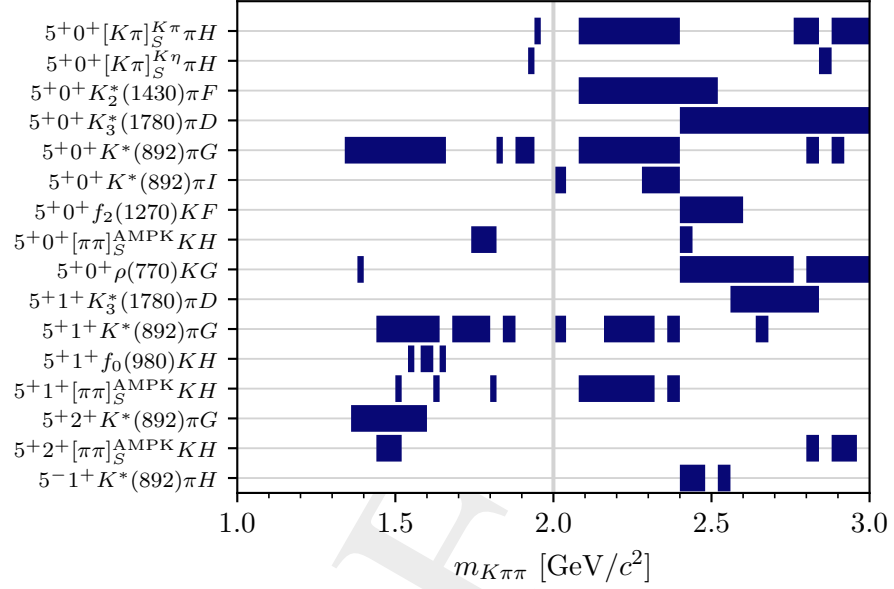


Figure D.16: Mass ranges of selected waves with  $J = 5$  in the range  $0.15 \leq t' < 0.24$  ( $\text{GeV}/c^2$ )<sup>2</sup>. The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

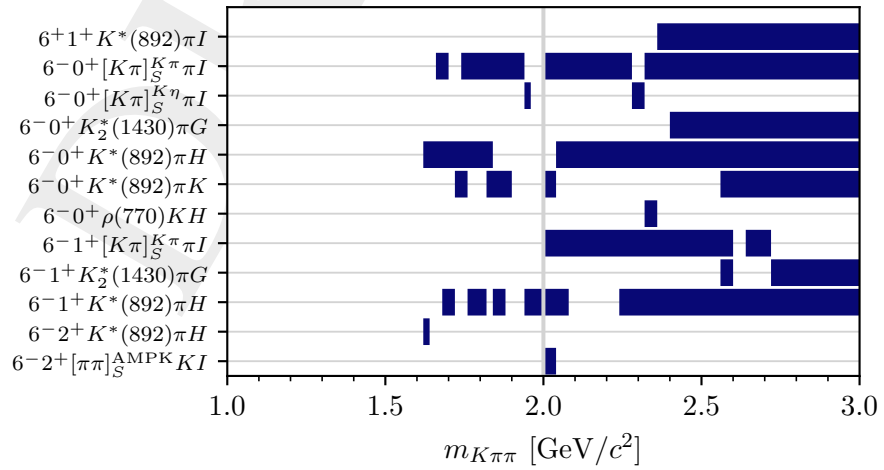


Figure D.17: Mass ranges of selected waves with  $J = 6$  in the range  $0.15 \leq t' < 0.24$  ( $\text{GeV}/c^2$ )<sup>2</sup>. The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

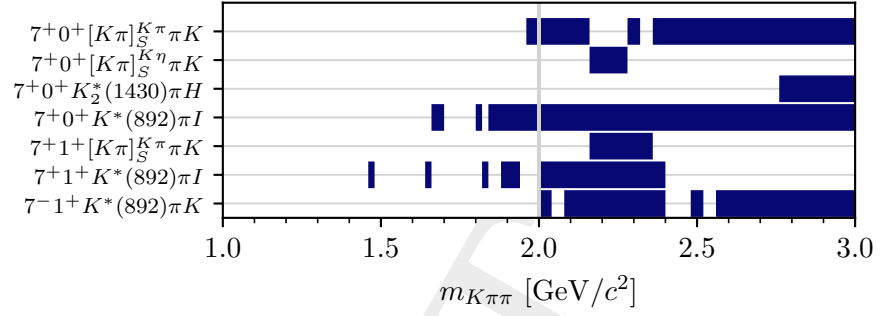


Figure D.18: Mass ranges of selected waves with  $J = 7$  in the range  $0.15 \leq t' < 0.24$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

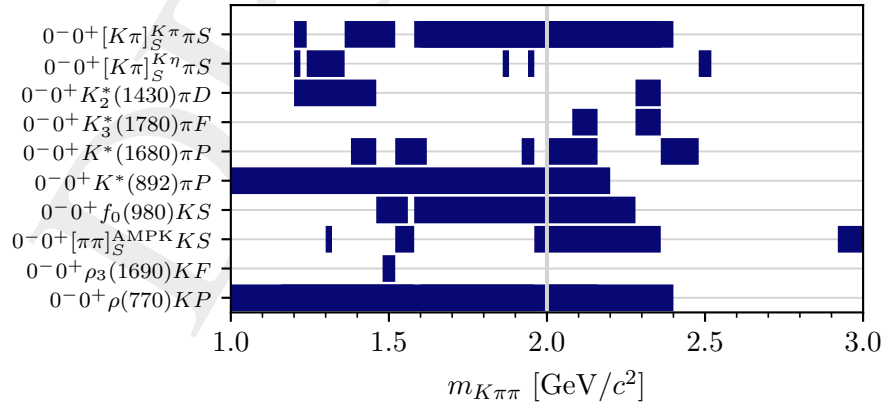


Figure D.19: Mass ranges of selected waves with  $J = 0$  in the range  $0.24 \leq t' < 0.34$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

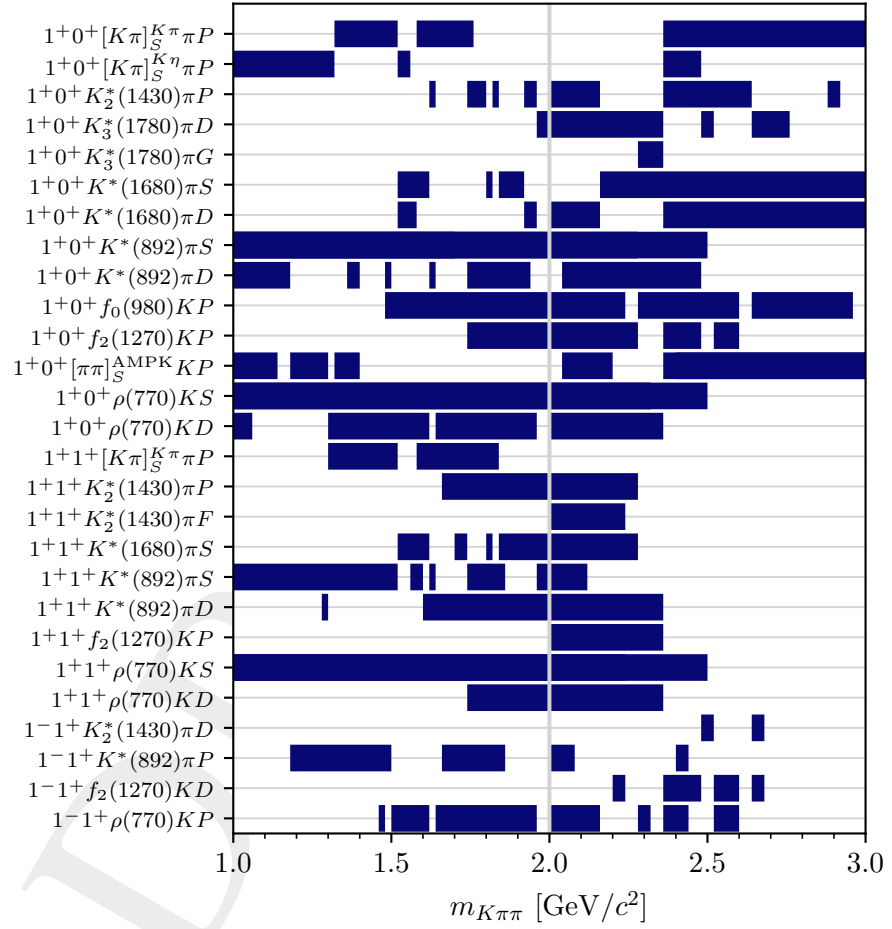


Figure D.20: Mass ranges of selected waves with  $J = 1$  in the range  $0.24 \leq t' < 0.34$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

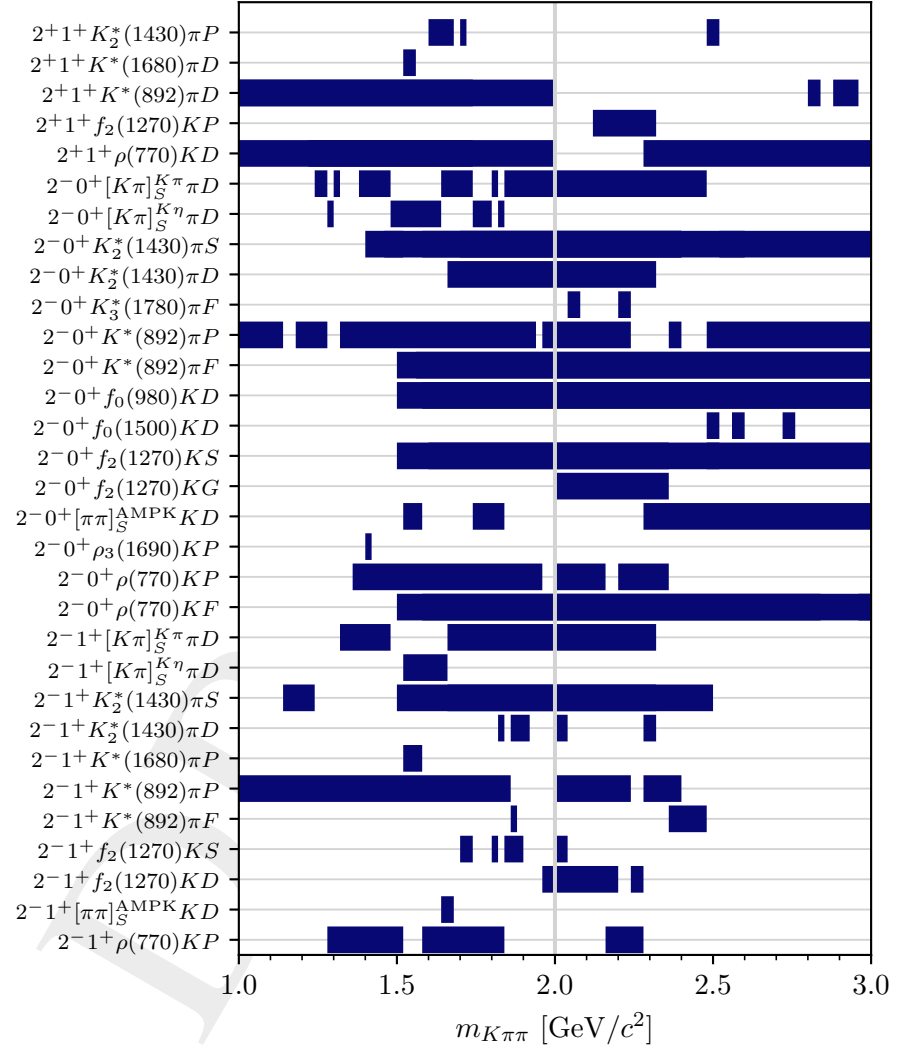


Figure D.21: Mass ranges of selected waves with  $J = 2$  in the range  $0.24 \leq t' < 0.34$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

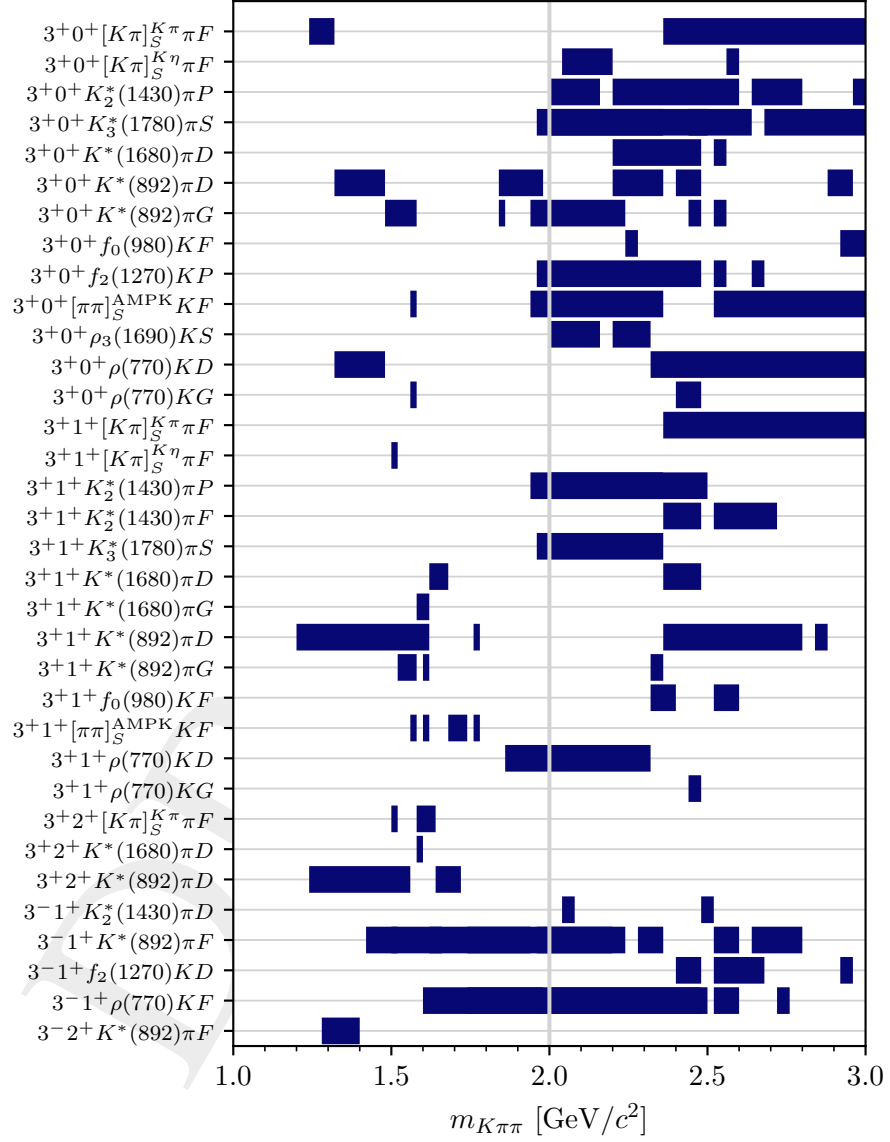


Figure D.22: Mass ranges of selected waves with  $J = 3$  in the range  $0.24 \leq t' < 0.34 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.



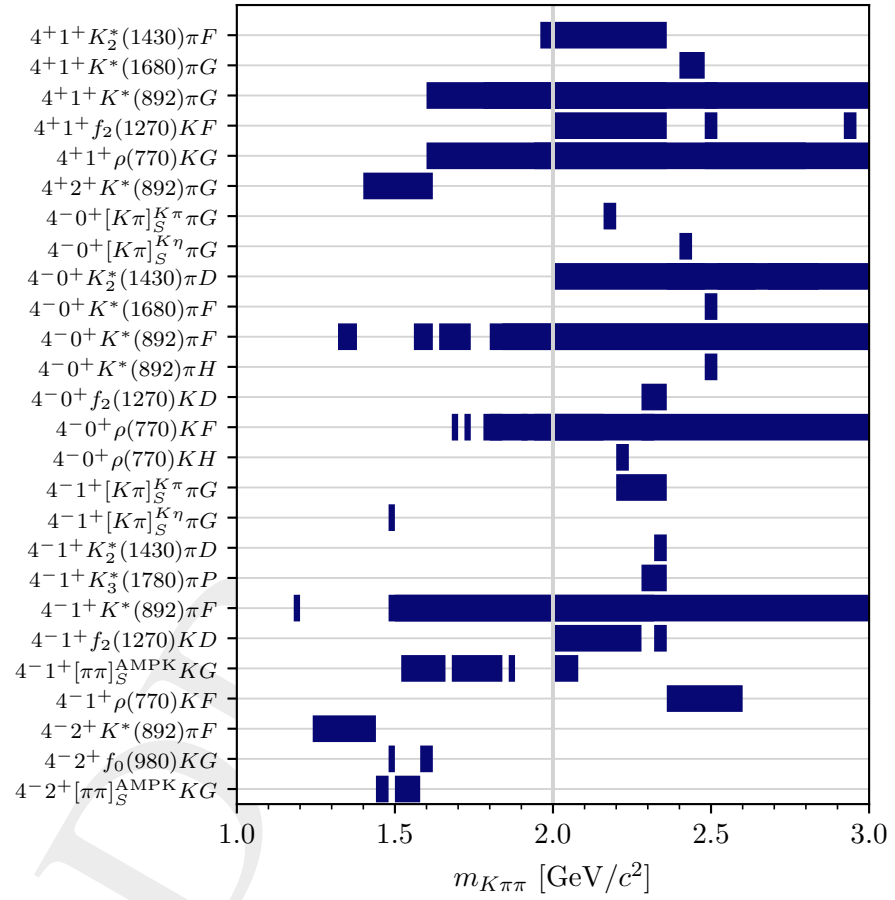


Figure D.23: Mass ranges of selected waves with  $J = 4$  in the range  $0.24 \leq t' < 0.34 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

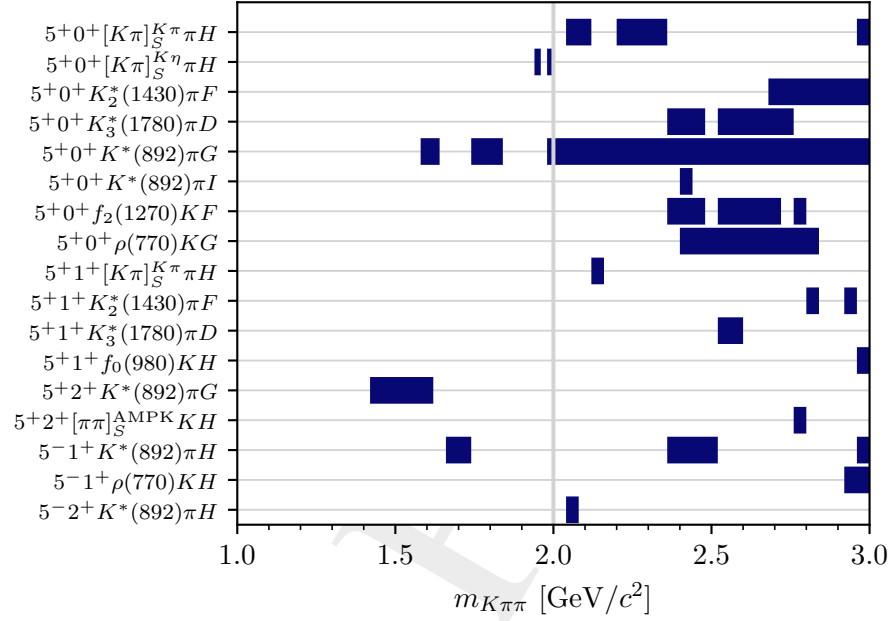


Figure D.24: Mass ranges of selected waves with  $J = 5$  in the range  $0.24 \leq t' < 0.34 \text{ (GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

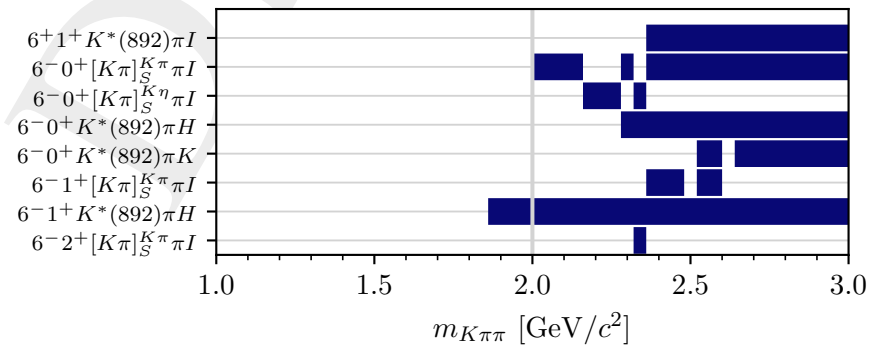


Figure D.25: Mass ranges of selected waves with  $J = 6$  in the range  $0.24 \leq t' < 0.34 \text{ (GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

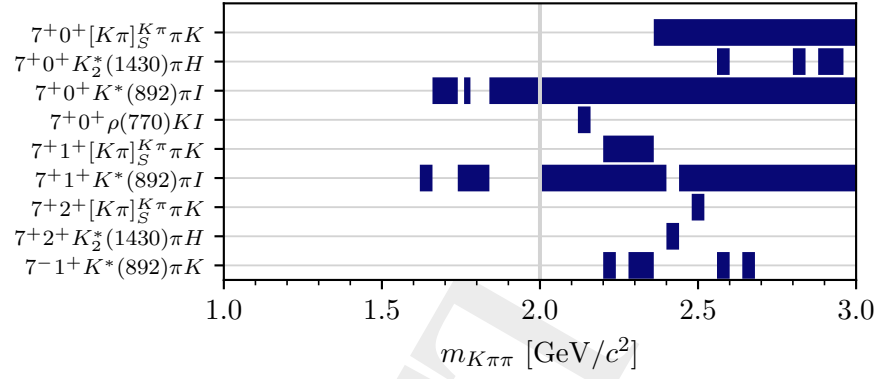


Figure D.26: Mass ranges of selected waves with  $J = 7$  in the range  $0.24 \leq t' < 0.34$  (GeV/c)<sup>2</sup>. The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from 20 MeV/c<sup>2</sup> to 40 MeV/c<sup>2</sup> wide bins.

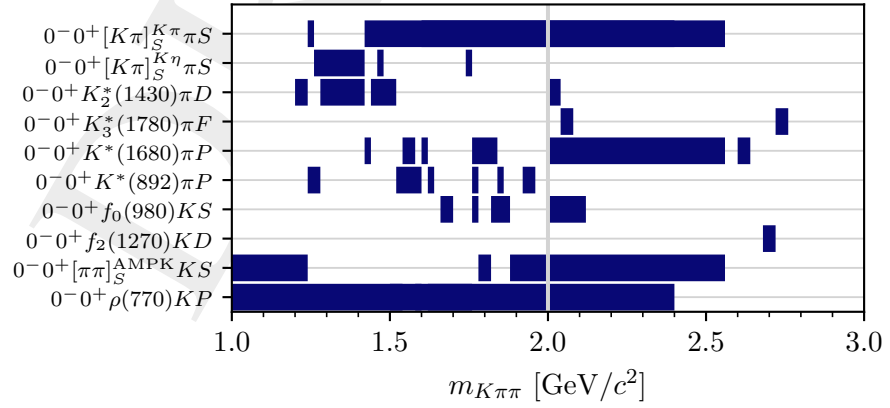


Figure D.27: Mass ranges of selected waves with  $J = 0$  in the range  $0.34 \leq t' < 1.00$  (GeV/c)<sup>2</sup>. The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from 20 MeV/c<sup>2</sup> to 40 MeV/c<sup>2</sup> wide bins.

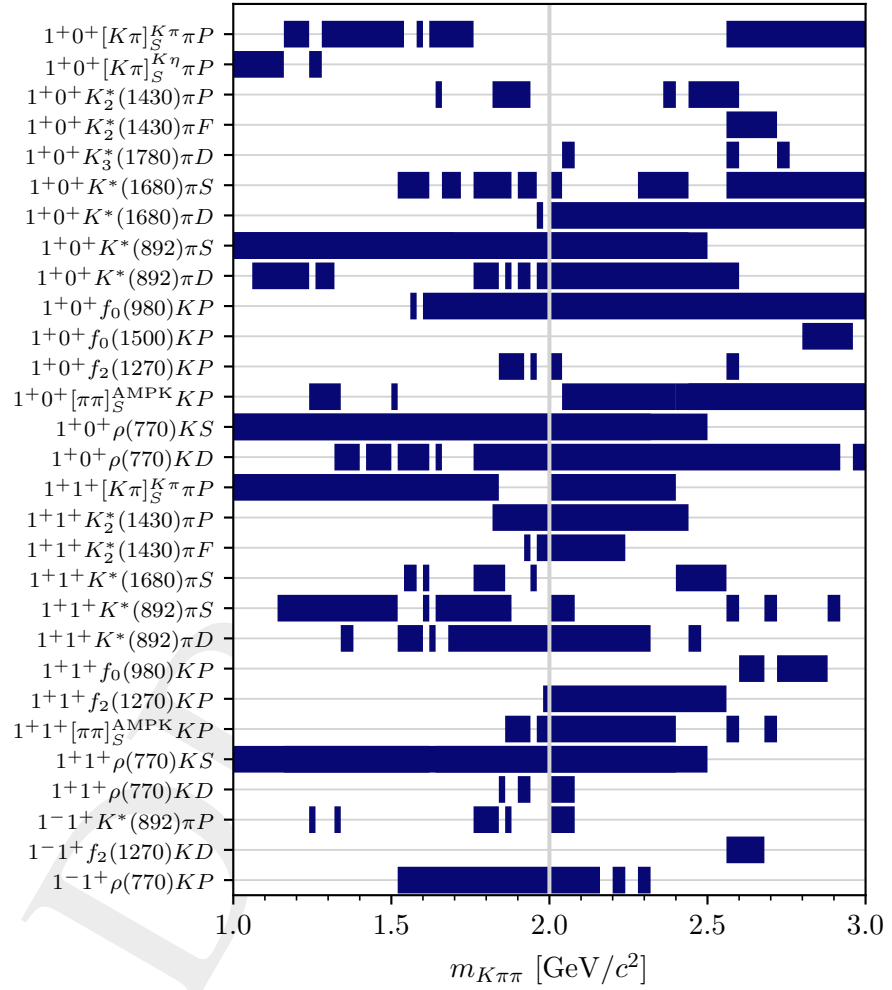


Figure D.28: Mass ranges of selected waves with  $J = 1$  in the range  $0.34 \leq t' < 1.00$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

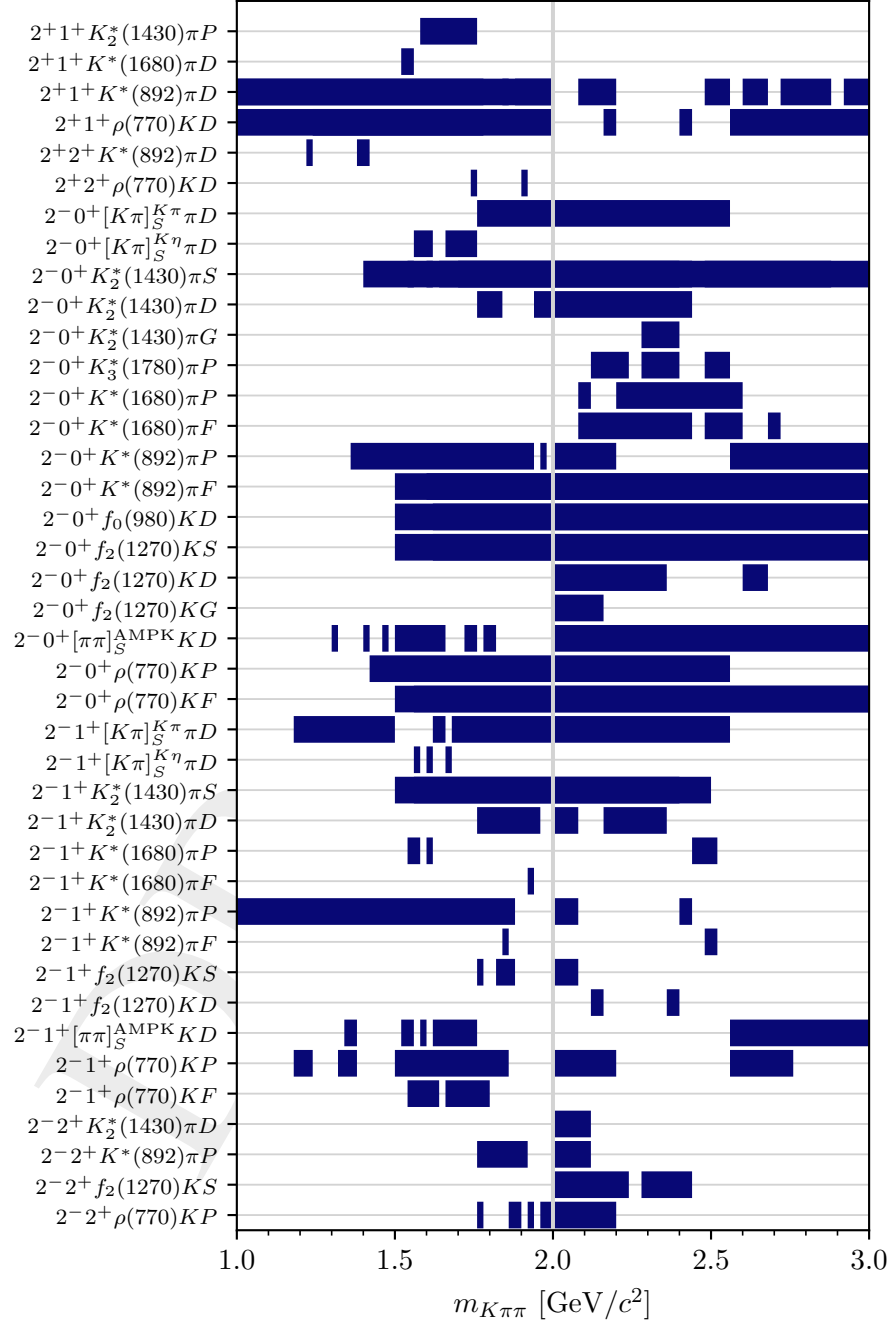


Figure D.29: Mass ranges of selected waves with  $J = 2$  in the range  $0.34 \leq t' < 1.00$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

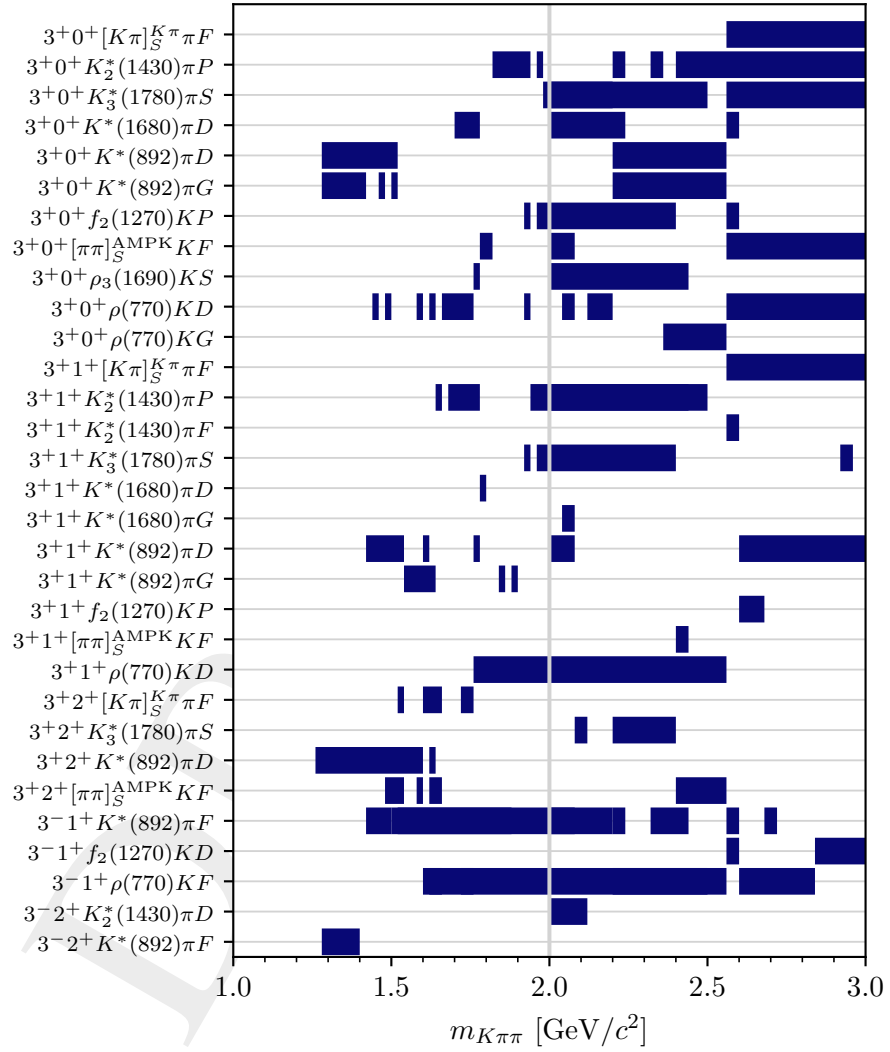


Figure D.30: Mass ranges of selected waves with  $J = 3$  in the range  $0.34 \leq t' < 1.00$  ( $\text{GeV}/c^2$ ). The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

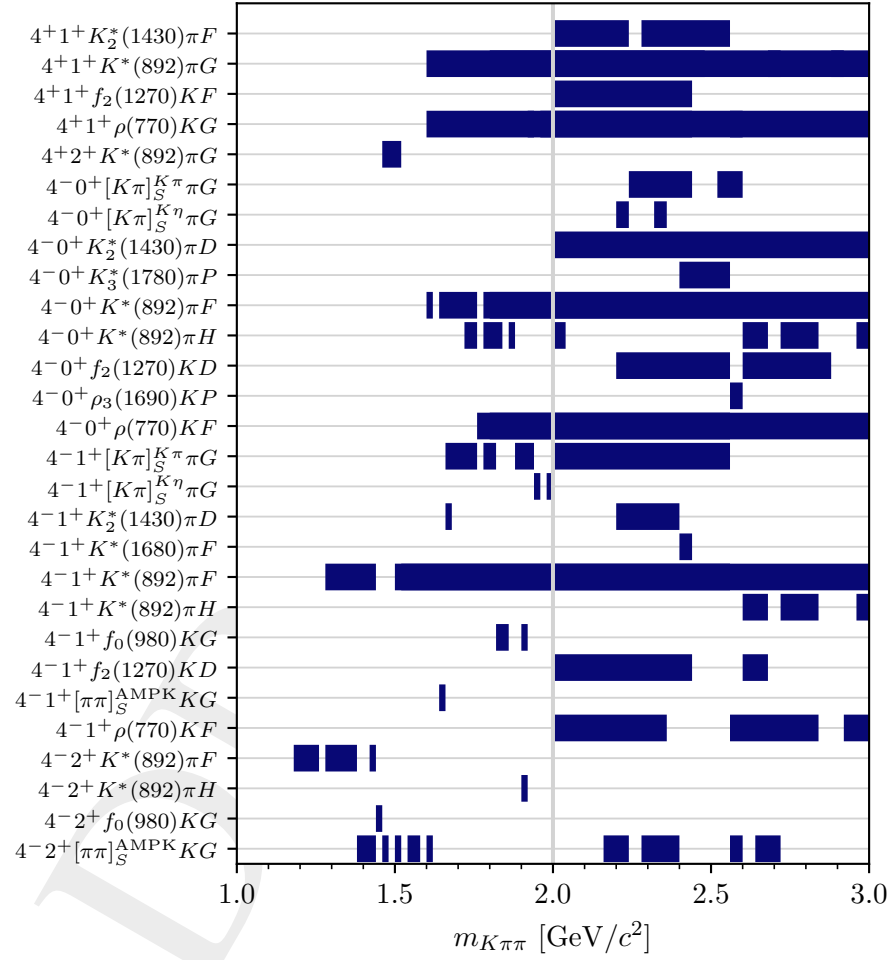


Figure D.31: Mass ranges of selected waves with  $J = 4$  in the range  $0.34 \leq t' < 1.00 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

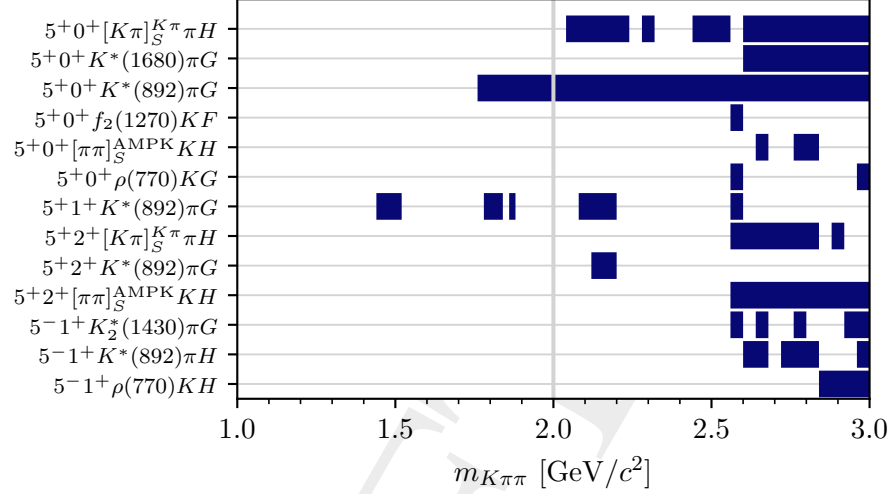


Figure D.32: Mass ranges of selected waves with  $J = 5$  in the range  $0.34 \leq t' < 1.00 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

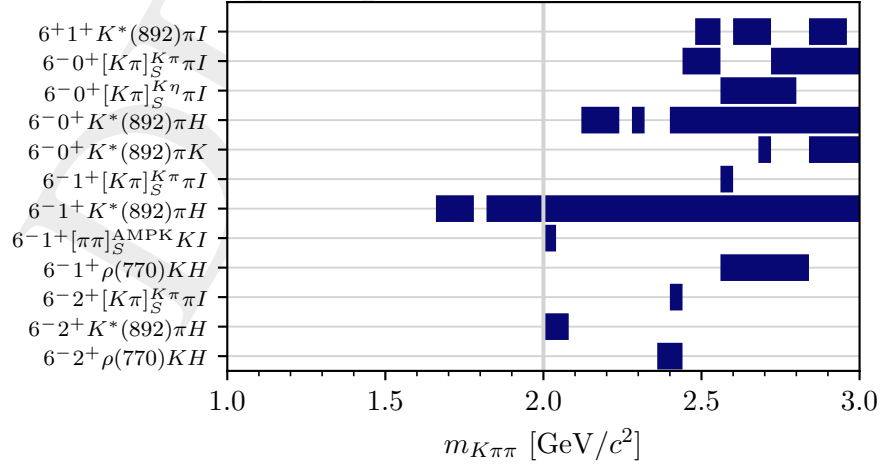


Figure D.33: Mass ranges of selected waves with  $J = 6$  in the range  $0.34 \leq t' < 1.00 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.



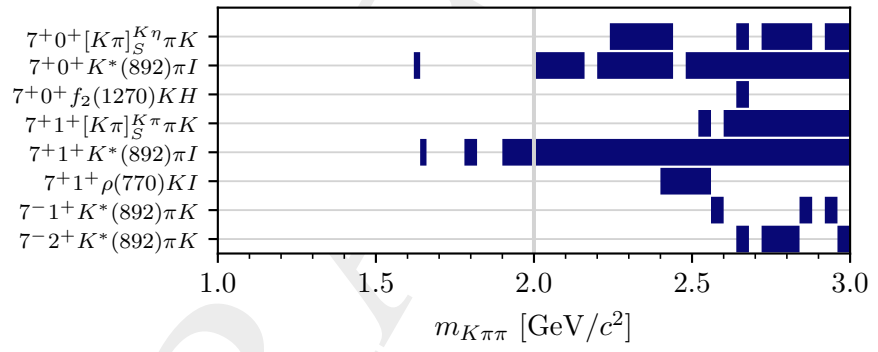


Figure D.34: Mass ranges of selected waves with  $J = 7$  in the range  $0.34 \leq t' < 1.00 (\text{GeV}/c)^2$ . The gray vertical line indicates the mass where the  $m_{K\pi\pi}$  binning changes from  $20 \text{ MeV}/c^2$  to  $40 \text{ MeV}/c^2$  wide bins.

## 6154 D.2 Experimental Acceptance and Agreement between 6155 Partial-Wave Model and Data

6156 In this section, we present plots to show the acceptance in the kinematic variables of the  
6157 reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  and the agreement between the results of the PWD fit, i.e.  
6158 PWD predictions for the kinematic distributions in the  $K^- \pi^- \pi^+$  phase-space variables, and the  
6159 measured data. Details on how we determined the PWD predictions can be found in section 5.6  
6160 and appendix C.

6161 The five-dimensional phase space of the  $K^- \pi^- \pi^+$  final state can be represented by four angles  
6162 and the invariant mass of one of the three two-body subsystems. Different representations are  
6163 possible (see sections 5.1.1 and 5.6 for details). In figures D.36 to D.41, we consider the  $\pi^- \pi^+$   
6164 isobar system. In figures D.42 to D.47, we consider the  $K^- \pi^+$  isobar system. Table D.2 gives an  
6165 overview over these figures. We split the analyzed  $m_{K\pi\pi}$  range into three sub-ranges: (i) the mass  
6166 range of the  $K_1$  double-peak,  $1.0 \leq m_{K\pi\pi} < 1.5 \text{ GeV}/c^2$ ; (ii) the mass range of the peak of the  $K_2$   
6167 resonances,  $1.5 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$ ; and (iii) the high-mass range,  $2.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$ .  
6168 The agreement between PWD model and data is discussed in section 5.6.

Table D.2: Figures showing the agreement between the results of the PWD and the measured data as a function of individual phase-space variables and as a function of two two-body decay angles. In addition, we show the acceptance as a function of the two-body decay angles using a common scale for the acceptance.

		$m_{K\pi\pi}$ range in $\text{GeV}/c^2$	[1.0, 1.5]	[1.5, 2.0]	[2.0, 3.0]
$\pi^- \pi^+$ isobar system	individual phase-space variables		D.36	D.38	D.40
	correlation of decay angles		D.37	D.39	D.41
$K^- \pi^+$ isobar system	individual phase-space variables		D.42	D.44	D.46
	correlation of decay angles		D.43	D.45	D.47

6169 In addition, we present estimates of the experimental acceptance as a function of different  
6170 kinematic variables. The acceptance is strongly modulated in particular in the Gottfried-Jackson  
6171 angles as, for example, shown in figure D.39e. Furthermore, the acceptance strongly depends  
6172 on  $m_{K\pi\pi}$  (compare, for example, figures D.39e and D.41e). This strong modulation of the  
6173 acceptance is caused by the limited momentum range of the final-state particle identification by  
6174 the RICH detector (see section 3.2.2).

6175 The acceptance depends on all kinematic variables. Showing the acceptance as a function of  
6176 only a subset of the kinematic variables implies marginalization over the not shown kinematic  
6177 variables. For example, showing the acceptance as a function of  $m_{K\pi\pi}$  in figure D.35a implies  
6178 marginalization over  $t'$  and the five phase-space variables of the  $K^- \pi^- \pi^+$  system. As, the  
6179 acceptance depends in a correlated way on  $m_{K\pi\pi}$ ,  $t'$ , and on the  $K^- \pi^- \pi^+$  phase-space variables,  
6180 the marginalized acceptance at a given  $m_{K\pi\pi}$  depends on the distributions in  $t'$  and the  $K^- \pi^- \pi^+$

6181 phase-space variables used for the marginalization. As we want to show the acceptance for the  
 6182 reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ , we used for the acceptance plots shown in figures D.35 to D.47  
 6183 and in figure 5.23b the physical kinematic distribution as predicted by the PWD model for the  
 6184 reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  for the marginalization. The acceptance is calculated as the ratio  
 6185 of the number of reconstructed events and the number of produced events as predicted by the  
 6186 PWD model.<sup>[d]</sup>

6187 Figure D.35a shows the average acceptance for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  as a function  
 6188 of  $m_{K\pi\pi}$ . In the region  $m_{K\pi\pi} < 1.6 \text{ GeV}/c^2$ , the acceptance is approximately constant and has a  
 6189 low value of about 2%. Compared to the acceptance for a sample that is distributed uniformly  
 6190 in phase-space, the acceptance for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  as predicted using the  
 6191 PWD model is lower in this  $m_{K\pi\pi}$  region (cf. figures C.4b and D.35a). The  $m_{K\pi\pi}$  region below  
 6192 about  $1.6 \text{ GeV}/c^2$  is affected by the leakage effect discussed in section 5.9, which leads to an  
 6193 overestimation of the number of produced events and thus to a strong bias for the estimate of  
 6194 the average acceptance towards smaller values in this  $m_{K\pi\pi}$  region. The PWD prediction for  
 6195 the distributions of reconstructed events is not affected by the leakage effect. Above about  
 6196  $1.6 \text{ GeV}/c^2$ , the acceptance rises steeply to a value of about 10% in the mass region of the  $K_2$   
 6197 ground states around  $1.8 \text{ GeV}/c^2$ . After this region, the rise is less steep. Above  $2.5 \text{ GeV}/c^2$ , the  
 6198 acceptance starts to saturate at a value of about 22%, which is slightly higher than the acceptance  
 6199 of about 19% for a sample that is distributed uniformly in phase-space. The distribution in  
 6200  $\cos \theta_{\text{GJ}}^{K\pi}$  strongly peaks at 1 in this  $m_{K\pi\pi}$  region (see figure 5.24a). For this kinematics, the  
 6201 bachelor  $\pi^-$  goes in backward direction with respect to the direction of the beam  $K^-$  in the  
 6202 Gottfried-Jackson frame. This translates to a slow  $\pi^-$  in the laboratory frame which is more  
 6203 likely identified by the RICH. Thus, the acceptance for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  is  
 6204 higher in this mass region compared to a sample that is distributed uniformly in phase-space, i.e.  
 6205 whose  $\cos \theta_{\text{GJ}}^{K\pi}$  distribution is flat.

6206 The average acceptance as a function of  $m_{\pi^- \pi^+}$  shown in figure D.35b is roughly constant, but  
 6207 exhibits structures in the mass regions of some of the  $\pi^- \pi^+$  resonances that we observe in this  
 6208 distribution (see figure 4.7b). For example, the acceptance exhibits a dip in the  $m_{\pi^- \pi^+}$  region  
 6209 of the  $f_0(980)$  isobar resonance at about  $1 \text{ GeV}/c^2$  and rises again in the mass region of the  
 6210  $f_2(1270)$  isobar resonance at about  $1.3 \text{ GeV}/c^2$ . As both isobar resonances have different spin,  
 6211 the correspondingly different angular distributions of their decay and the strong modulation of  
 6212 the acceptance in the decay angles can explain the different average acceptances.

6213 The acceptance effects discussed above show, that the measured distributions can be interpreted  
 6214 only at a qualitative level. An acceptance correction that takes into account the full high-  
 6215 dimensional dependence of the acceptance on all kinematic variables is mandatory in order to  
 6216 interpret the data on a quantitative level as done in the partial-wave analysis.

<sup>[d]</sup> The PWD prediction for the number of reconstructed events was obtained by weighting reconstructed phase-space pseudodata. The number of produce events as predicted by the PWD model was obtained by weighting produced phase-space pseudodata. The weights are proportional to the model intensity in equation (5.16) using the results of the PWD fit to the  $K^- \pi^- \pi^+$  sample. See appendix C for details.

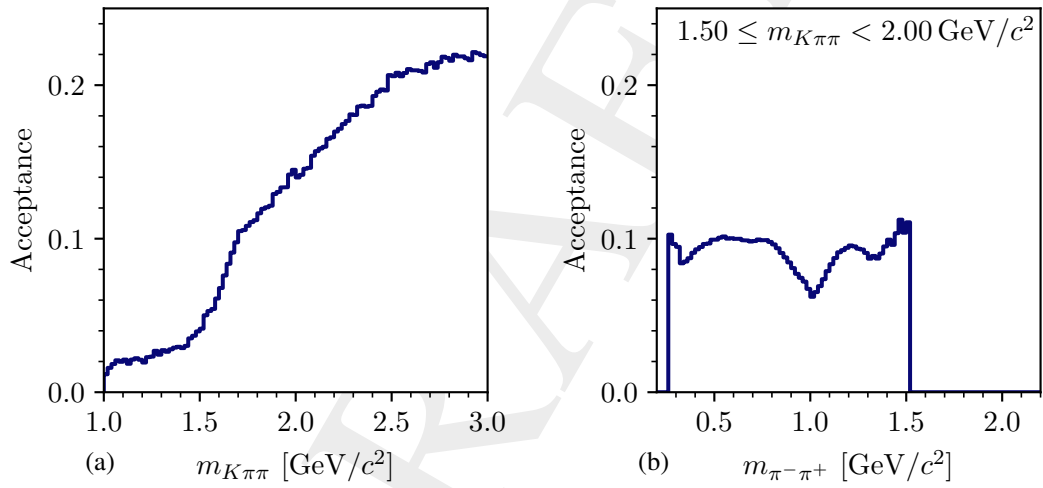


Figure D.35: Marginalized acceptance for the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$ . (a) shows the acceptance as a function of  $m_{K\pi\pi}$ . (b) shows the acceptance as a function of  $m_{\pi^-\pi^+}$  in the range  $1.5 \leq m_{K\pi\pi} < 2.0$  GeV/c<sup>2</sup>.

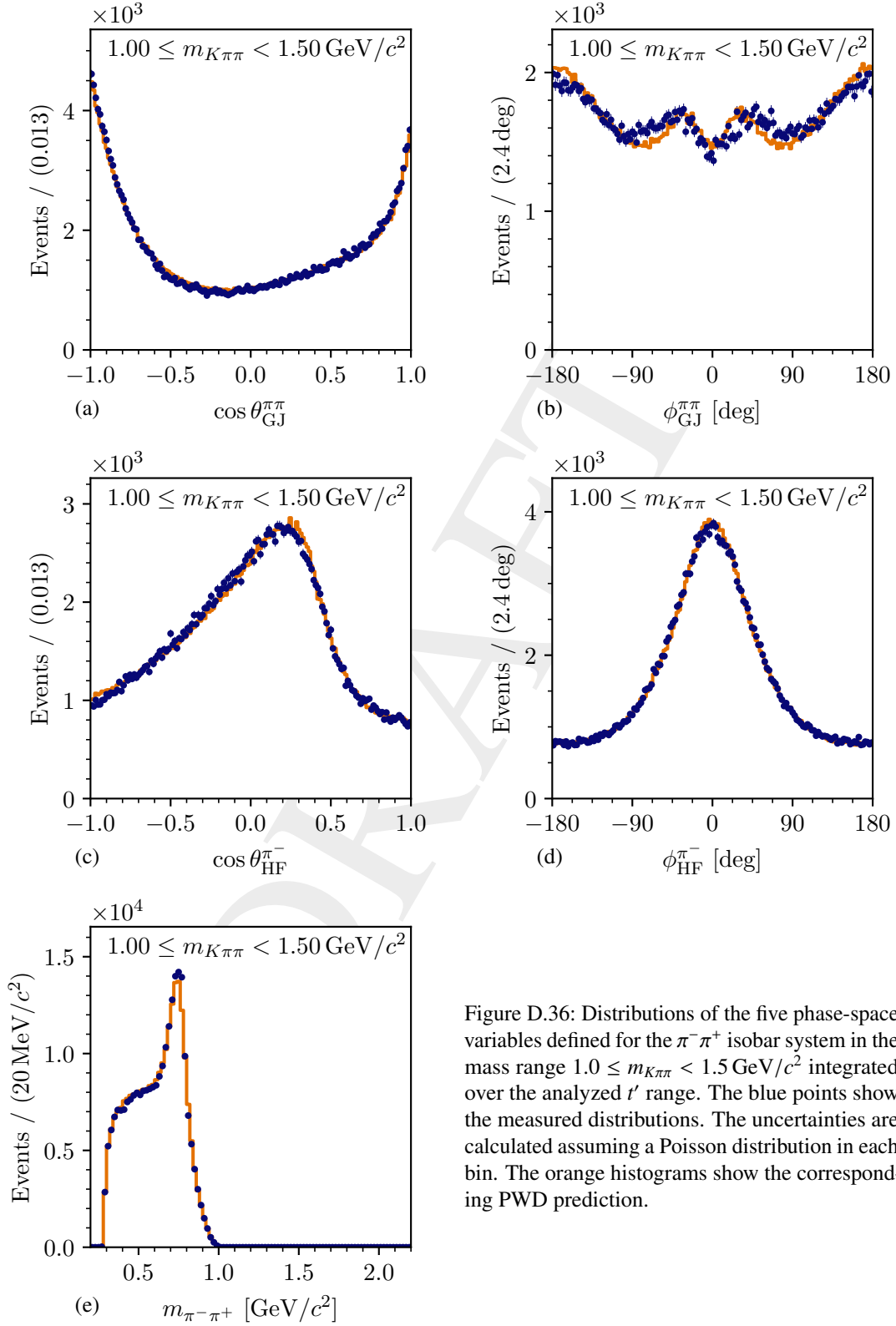


Figure D.36: Distributions of the five phase-space variables defined for the  $\pi^- \pi^+$  isobar system in the mass range  $1.0 \leq m_{K\pi\pi} < 1.5 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD prediction.

## D Partial-Wave Decomposition

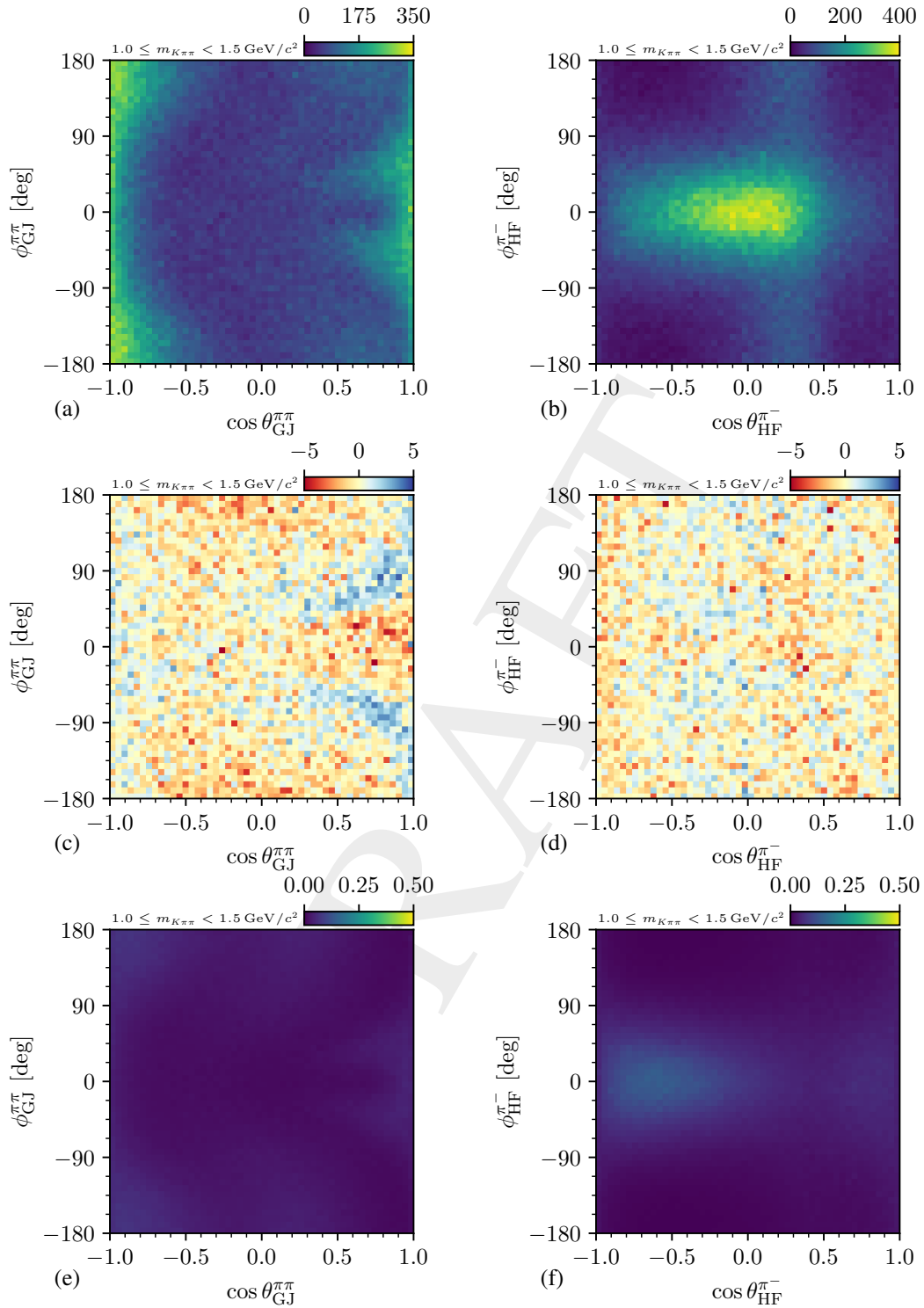


Figure D.37: Distributions of the four two-body decay angles defined for the  $\pi^-\pi^+$  isobar system in the mass range  $1.0 \leq m_{K\pi\pi} < 1.5 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The top row shows the measured distributions, the middle row shows the difference between the measured number of events and the corresponding PWD prediction divided by the square root of the PWD prediction, and the lower row shows the acceptance.

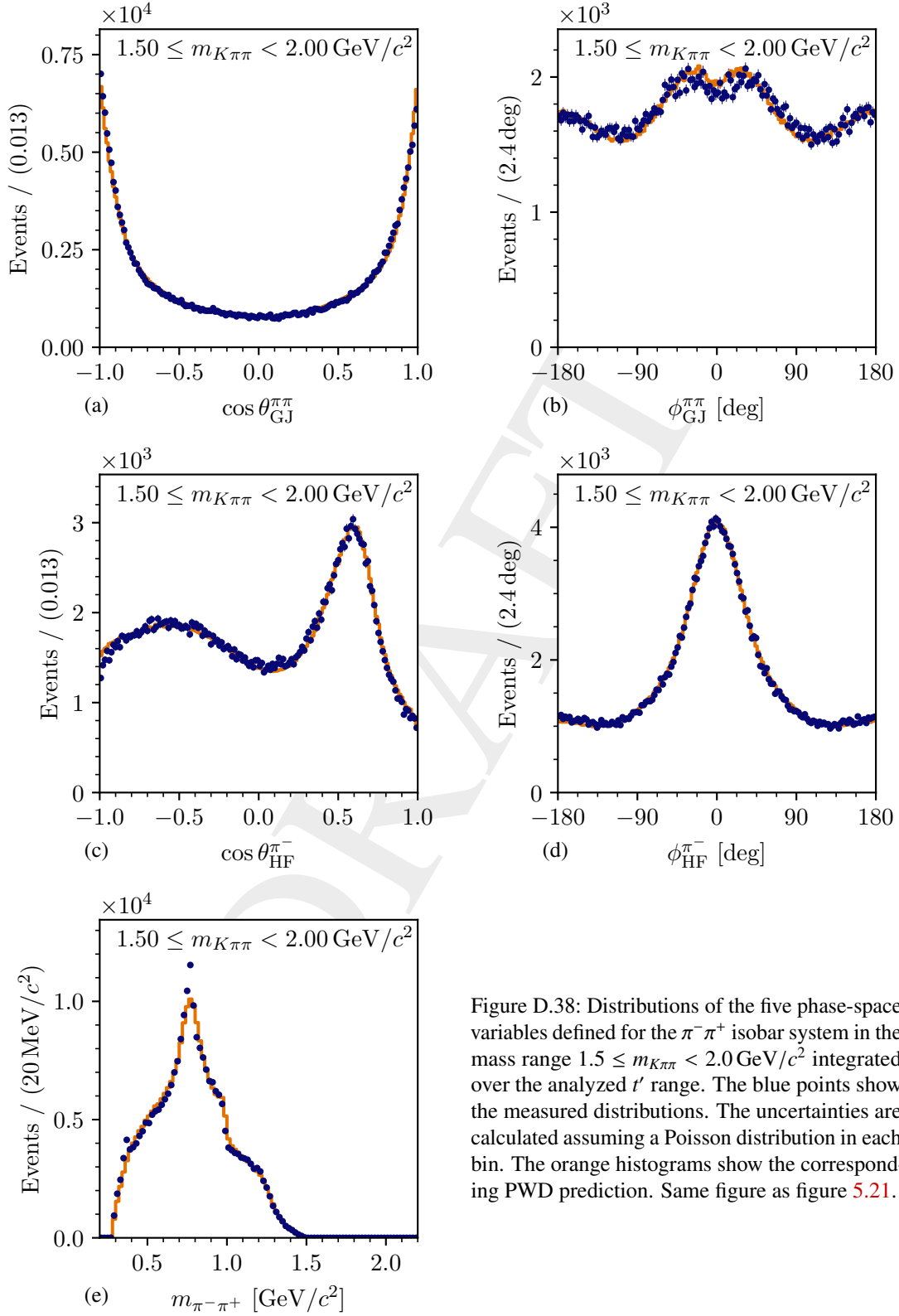


Figure D.38: Distributions of the five phase-space variables defined for the  $\pi^- \pi^+$  isobar system in the mass range  $1.5 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD prediction. Same figure as figure 5.21.

## D Partial-Wave Decomposition

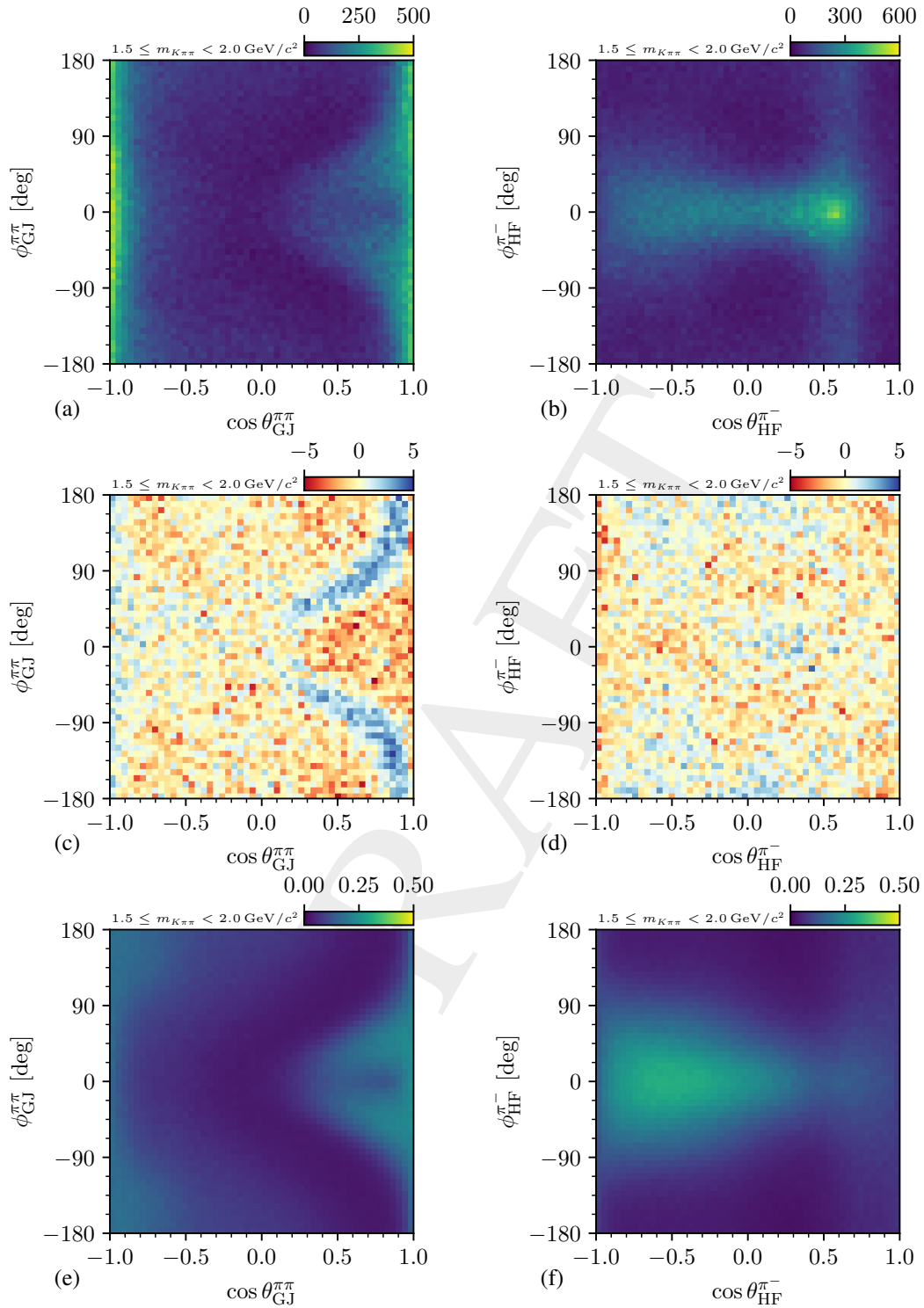


Figure D.39: Distributions of the four two-body decay angles defined for the  $\pi^- \pi^+$  isobar system in the mass range  $1.5 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The top row shows the measured distributions, the middle row shows the difference between the measured number of events and the corresponding PWD prediction divided by the square root of the PWD prediction, and the lower row shows the acceptance.



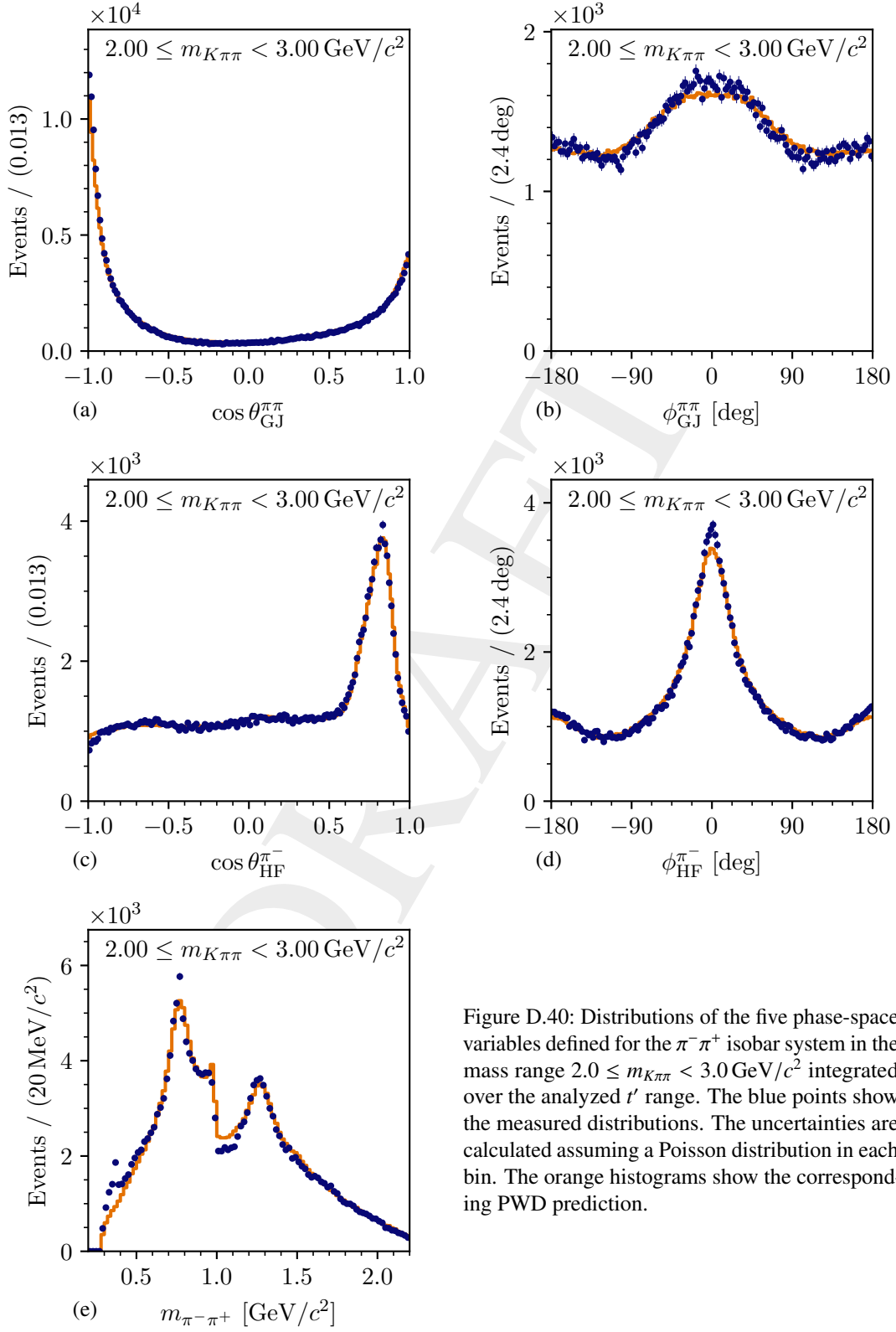


Figure D.40: Distributions of the five phase-space variables defined for the  $\pi^- \pi^+$  isobar system in the mass range  $2.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD prediction.

## D Partial-Wave Decomposition

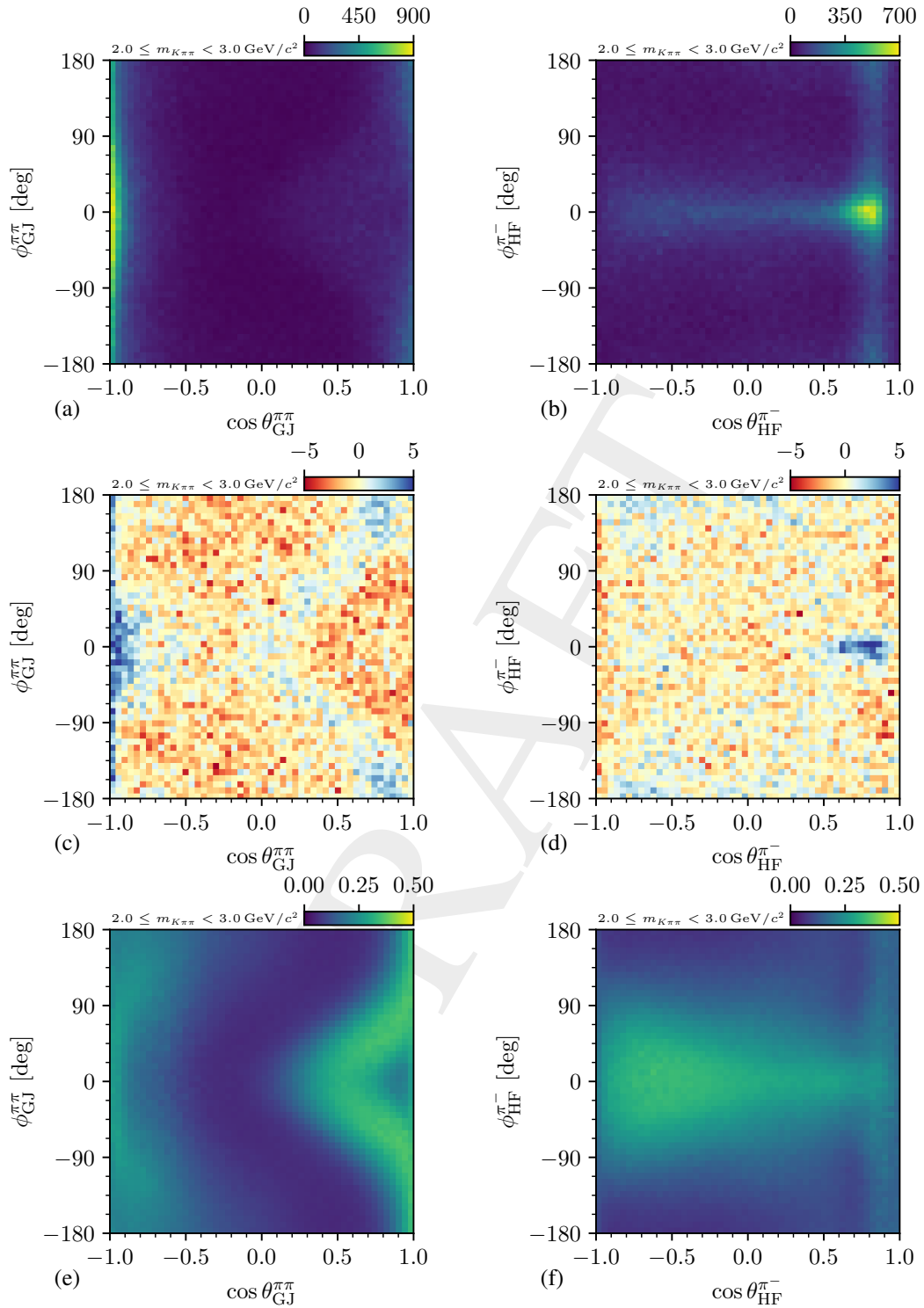


Figure D.41: Distributions of the four two-body decay angles defined for the  $\pi^-\pi^+$  isobar system in the mass range  $2.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The top row shows the measured distributions, the middle row shows the difference between the measured number of events and the corresponding PWD prediction divided by the square root of the PWD prediction, and the lower row shows the acceptance.

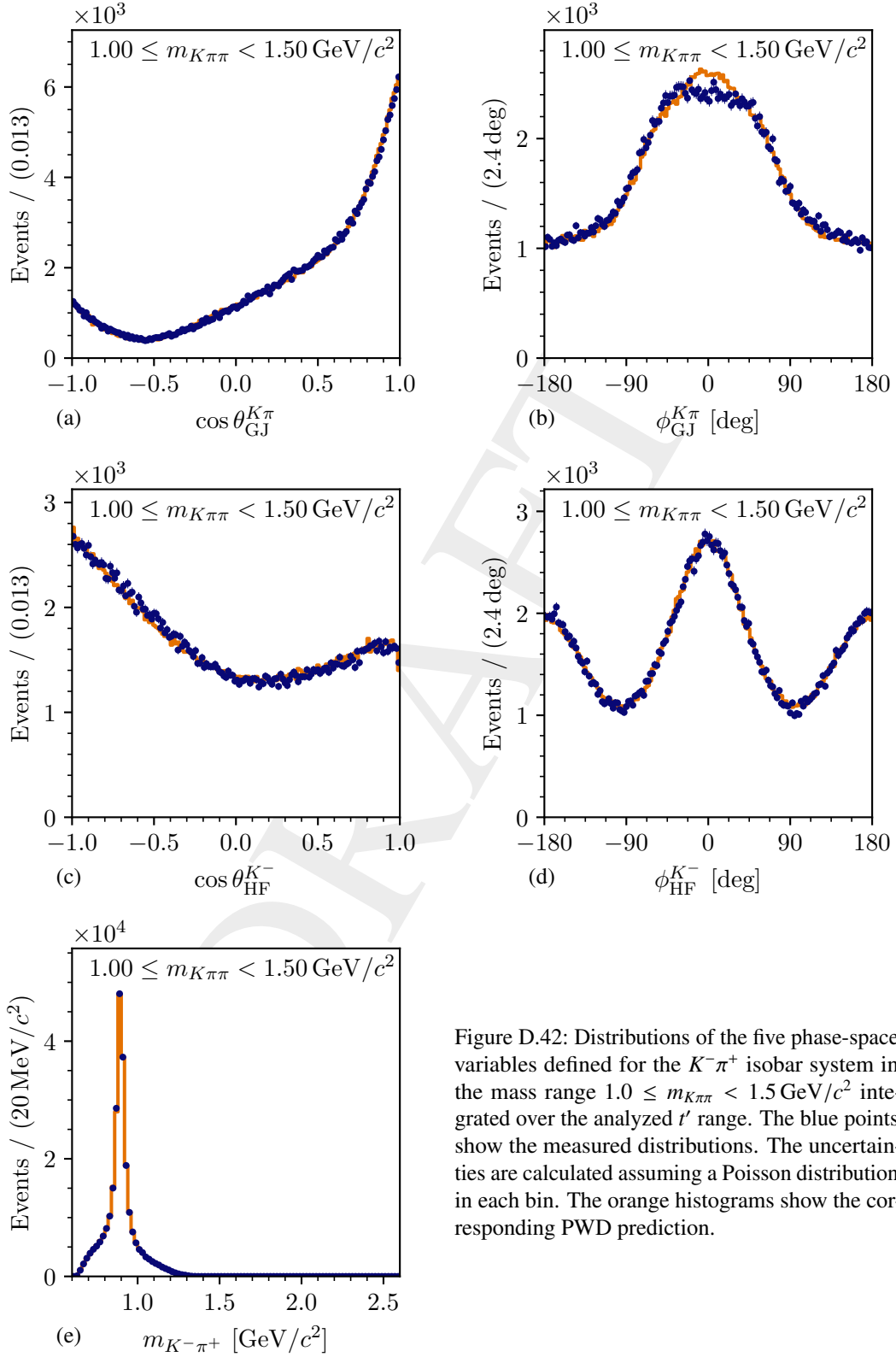


Figure D.42: Distributions of the five phase-space variables defined for the  $K^- \pi^+$  isobar system in the mass range  $1.0 \leq m_{K\pi\pi} < 1.5 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD prediction.

## D Partial-Wave Decomposition

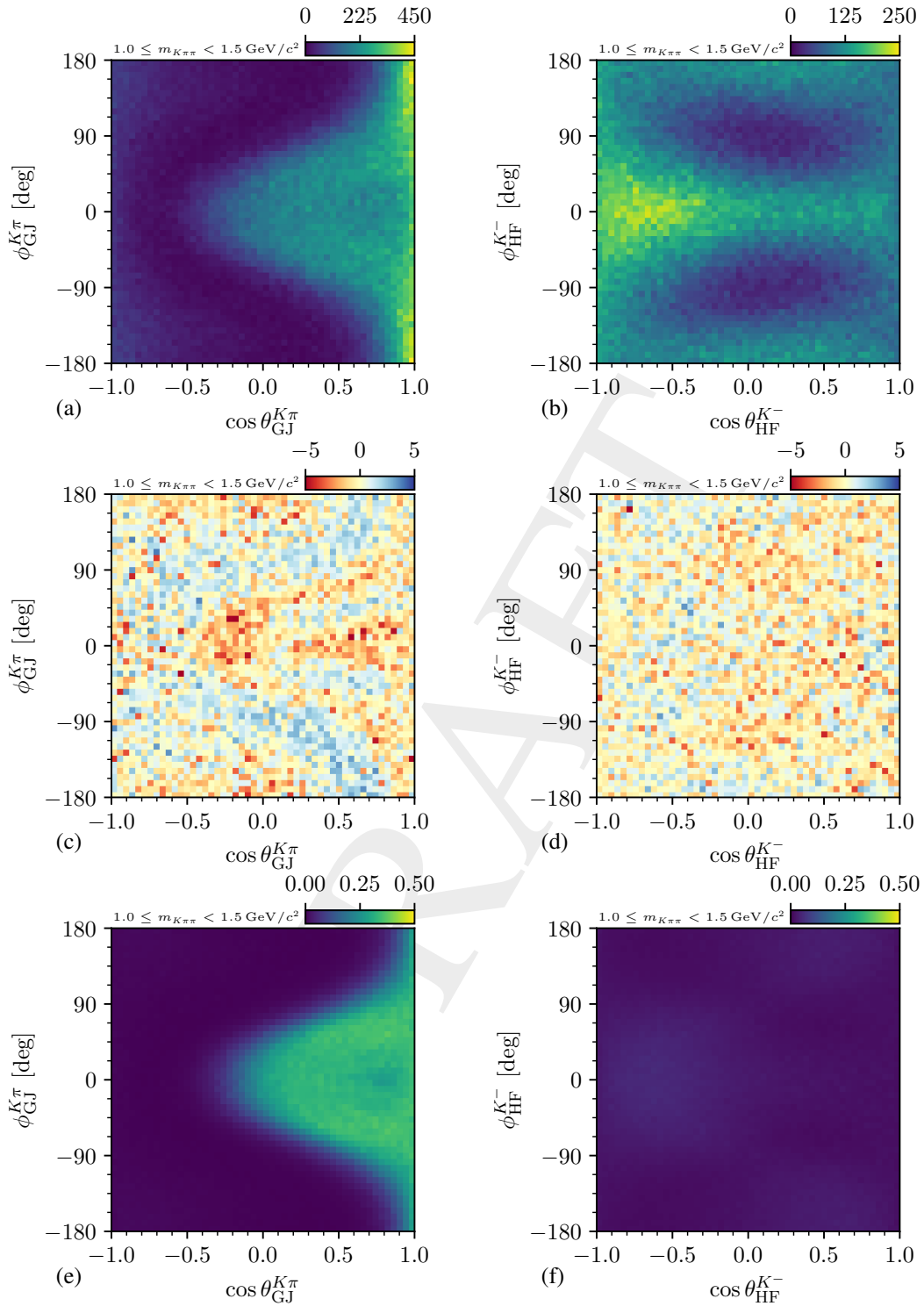


Figure D.43: Distributions of the four two-body decay angles defined for the  $K^-\pi^+$  isobar system in the mass range  $1.0 \leq m_{K\pi\pi} < 1.5 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The top row shows the measured distributions, the middle row shows the difference between the measured number of events and the corresponding PWD prediction divided by the square root of the PWD prediction, and the lower row shows the acceptance.

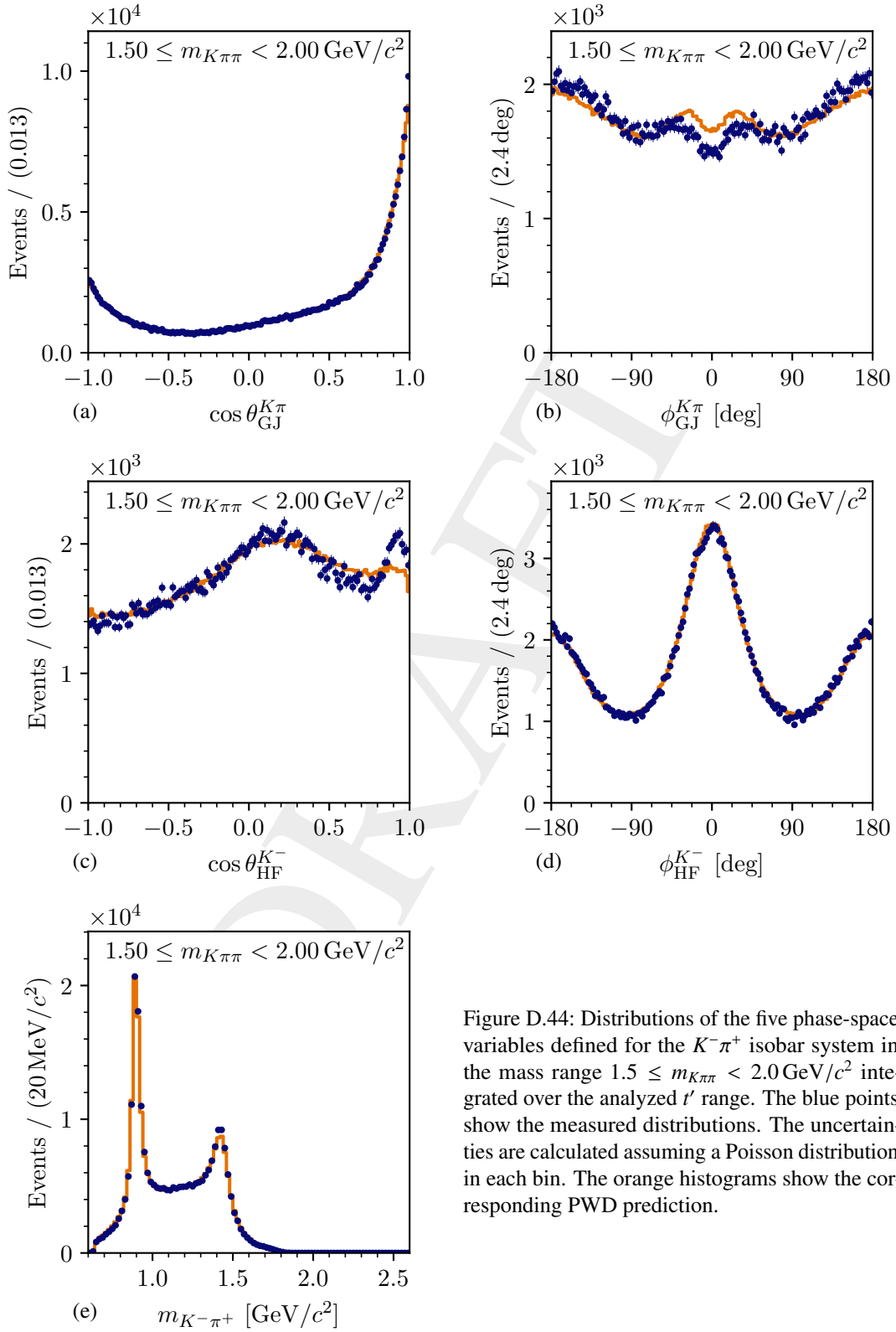


Figure D.44: Distributions of the five phase-space variables defined for the  $K^- \pi^+$  isobar system in the mass range  $1.5 \leq m_{K\pi\pi} < 2.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD prediction.

## D Partial-Wave Decomposition

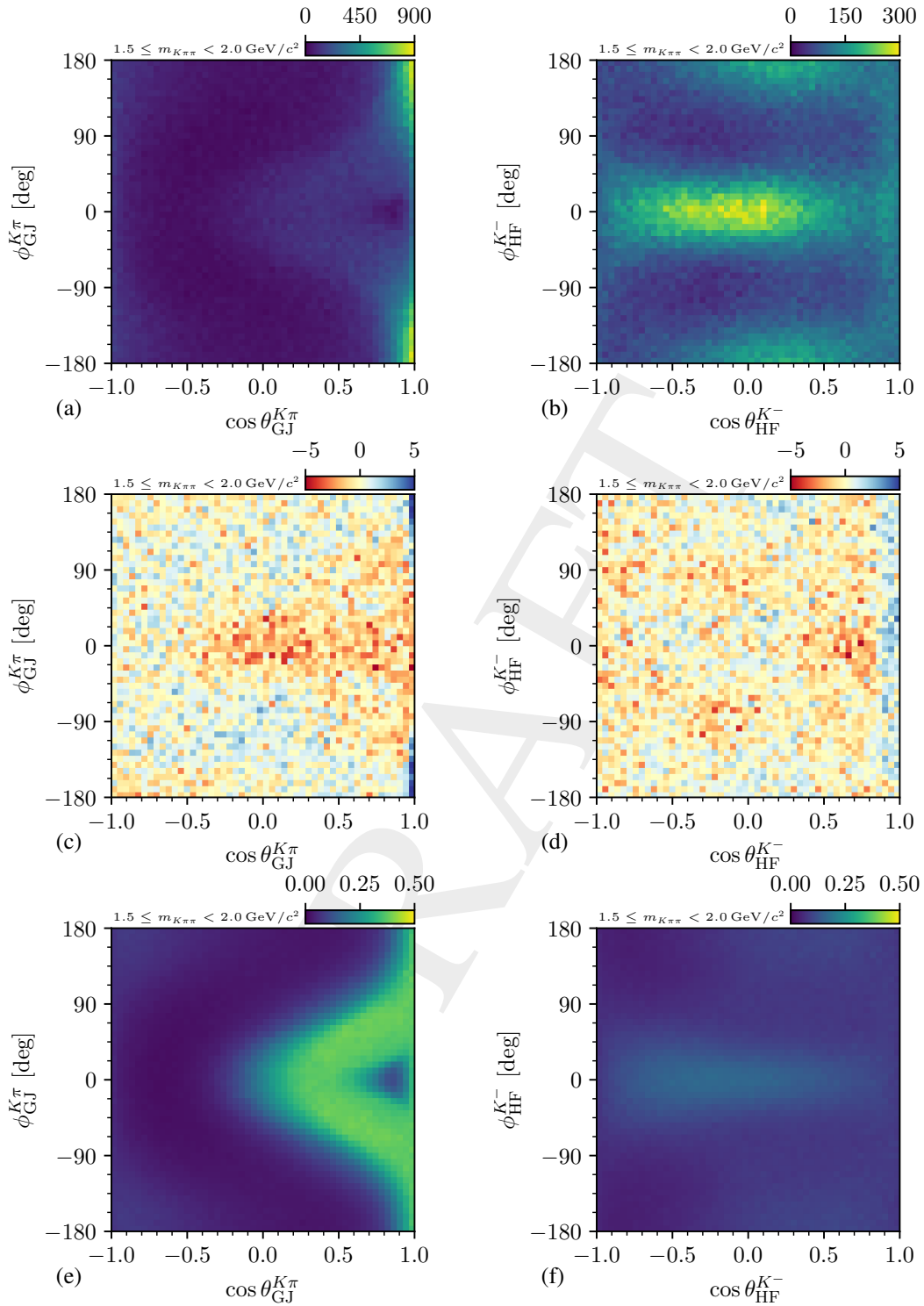


Figure D.45: Distributions of the four two-body decay angles defined for the  $K^- \pi^+$  isobar system in the mass range  $1.5 \leq m_{K\pi} < 2.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The top row shows the measured distributions, the middle row shows the difference between the measured number of events and the corresponding PWD prediction divided by the square root of the PWD prediction, and the lower row shows the acceptance.

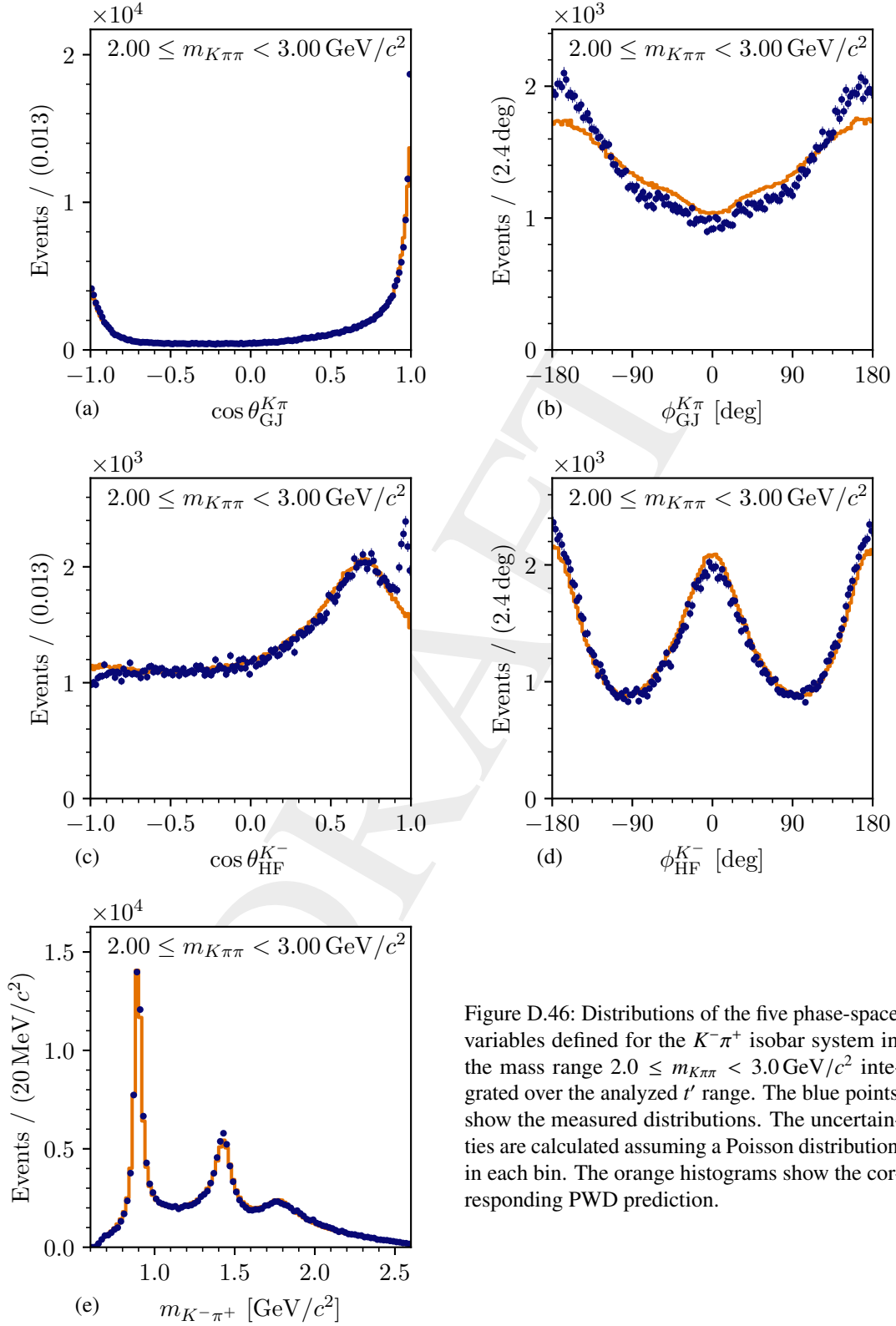


Figure D.46: Distributions of the five phase-space variables defined for the  $K^-\pi^+$  isobar system in the mass range  $2.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The blue points show the measured distributions. The uncertainties are calculated assuming a Poisson distribution in each bin. The orange histograms show the corresponding PWD prediction.

## D Partial-Wave Decomposition

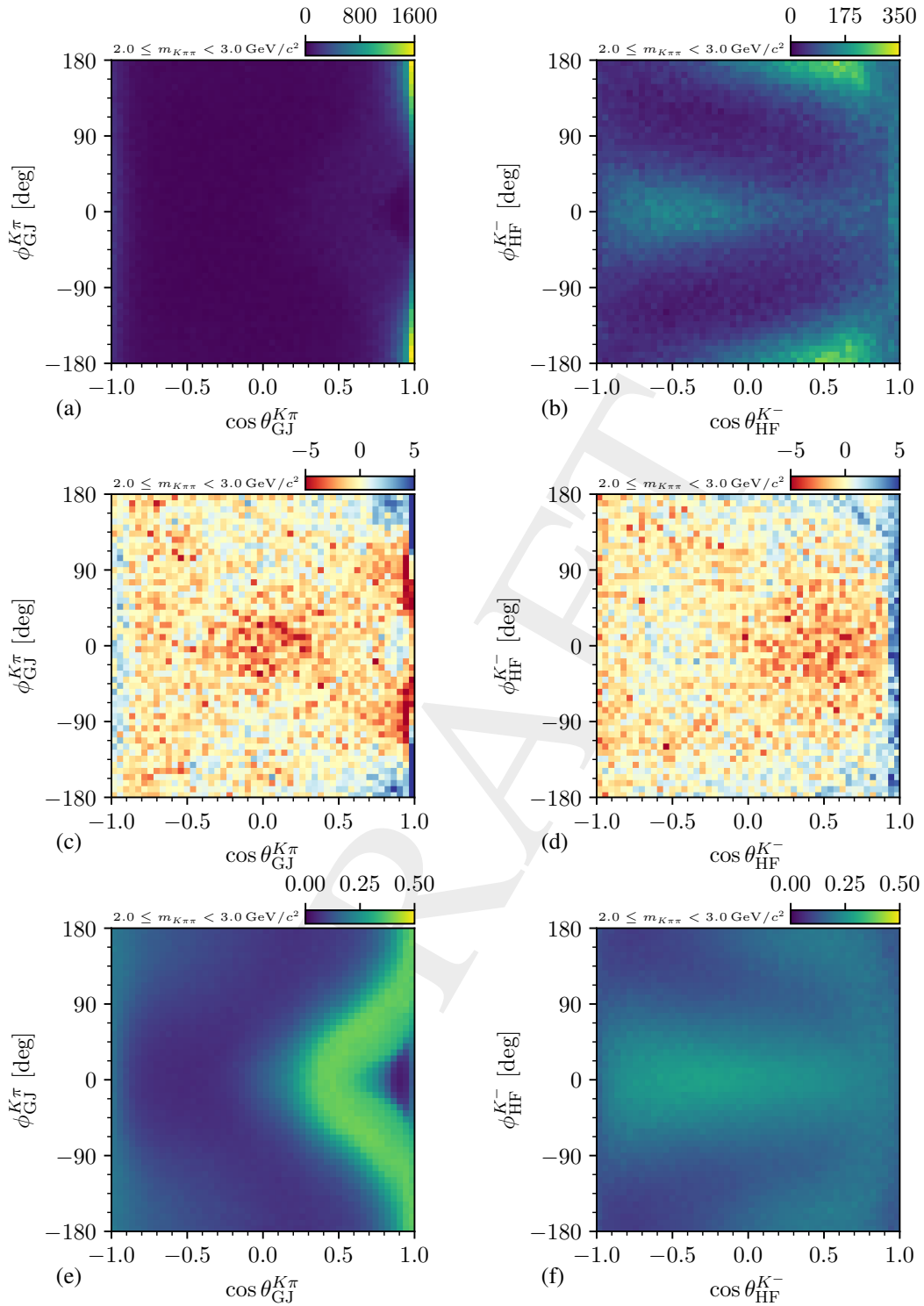


Figure D.47: Distributions of the four two-body decay angles defined for the  $K^- \pi^+$  isobar system in the mass range  $2.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$  integrated over the analyzed  $t'$  range. The top row shows the measured distributions, the middle row shows the difference between the measured number of events and the corresponding PWD prediction divided by the square root of the PWD prediction, and the lower row shows the acceptance.



6217

## D.3 Phase-Space Integral Matrix and Overlaps

6218 Figure D.48a shows the magnitude of the elements of the phase-space integral matrix as given in  
 6219 equation (5.22) at  $m_{K\pi\pi} = 1.31 \text{ GeV}/c^2$  in the lowest  $t'$  bin. As stated in section 5.9, for most  
 6220 waves we observe only small overlaps (dark blue regions) due to the orthogonality of the Wigner  
 6221  $D$ -functions. However, there are some exceptions. For example, the  $0^- 0^+ [K\pi]_S^{K\pi} \pi S$  and  $0^- 0^+$   
 6222  $[\pi\pi]_S^{\text{AMPK}} K S$  waves have an overlap close to one (see (i) in figure D.48a). As the spins as well  
 6223 as the orbital angular momenta of both waves are the same, i.e. zero, they differ only by the  
 6224 different isobar amplitudes that correspond to  $[K\pi]_S^{K\pi}$  and  $[\pi\pi]_S^{\text{AMPK}}$ . In the low  $m_{K^-\pi^+}$  and  $m_{\pi^-\pi^+}$   
 6225 ranges kinematically accessible at  $m_{K\pi\pi} = 1.31 \text{ GeV}/c^2$ , these isobar amplitudes are similar (see  
 6226 figures 5.4 and 5.5). Thus, the decay amplitudes become similar and the corresponding overlap  
 6227 becomes large. A similar case are the  $1^+ 0^+ [K\pi]_S^{K\pi} \pi P$  and  $1^+ 0^+ [K\pi]_S^{K\eta} \pi P$  waves, where we  
 6228 observe a large overlap marked by (ii).

6229 Also, we find modest overlaps of about 0.5 between various waves marked by (iii) and (iv), e.g.  
 6230 between the  $1^+ 0^+ [K\pi]_S^{K\pi} \pi P$  and  $1^+ 0^+ \rho(770) K S$  waves. Both waves have the same  $J^P M^E$   
 6231 quantum numbers. For the  $1^+ 0^+ [K\pi]_S^{K\pi} \pi P$  wave, the  $K^-\pi^+$  system is in an  $S$  wave and the  
 6232  $\pi^-\pi^+$ -isobar system is in a  $P$  wave. For the  $1^+ 0^+ \rho(770) K S$  wave, the  $K^-\pi^+$ -isobar system is in an  
 6233  $S$  wave and the  $\pi^-\pi^+$  system is in a  $P$  wave. Thus, the angular distribution of both waves are  
 6234 similar. However, they are not identical and both waves clearly differ in the isobar amplitude.  
 6235 Thus, the overlap is smaller than one, which means that the waves can be separated in principle  
 6236 in the PWD. This holds for all waves with similar overlap values.

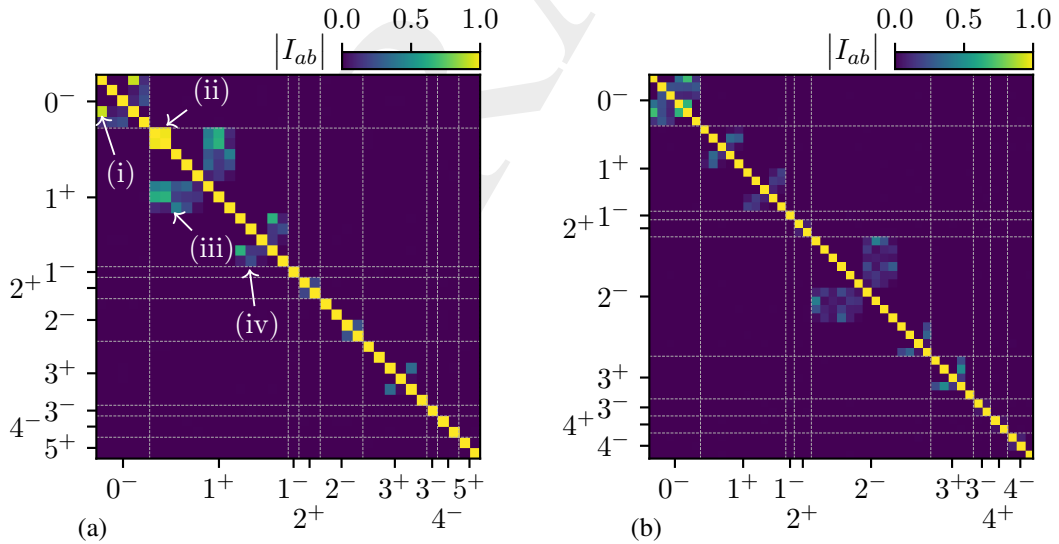


Figure D.48: Magnitude of the elements of the phase-space integral matrix for the wave set in the kinematic cell at (a)  $m_{K\pi\pi} = 1.31 \text{ GeV}/c^2$  and (b)  $m_{K\pi\pi} = 1.91 \text{ GeV}/c^2$  in the lowest  $t'$  bin. For simplicity, the incoherent flat wave is not shown and in (b) we show only waves with  $J \leq 4$ .

6237 Figure D.48b shows the magnitude of the elements of the phase-space integral-matrix at a  
 6238 higher mass of  $m_{K\pi\pi} = 1.91 \text{ GeV}/c^2$  in the lowest  $t'$  bin. Overall, the overlaps are smaller in  
 6239 the high- $m_{K\pi\pi}$  region than in the low- $m_{K\pi\pi}$  region and we do not observe overlaps as large as  
 6240 those marked with (i) and (ii) in figure D.48a. The reason for this is, that at higher  $m_{K\pi\pi}$  the  
 6241 phase-space is larger, i.e. a larger range in  $m_{\pi^-\pi^+}$  and  $m_{K^-\pi^+}$  is kinematically accessible. Thus,  
 6242 we explore more of the isobar amplitude in the PWD, which improves the separation of, e.g.,  
 6243 the  $0^- 0^+ [K\pi]_S^{K\pi} \pi S$  and  $0^- 0^+ [\pi\pi]_S^{\text{AMPK}} K S$  waves. Similar to some  $1^+$  waves in the low- $m_{K\pi\pi}$   
 6244 region, we find modest overlaps between some  $2^-$  waves in the high- $m_{K\pi\pi}$  region. The latter one  
 6245 is dominated by  $2^-$  resonances and thus more  $2^-$  waves were selected for the wave set in the  
 6246 shown  $(m_{K\pi\pi}, t')$  cell.

6247 Partial waves with large overlaps can lead to artifacts, i.e. wrong estimates for the spin-density  
 6248 matrix elements in the PWD. This is because the decay amplitudes, which are similar for  
 6249 overlapping waves, may cancel each other via destructive interference in a large region of the  
 6250 phase space in the coherent sum of the model intensity given by equation (5.16). Although the  
 6251 intensities of the partial waves in such a destructive interference may become artificially large,  
 6252 they change the model intensity only marginally. Thus, destructive interference may be misused  
 6253 by the PWD fit to describe statistical fluctuations or small imperfections in the model.

6254 Such destructive interference effects from overlapping waves are known, e.g. from the COMPASS  
 6255  $\pi^-\pi^-\pi^+$  analysis [43]. We do not observe large destructive interference effects from overlapping  
 6256 waves in the partial waves shown in this work. A reason is that the wave set obtained from  
 6257 the wave-set selection described in section 5.2 was designed to disfavor overlapping waves by  
 6258 imposing  $m_{K\pi\pi}$  thresholds for waves with heavy isobars (see section 5.2.4).

## 6259 D.4 $\pi^-\pi^-\pi^+$ Pseudodata Studies

### 6260 D.4.1 The $\pi^-\pi^-\pi^+$ Pseudodata Model

6261 The PWD model used to generate the  $\pi^-\pi^-\pi^+$  pseudodata sample was obtained from the so-far  
 6262 world's largest sample of the reaction  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$  collected by COMPASS during  
 6263 the 2008 diffraction data taking.<sup>[e]</sup> This  $\pi^-\pi^-\pi^+$  sample was first analyzed and published in  
 6264 ref. [39]. Based on these results, an improved analysis was performed and will be presented  
 6265 in ref. [43].<sup>[f]</sup> An improved event reconstruction of the raw data with a refined time-resolved  
 6266 detector alignment. Also, the event selection was fine-tuned; i.e. some cut parameters were  
 6267 optimized for the updated data sample, the cut to suppress central-production reactions was

<sup>[e]</sup> The 2009 diffraction data set was not used in the  $\pi^-\pi^-\pi^+$  analysis when obtaining the model for the  $\pi^-\pi^-\pi^+$  pseudodata, yet.

<sup>[f]</sup> As the analysis of ref. [43] was not finished when obtaining the model for the  $\pi^-\pi^-\pi^+$  pseudodata, the final results that will be shown in ref. [43] may slightly differ from the model for the  $\pi^-\pi^-\pi^+$  pseudodata sample. However, the description of the measured  $\pi^-\pi^-\pi^+$  sample by the PWD model, which is the property of the PWD model that is important for generating pseudodata from, it should remain basically unchanged.

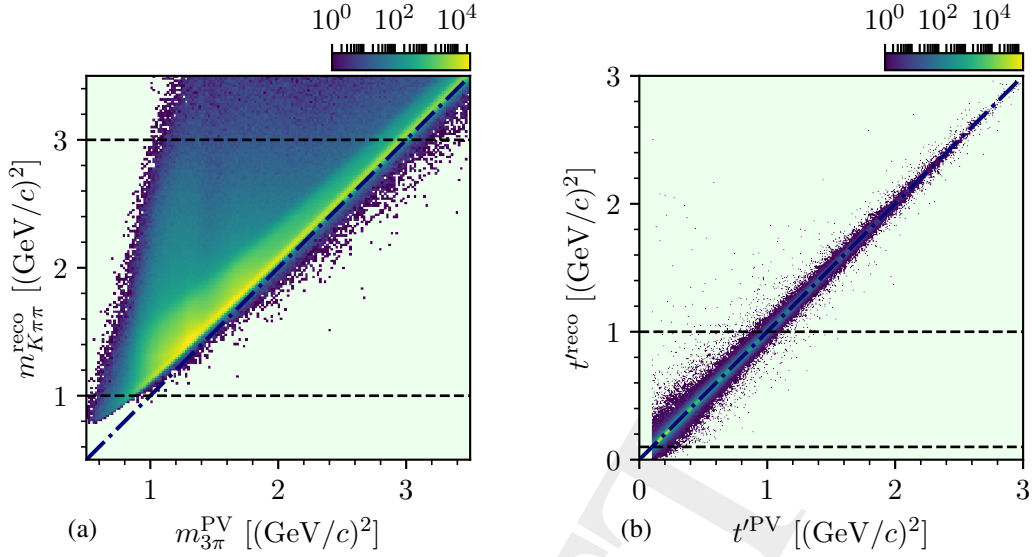


Figure D.49: Reconstructed versus true physical values (PV) for the  $\pi^-\pi^-\pi^+$  pseudodata sample reconstructed as  $K^-\pi^-\pi^+$  events: (a) for  $m_{K\pi\pi}$  and (b) for  $t'$ . The dashed horizontal black lines show the  $m_{K\pi\pi}$  and  $t'$  ranges analyzed in this work. The dash-dotted blue lines represents  $m_{K\pi\pi}^{\text{reco}} = m_{3\pi}^{\text{PV}}$  and  $t'^{\text{reco}} = t'^{\text{PV}}$ , respectively. The reconstructed sample without the beam-particle identification cut is shown. Regions without events are shown in light green.

6268 not applied, and the particle identification cuts to suppress beam kaons and final-state particles  
 6269 other than pions were improved using the methods developed in this work (see sections 3.1, 3.2,  
 6270 and 4.1). This yielded a measured  $\pi^-\pi^-\pi^+$  sample of about  $70.4 \times 10^6$  events in the kinematic  
 6271 region  $0.5 \leq m_{3\pi} < 3.5 \text{ GeV}/c^2$  and  $0.1 \leq t' < 3.0 (\text{GeV}/c)^2$ . This sample is significantly larger  
 6272 and covering a wider kinematic region as the one used ref. [39].

6273 Based on this  $\pi^-\pi^-\pi^+$  sample, a PWD was performed using the same approach as presented in  
 6274 section 5.1. The same wave set as in ref. [39] was used, which consists of 88 partial waves. The  
 6275 corresponding PWD model was formulated in terms of a rank=1 spin-density matrix for the  
 6276 positive-reflectivity waves, a rank=2 spin-density matrix for the negative-reflectivity waves, and  
 6277 an incoherent flat wave. A fine binning in  $m_{3\pi}$  and  $t'$  was used, i.e. the sample was split in 300  
 6278  $m_{3\pi}$  bins with a width of  $10 \text{ MeV}/c^2$  and 33 non-equidistant  $t'$  bins, which were chosen such that  
 6279 a similar number of events enters each  $t'$  bin.

6280 We used the results of this PWD as an input to generate a  $\pi^-\pi^-\pi^+$  pseudodata sample in the  
 6281 kinematic ranges  $0.5 \leq m_{3\pi} < 3.5 \text{ GeV}/c^2$  and  $0.1 \leq t' < 3.0 (\text{GeV}/c)^2$ . Then, we reconstructed  
 6282 this produced  $\pi^-\pi^-\pi^+$  pseudodata sample as  $K^-\pi^-\pi^+$  events in order to study the  $\pi^-\pi^-\pi^+$  contam-  
 6283 ination of the measured  $K^-\pi^-\pi^+$  sample (see section 5.10). To test whether the  $\pi^-\pi^-\pi^+$  kinematic  
 6284 range is sufficient to cover the analyzed  $K^-\pi^-\pi^+$  range of  $1.0 \leq m_{K\pi\pi} < 3.0 \text{ GeV}/c^2$  and  $0.1 \leq t'$   
 6285  $< 1.0 (\text{GeV}/c)^2$ , we show in figure D.49 the reconstructed values (reco) under the  $K^-\pi^-\pi^+$  event  
 6286 hypothesis versus the true physical values (PV) with which the  $\pi^-\pi^-\pi^+$  pseudodata event was  
 6287 produced.

6288 The reconstructed value for  $m_{K\pi\pi}$ , i.e.

$$m_{K\pi\pi}^{\text{reco}} = \sqrt{(p_{K^-}^{\text{reco}} + p_{\pi^-}^{\text{reco}} + p_{\pi^+}^{\text{reco}})^2}, \quad (\text{D.1})$$

6289 is given by the reconstructed three-momenta of the final-state particles and their mass assumptions,  
 6290 which yields the four-momenta  $p_{h^\pm}^{\text{reco}}$  of the final-state particles. For the final-state  $\pi^-$  that  
 6291 was erroneously identified as  $K^-$  in the reconstructed  $\pi^- \pi^- \pi^+$  pseudodata sample, this mass  
 6292 assumption is wrong. Typically,  $m_{K\pi\pi}^{\text{reco}}$  is as large or larger than the value  $m_{3\pi}^{\text{PV}}$  with which the event  
 6293 was produced (see figure D.49a). Just above the  $\pi^- \pi^- \pi^+$  threshold at about  $m_{3\pi}^{\text{PV}} = 0.5 \text{ GeV}/c^2$ ,  
 6294 the difference between  $m_{K\pi\pi}^{\text{reco}}$  and  $m_{3\pi}^{\text{PV}}$  is given mainly by the mass difference between the final-  
 6295 state  $K^-$  and  $\pi^-$ , because of the wrong mass assumption for one of the final-state  $\pi^-$ . With  
 6296 increasing  $m_{3\pi}^{\text{PV}}$ , this relation is smeared out, because of the larger momenta of the final-state  
 6297 particles, which have a larger influence on  $m_{K\pi\pi}^{\text{reco}}$  (see equation (D.1)). From the distribution in  
 6298 figure D.49a we do not expect events with  $m_{3\pi}^{\text{PV}} < 0.5 \text{ GeV}/c^2$  or  $m_{3\pi}^{\text{PV}} > 3.5 \text{ GeV}/c^2$  to enter the  
 6299 analyzed  $m_{K\pi\pi}^{\text{reco}}$  region (dashed horizontal lines). Thus, the  $m_{3\pi}^{\text{PV}}$  range in which we generated  
 6300 pseudodata events is sufficient to cover the analyzed  $m_{K\pi\pi}^{\text{reco}}$  range.

6301 As expected, the reconstructed squared four-momentum transfer  $t'^{\text{reco}}$  scatters around the true  
 6302 physical value  $t'^{\text{PV}}$  with which the event was produced (see figure D.49b), as expected. We do  
 6303 not expect events with  $t'^{\text{PV}} > 3.0 (\text{GeV}/c)^2$  to enter the analyzed  $t'^{\text{reco}}$  region (dashed horizontal  
 6304 lines). However, the lower limit of the analyzed  $t'$  range of  $0.1 (\text{GeV}/c)^2$  is the same for both  
 6305 analysis. It is given by the minimum energy necessary for the recoil proton to produce a signal  
 6306 in the recoil-proton detector (see section 2.2). Due to the finite resolution in  $t'^{\text{reco}}$  of about  
 6307  $0.006 (\text{GeV}/c)^2$  (see figure C.5b), a small fraction of events with  $t'^{\text{PV}} < 0.1 (\text{GeV}/c)^2$  may enter  
 6308 the analyzed  $t'^{\text{reco}}$  range. However, we do not have a PWD model for  $t'^{\text{PV}} < 0.1 (\text{GeV}/c)^2$  and  
 6309 thus we cannot generate pseudodata for this range. Hence, we neglect these events in the low  
 6310  $t'^{\text{reco}}$  region of the reconstructed  $\pi^- \pi^- \pi^+$  pseudodata sample. Due to the exponential shape of  
 6311 the  $t'^{\text{PV}}$  distribution, this bin-migration effect may lead to a slight underestimation of the number  
 6312 of  $\pi^- \pi^- \pi^+$  background events in the lowest  $t'$  bin. However, given the good resolution in  $t'^{\text{reco}}$ ,  
 6313 we expect this effect to be negligible.

6314 In conclusion, the PWD model from the COMPASS  $\pi^- \pi^- \pi^+$  analysis is well suited to generate  
 6315 a realistic pseudodata sample for the reaction  $\pi^- + p \rightarrow \pi^- \pi^- \pi^+ + p$ , which allows us to study  
 6316 the  $\pi^- \pi^- \pi^+$  background in the  $K^- \pi^- \pi^+$  sample. The results of this study are discussed in  
 6317 sections 5.10.1 and 5.10.2.

#### 6318 D.4.2 Acceptance of the $K^- \pi^- \pi^+$ Event Selection for $\pi^- \pi^- \pi^+$ Events

6319 As discussed in section 5.10.1, we expect about 6.7%  $\pi^- \pi^- \pi^+$  background in the  $K^- \pi^- \pi^+$   
 6320 sample. This amount of  $\pi^- \pi^- \pi^+$  background is given by the beam-particle miss-identification  
 6321 probability; the acceptance of the final-state event selection, i.e. the  $K^- \pi^- \pi^+$  event selection  
 6322 without the beam-particle identification; and potentially different cross-sections for the reactions

6323  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  and  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$ . The amount of  $\pi^-\pi^-\pi^+$  background is about  
 6324 twice as large as the expected impurity from beam pions in a kaon-beam sample selected by the  
 6325 CEDARs, which is about 3% (see section 3.1.6). By comparing the acceptance of the  $K^-\pi^-\pi^+$   
 6326 final-state event selection for  $\pi^-\pi^-\pi^+$  pseudodata events and for  $K^-\pi^-\pi^+$  pseudodata events, we  
 6327 found that the acceptance for  $\pi^-\pi^-\pi^+$  events is about twice as large as the acceptance for  $K^-\pi^-\pi^+$   
 6328 events. This explains the two-times larger amount of  $\pi^-\pi^-\pi^+$  background compared to the naïve  
 6329 expectation from the impurity from beam pions in a kaon-beam sample.

6330 The main reason for the comparably high acceptance of the final-state event selection for  $\pi^-\pi^-\pi^+$   
 6331 events is that in the  $K^-\pi^-\pi^+$  event selection we required only one of the two negative final-state  
 6332 particles to be identified. The  $\pi^-$  is identified for most of the events (see figure 4.3). Events of  
 6333 the reaction  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  have one final-state  $\pi^-$  to be identified, while events of the  
 6334 reaction  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$  have two  $\pi^-$  and thus a higher probability to be accepted. In  
 6335 principle, the final-state particle identification veto should reject  $\pi^-\pi^-\pi^+$  events (see section 4.1).  
 6336 However, only few  $\pi^-\pi^-\pi^+$  events are rejected, because the positive final-state particle is a  $\pi^+$   
 6337 in both reactions and because it is kinematically very improbable to simultaneously identify  
 6338 both negative final-state particles (see section 4.1). Also, the other event selection cuts do not  
 6339 suppress  $\pi^-\pi^-\pi^+$  events with respect to  $K^-\pi^-\pi^+$  events. Figure D.50 shows the distributions of  
 6340 the  $\pi^-\pi^-\pi^+$  pseudodata sample reconstructed as  $K^-\pi^-\pi^+$  events (red histograms) in the kinematic  
 6341 variables used to impose energy and momentum conservation in the event selection as discussed  
 6342 in section 4.1. They exhibit peaks that are similar to those of the measured  $K^-\pi^-\pi^+$  sample  
 6343 (blue histograms). Thus, also the cuts (gray vertical lines) on energy conservation, i.e. on  $E_{\text{beam}}$ ,  
 6344 and on momentum conservation, i.e. on  $\Delta\phi_{\text{recoil}}$ , do not suppress the  $\pi^-\pi^-\pi^+$  background in the  
 6345  $K^-\pi^-\pi^+$  sample.

6346 In summary, the amount of  $\pi^-\pi^-\pi^+$  background is mainly caused by the limited kinematic range  
 6347 of the final-state particle identification. Since the relative amount of  $\pi^-\pi^-\pi^+$  background in the  
 6348  $K^-\pi^-\pi^+$  sample is dominantly explained by acceptance effects, the cross-sections of the reactions  
 6349  $K^- + p \rightarrow K^-\pi^-\pi^+ + p$  and  $\pi^- + p \rightarrow \pi^-\pi^-\pi^+ + p$  have a similar scale. This is consistent with  
 6350 measurements of the total  $Kp$  and  $\pi p$  cross-sections [9].

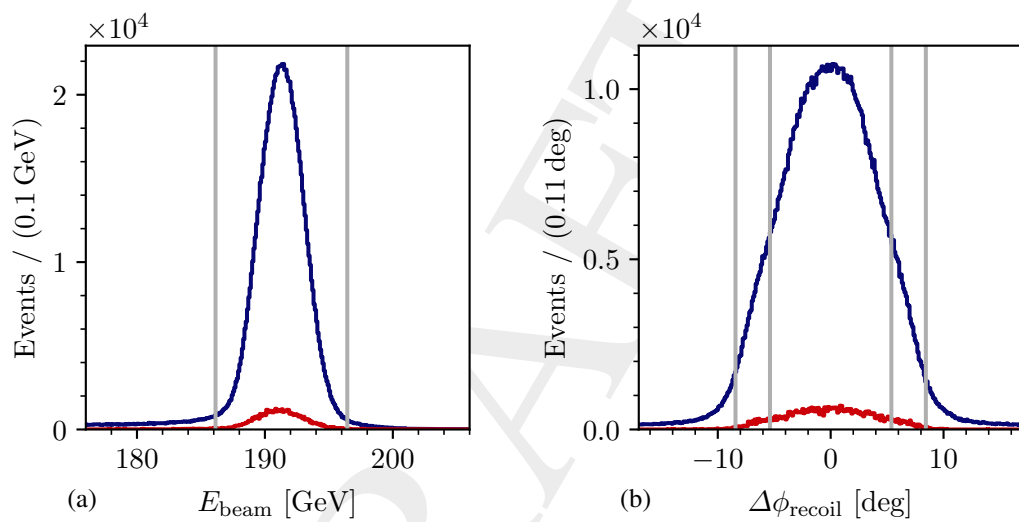


Figure D.50: Distribution of the kinematic variables used to select exclusive events. The red histograms show the  $\pi^-\pi^-\pi^+$  pseudodata sample reconstructed as  $K^-\pi^-\pi^+$  events (see section 5.10) and scaled such that the number of reconstructed  $\pi^-\pi^-\pi^+$  pseudodata events corresponds to the predicted amount of  $\pi^-\pi^-\pi^+$  background in the  $K^-\pi^-\pi^+$  sample. The blue histograms show the measured  $K^-\pi^-\pi^+$  sample (same as figure 4.4). (a) shows the distribution of the reconstructed beam energy after all cuts except for the cut on  $E_{\text{beam}}$ . (b) shows the distribution of  $\Delta\phi_{\text{recoil}}$ , which is a measure of momentum conversation (see section 4.1), after all cuts except for the cut on  $\Delta\phi_{\text{recoil}}$ . The gray lines represent the applied cuts.

## E The Resonance Model Fit

### E.1 The 10-Wave RMF

#### E.1.1 The 10-Wave RMF Model

An overview over the 10-wave RMF model is given in section 6.2.1 and it is also summarized in table 6.1. Here, we provide additional, mainly technical details of the 10-wave RMF model.

Table E.1 lists the eight resonance components included in the 10-wave RMF. For all resonance components, we used the relativistic Breit-Wigner amplitude given in equation (5.39) with a dynamic width that takes into account a single decay channel given in the last column in table E.1. The same decay channel is used for all resonances that belong to the same  $J^P$  sector, i.e. the dominant decay channel of the dominant resonance. We chose the parameter limits for the  $m_0$  and  $\Gamma_0$  parameters (second column in table E.1) to be as little restrictive as possible in order to prevent the results ending up on these limits, which would bias our results. Resonance components representing ground or excited states of the same  $J^P$  sector have non-overlapping  $m_0$  limits. For example, this prevents interchange of resonance components, which would lead to ambiguities in the RMF. The upper limit for  $\Gamma_0$  of  $600 \text{ MeV}/c^2$  is the same for all resonance components. It is much larger than the width of the broadest of the included resonances as measured by previous experiments, which is the  $K_2(1820)$  with a width of about  $276 \text{ MeV}/c^2$  [91]. The lower limits for the  $\Gamma_0$  parameters were optimized for each resonance to suppress solutions with unrealistically small widths. We chose these limits to be smaller than any previous  $\Gamma_0$  measurement of the corresponding state. Furthermore, we selected the start-parameter ranges for  $m_0$  and  $\Gamma_0$  such that their cover a reasonable range including previous measurements [91] plus a safety margin. Hence, we do not expect bias from the choice of the start-parameter ranges. As the  $K_1(1400)$  is only a small signal in the two included  $1^+$  waves, we could not determine its mass and width reliably (see section 6.3.3). Thus, we fixed the  $m_0$  and  $\Gamma_0$  parameters of the  $K_1(1400)$  component to the corresponding PDG average values [91] as listed in table E.1.

For the non-resonant and effective background components, we used in most of the waves the simplified shape given in equations (6.11) and (6.17) as listed in table 6.1. The parameter limits of  $-0.1 \leq b_k < 130.0 (\text{GeV}/c)^{-2}$  were chosen to be much larger than the expected range of  $b_k$ , e.g. larger than the typical values for  $b_k$  obtained in the COMPASS  $\pi^-\pi^-\pi^+$  analysis [41]. The start parameter range was chosen to be  $1.0 \leq b_k < 10.0 (\text{GeV}/c)^{-2}$ . For those components that are parameterized by extended non-resonant and effective background shapes in equations (6.8)

Table E.1: Resonance components included in the set  $\mathbb{S}_d$  in equation (6.6) for the 10 partial waves listed in table 6.1. In addition, we list the fit-parameter limits and the start-parameter ranges (see text) for the mass parameters  $m_0$  and width parameters  $\Gamma_0$ . The resonance parameters of the  $K_1(1400)$  component were fixed in the RMF to the PDG average values [91]. The last column shows the decay mode that we assumed when calculating the dynamic width of the resonance in equation (5.40).

Resonance	Parameter	Limits [MeV/ $c^2$ ]		Start Ranges [MeV/ $c^2$ ]		Fixed Values [MeV/ $c^2$ ]	Decay Mode for $\Gamma(m)$
$K_1(1270)$	$m_0$	1200	1500	1270	1290	—	$K^*(892)\pi S$
	$\Gamma_0$	50	600	80	130	—	
$K_1(1400)$	$m_0$	—	—	—	—	1403	$K^*(892)\pi S$
	$\Gamma_0$	—	—	—	—	174	
$K_1(1630)$	$m_0$	1550	2300	1600	1900	—	$K^*(892)\pi S$
	$\Gamma_0$	50	600	120	350	—	
$K_2^*(1430)$	$m_0$	1300	1500	1425	1435	—	$K\pi S$
	$\Gamma_0$	80	600	105	115	—	
$K_2(1770)$	$m_0$	1700	1790	1700	1790	—	$K^*(892)\pi P$
	$\Gamma_0$	100	600	150	250	—	
$K_2(1820)$	$m_0$	1800	2000	1820	1850	—	$K^*(892)\pi P$
	$\Gamma_0$	100	600	150	250	—	
$K_2(2250)$	$m_0$	2100	2450	2200	2280	—	$K^*(892)\pi P$
	$\Gamma_0$	50	600	150	250	—	
$K_4^*(2045)$	$m_0$	2000	2400	2050	2080	—	$K^*(892)\pi G$
	$\Gamma_0$	100	600	150	250	—	

6382 and (6.18), respectively, we chose the parameter limits  $-5.0 \leq a_k < 30.0$  and  $-500.0 \leq c_k$   
6383  $< 500.0$ , and the start-parameter ranges  $0.1 \leq a_k < 1.0$  and  $-3.0 \leq c_k < 3.0$ .

6384 There are a few exceptions from these parameter limits and start-parameter ranges that we had to  
6385 introduce to improve the fit stability and convergence rate:

- 6386 • The non-resonant components in the  $2^+$  waves turned out to be small (see section 7.2). In  
6387 combination with the rather narrow  $m_{K\pi\pi}$  fit ranges, in which we considered data from  
6388 these  $2^+$  waves, we were not able to reliably determine the shape parameter  $b_k$  of the non-  
6389 resonant components in these waves. In most of the cases, our estimates for the  $b_k$  ended  
6390 up at the lower parameter limit of  $-0.1 \text{ (GeV}/c)^{-2}$ . Hence, we fixed the  $b_k$  parameters of  
6391 the non-resonant components in the  $2^+$  waves to  $b_k = -0.1 \text{ (GeV}/c)^{-2}$ .
- 6392 • Similarly, the  $b_k$  parameter of the non-resonant component in the  $2^- 0^+ K^*(892)\pi F$  wave  
6393 could not be determined from the limited  $m_{K\pi\pi}$  fit range of this wave. In order to obtain



6394 an estimate for  $b_k$ , we performed an RMF with an extended upper  $m_{K\pi\pi}$  fit range for this  
 6395 wave. This fit yielded a value of  $b_k = 1.616 (\text{GeV}/c)^{-2}$ . Then, we fixed  $b_k$  to this value in  
 6396 all others RMFs.<sup>[a]</sup>

6397 • We fine-tuned some start-parameter ranges and parameter limits based on the results of  
 6398 first RMFs in order to improve the speed of convergence of the fit and thereby reduce the  
 6399 computational costs:

6400 – We changed the start-parameter ranges of the non-resonant component of the  $2^- 0^+$   
 6401  $K_2^*(1430)\pi S$  wave to  $3.0 \leq a_k < 5.0$  and  $2.0 \leq c_k < 3.0$ .

6402 – We changed the start-parameter ranges of the effective background component of the  
 6403  $2^- 0^+ K_2^*(1430)\pi S$  wave to  $7.0 \leq a_k < 8.0$  and  $3.3 \leq c_k < 3.4$ .

6404 – We changed the start-parameter ranges of the effective background component of the  
 6405  $4^+ 1^+ K^*(892)\pi G$  wave to  $4.0 \leq a_k < 6.0$  and  $1.5 \leq c_k < 1.6$ .

6406 – We changed the parameter limits of the effective background component of the  $2^- 0^+$   
 6407  $K_2^*(1430)\pi S$  wave to  $-0.5 \leq a_k < 30.0$ .

6408 – We changed the parameter limits of the effective background component of the  $2^- 0^+$   
 6409  $f_2(1270)\pi S$  wave to  $-0.1 \leq b_k < 200 (\text{GeV}/c)^{-2}$ .

6410 • The intensity spectrum of the  $4^+ 1^+ K^*(892)\pi G$  wave exhibits an enhanced low-mass tail  
 6411 below  $m_{K\pi\pi} \approx 2 \text{ GeV}/c^2$  as shown in figure 5.20b. As the pre-factor in equation (6.6),  
 6412 which encodes the  $m_{K\pi\pi}$  dependence of the production and the phase space, suppresses the  
 6413 transition amplitude at low  $m_{K\pi\pi}$ , the RMF yielded very large values for  $a_k$  in equation (6.8)  
 6414 to compensate for the suppression when trying to reproduce this enhanced low-mass tail. To  
 6415 take this into account we dropped this pre-factor in the model of the effective background  
 6416 in the  $4^+ 1^+ K^*(892)\pi S$  wave in equation (6.16), i.e. we used the following modified  
 6417 version of equation (6.18):

$$\mathcal{D}_k^{\text{eBKG}}(m_{K\pi\pi}; a_k, c_k) = \frac{\mathcal{D}_k^{\text{NR}}(m_{K\pi\pi}; a_k, c_k)}{\sqrt{\mathfrak{R}_a(m_{K\pi\pi})m_{K\pi\pi}\mathcal{P}_{\mathbb{P}}(m_{K\pi\pi}, t')}}. \quad (\text{E.1})$$

6418 As  $a_k$  has a different meaning in this parameterization, we applied different parameter  
 6419 limits of  $-5.0 \leq a_k < 60.0$ .

<sup>[a]</sup> As the RMF does not describe well the region  $m_{K\pi\pi} > 2 \text{ GeV}/c^2$  in the  $2^- 0^+ K^*(892)\pi F$  wave, we did not use the extended  $m_{K\pi\pi}$  fit range in the main analysis.

6420 **E.1.2 Results from the 10-Wave RMF**

6421 In this section, we summarize additional results from the 10-wave RMF that are not shown in the  
 6422 main text in section 6.2. The parameter estimates for the shape parameters of the non-resonant  
 6423 and effective background terms are listed in tables E.2 and E.3, respectively. The spin-density  
 6424 matrices of the 10-wave RMF from the four analyzed  $t'$  bins are shown in figures E.1 to E.4.

Table E.2: Estimates for the shape parameters of the non-resonant components as obtained from the 10-wave RMF described in section 6.2. The statistical and systematic uncertainties are not given. Values of shape parameters that were fixed in the RMF (see appendix E.1.1) are marked by (\*).

Partial wave	Parameter	Value
$2^-0^+ \bar{K}_2^*(1430)\pi S$	$c$	3.00
	$a$	11.0
$1^+0^+ \rho^0(770)KS$	$b [(\text{GeV}/c)^{-2}]$	4.03
$1^+1^+ \rho^0(770)KS$	$b [(\text{GeV}/c)^{-2}]$	3.39
$2^+1^+ \bar{K}^*(892)\pi D$	$b [(\text{GeV}/c)^{-2}]$	(*) -0.1
$2^+1^+ \rho^0(770)KD$	$b [(\text{GeV}/c)^{-2}]$	(*) -0.1
$2^-0^+ \bar{K}^*(892)\pi S$	$b [(\text{GeV}/c)^{-2}]$	(*) 1.616
$2^-0^+ \rho^0(770)KF$	$b [(\text{GeV}/c)^{-2}]$	8.6
$2^-0^+ f_2(1270)KS$	$b [(\text{GeV}/c)^{-2}]$	7.4
$4^+1^+ \bar{K}^*(892)\pi G$	$b [(\text{GeV}/c)^{-2}]$	19
$4^+1^+ \rho^0(770)KG$	$b [(\text{GeV}/c)^{-2}]$	3.1

Table E.3: Estimates for the shape parameters of the effective background components as obtained from the 10-wave RMF described in section 6.2. The statistical and systematic uncertainties are not given.

Partial wave	Parameter	Value
$2^-0^+ \bar{K}_2^*(1430)\pi S$	$c$	3.88
	$a$	12.91
$4^+1^+ \bar{K}^*(892)\pi G$	$c$	2.05
	$a$	7
$1^+0^+ \rho^0(770)KS$	$b [(\text{GeV}/c)^{-2}]$	5.7
$1^+1^+ \rho^0(770)KS$	$b [(\text{GeV}/c)^{-2}]$	13.01
$2^-0^+ \bar{K}^*(892)\pi F$	$b [(\text{GeV}/c)^{-2}]$	7
$2^-0^+ f_2(1270)KS$	$b [(\text{GeV}/c)^{-2}]$	0.1
$2^-0^+ \rho^0(770)KF$	$b [(\text{GeV}/c)^{-2}]$	3.5
$2^+1^+ \bar{K}^*(892)\pi D$	$b [(\text{GeV}/c)^{-2}]$	8.4
$2^+1^+ \rho^0(770)KD$	$b [(\text{GeV}/c)^{-2}]$	10.7
$4^+1^+ \rho^0(770)KG$	$b [(\text{GeV}/c)^{-2}]$	0.1

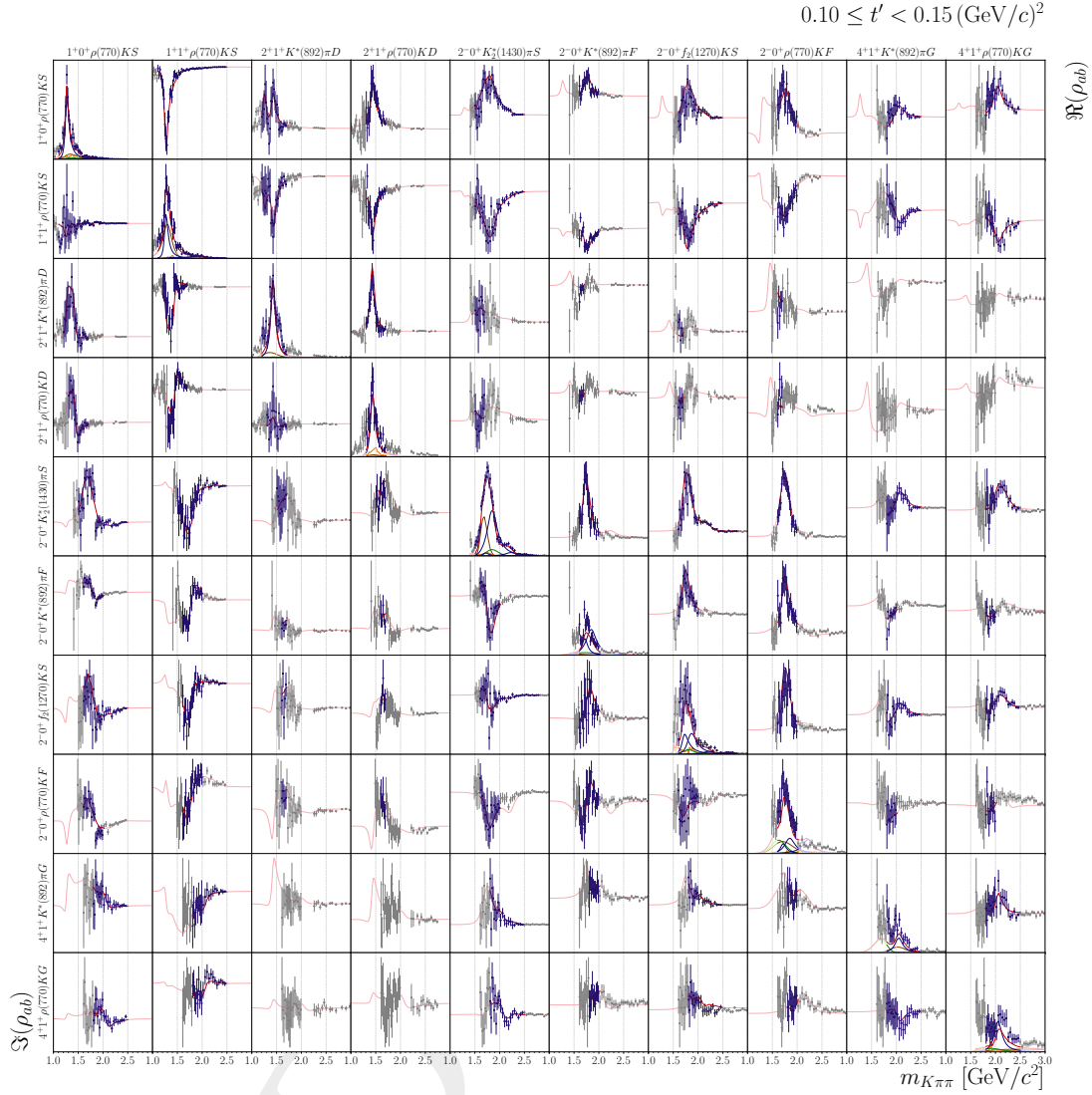


Figure E.1: Same figure as figure 6.2: Real and imaginary parts of the spin-density matrix elements, i.e.  $\Lambda_{ab}(m_{K\pi\pi}, t')$  in equation (6.19), as a function of  $m_{K\pi\pi}$  in the lowest of the four  $t'$  bins for the 10 partial waves that were included in the 10-wave RMF. The figures on the diagonal show the intensity spectra. The upper-right and lower-left off-diagonal figures show the real and imaginary parts of the off-diagonal elements of the spin-density matrix, respectively. The blue data points represent the measured spin-density matrix elements. The curves represent the result of the 10-wave RMF to these data points. The red curves represent the total RMF model. The blue curves represent the individual resonance components, the green curves the non-resonant components, the orange curves the  $\pi^-\pi^-\pi^+$  background components, and the brown curves the effective background components. The extrapolations beyond the  $m_{K\pi\pi}$  fit ranges are shown in lighter colors. The corresponding data points are shown in gray. The ranges of the vertical axes are different for each subplot. They are adjusted to the data shown in each subplot. Hence, we do not show tick marks for the vertical axes.

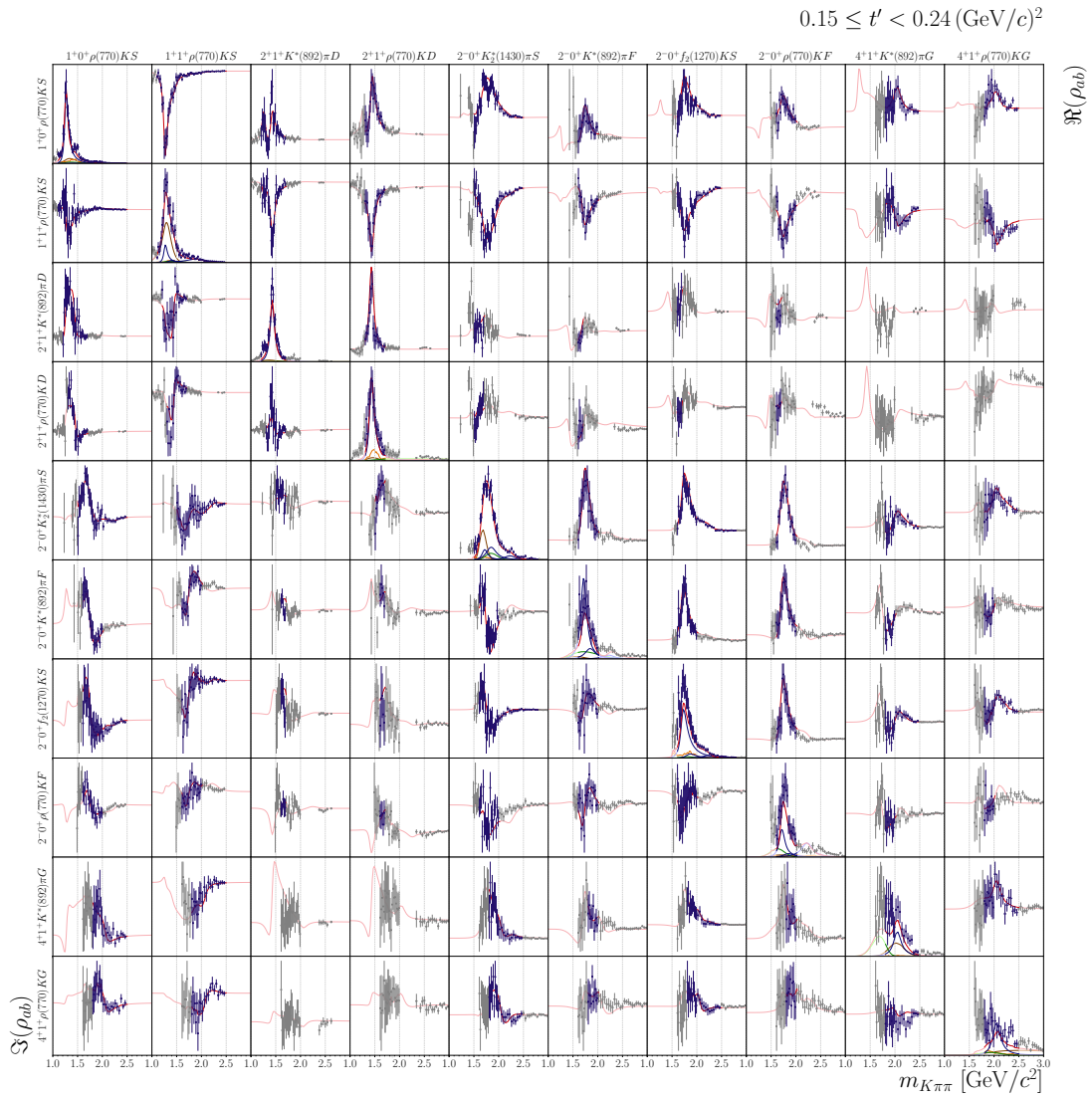


Figure E.2: Same as figure E.1 but for the second  $t'$  bin.

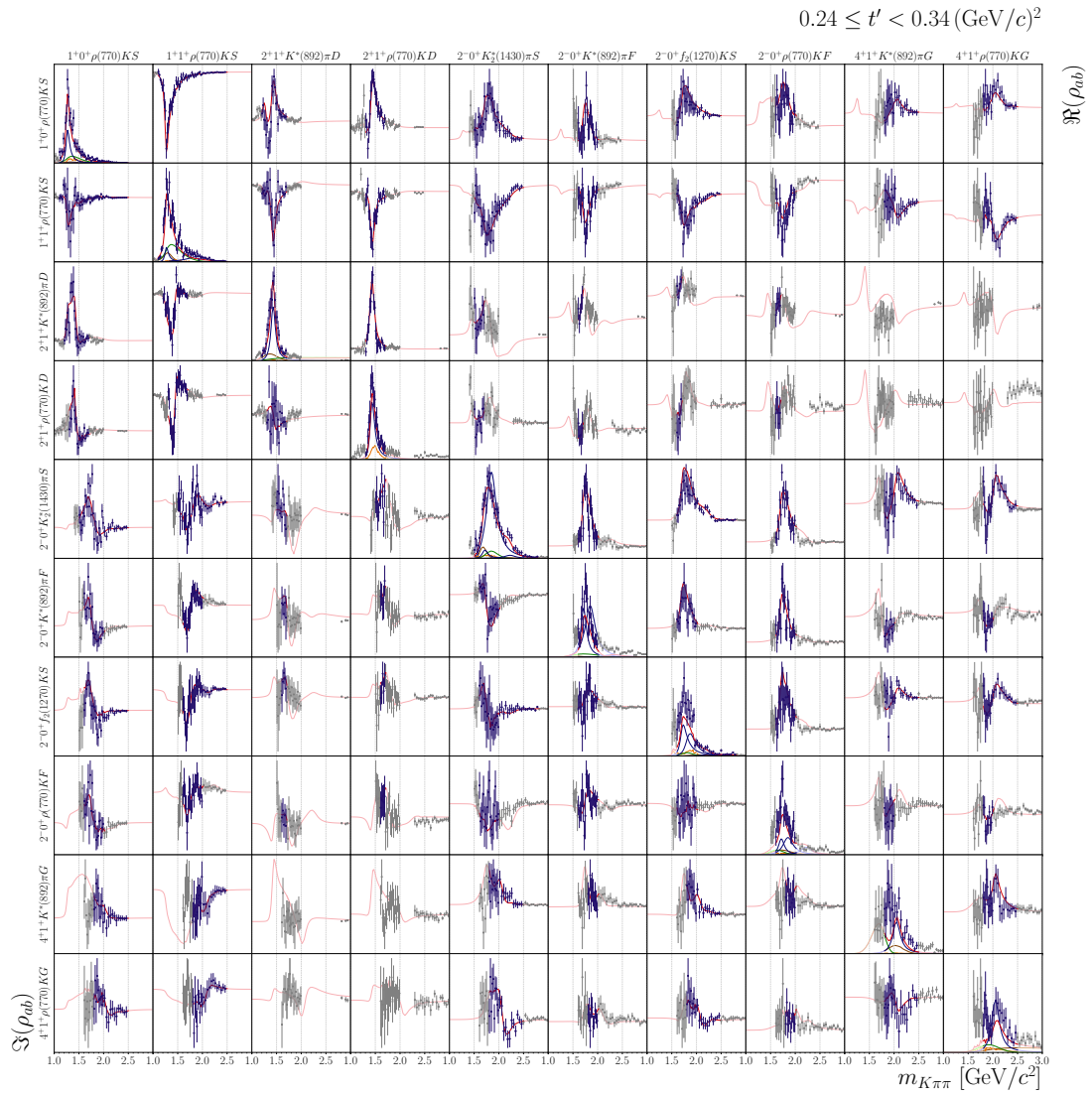


Figure E.3: Same as figure E.1 but for the third  $t'$  bin.

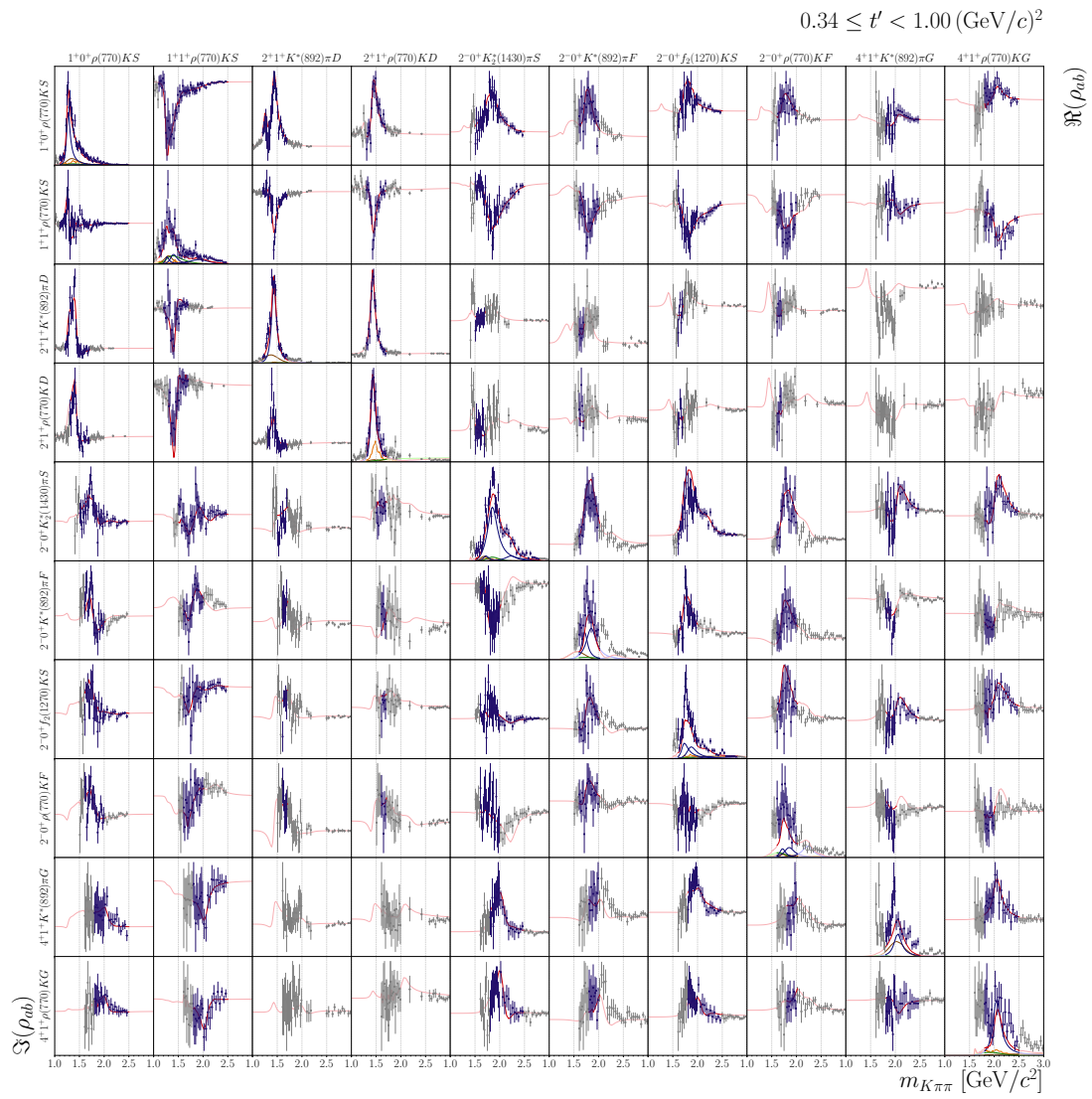


Figure E.4: Same as figure E.1 but for the fourth  $t'$  bin.

6425 **E.2 Extended Resonance-Model Fits of Waves with  $J^P = 0^-, 3^+,$**   
 6426  **$3^-,$  and  $4^-$** 

6427 In order to also study the resonance content of waves with  $J^P = 0^-, 3^+, 3^-,$  and  $4^-$ ; which were  
 6428 not included in the 10-wave RMF; we performed four extended RMFs, one per  $J^P$  sector. In  
 6429 these extended RMFs, we added waves of further interest to the 10-wave RMF model, which is  
 6430 described in section 6.2.1. The modeling of these additional waves and the fitting procedure is  
 6431 the same as used for the 10-wave RMF and described in section 6.1. Table E.4 lists the additional  
 6432 partial waves that were used in the extended RMFs and their model components. Table E.5 lists  
 6433 the additional resonance components in these waves. The results of the extended RMFs for the  
 6434  $0^-, 3^+, 3^-,$  and  $4^-$  waves are discussed in sections 7.5, 7.6, 7.7, and 7.8, respectively.

Table E.4: List of partial waves and model components included in the extended RMFs in addition to the waves and components of the 10-wave RMF, which are listed in table 6.1. The first column gives the  $J^P$  sectors, for which the extended RMF was performed. The second column lists the corresponding wave names. The third column lists the resonance components included in  $\mathbb{S}_a$  in equation (6.6). They are specified in table E.5. The fourth column lists the parameterization used for the dynamic amplitudes of the non-resonant components (NR). The fifth column lists the model for the  $\pi^- \pi^- \pi^+$  background components. The sixth column lists the parameterizations used for the dynamic amplitudes of the effective background components (eBKG) in equation (6.16). The last two columns list the  $m_{K\pi\pi}$  range, in which data from this partial wave is considered in the RMF.

RMF	Partial Wave	Resonances	NR	$\pi^- \pi^- \pi^+$	eBKG	$m_{K\pi\pi}$ Range [GeV/ $c^2$ ]
$0^-$	$0^- 0^+ \rho(770) \pi P$	$\left\{ \begin{array}{l} K(1460), \\ K(1630), \\ K(1830) \end{array} \right\}$	(6.11)	(6.15)	(6.17)	1.1 2.3
$3^+$	$3^+ 0^+ K_3^*(1780) \pi S$	$\left\{ K_3(2320) \right\}$	(6.11)	(6.15)	—	2.0 2.3
	$3^+ 1^+ K_2^*(1430) \pi P$	$\left\{ K_3(2320) \right\}$	(6.11)	(6.15)	(6.17)	2.0 2.5
$3^-$	$3^- 1^+ K^*(892) \pi F$	$\left\{ K_3^*(1780) \right\}$	(6.11)	(6.15)	(6.18)	1.6 2.0
	$3^- 1^+ \rho(770) K F$	$\left\{ K_3^*(1780) \right\}$	(6.8)	(6.15)	(6.17)	1.6 2.2
$4^-$	$4^- 1^+ K_2^*(1430) \pi D$	$\left\{ K_4(2500) \right\}$	(6.11)	(6.15)	(6.17)	2.1 2.8

Table E.5: Resonance components included in  $\mathbb{S}_a$  in equation (6.6) for the extended RMFs (labeled by the first column) in addition to the resonances listed in table E.1. The columns 4 and 5 list the parameter limits and start-parameter ranges (see text in section 6.1.6) for the mass and width parameters,  $m_0$  and  $\Gamma_0$ , respectively. The last column lists the decay mode that we assumed for the dynamic width of the resonance in equation (5.40).

RMF	Resonance	Parameter	Limits		Start Ranges		Decay
			[MeV/ $c^2$ ]		[MeV/ $c^2$ ]		
0 <sup>-</sup>	K(1460)	$m_0$	1300	1500	1400	1450	$K^*(892)\pi P$
		$\Gamma_0$	10	500	50	200	
	K(1630)	$m_0$	1500	1700	1600	1650	$K^*(892)\pi P$
		$\Gamma_0$	10	350	150	200	
	K(1830)	$m_0$	1800	1930	1820	1860	$K^*(892)\pi P$
		$\Gamma_0$	10	400	130	200	
3 <sup>+</sup>	$K_3(2320)$	$m_0$	2100	2500	2200	2450	$K_2^*(1430)\pi P$
		$\Gamma_0$	100	600	100	300	
3 <sup>-</sup>	$K_3^*(1780)$	$m_0$	1600	2000	1750	1820	$K_2^*(1430)\pi P$
		$\Gamma_0$	100	600	100	300	
4 <sup>-</sup>	$K_4(2500)$	$m_0$	2100	2650	2200	2450	$K^*(892)\pi F$
		$\Gamma_0$	100	600	100	300	



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## F The Freed-Isobar Analysis

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### F.1 Method

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In this section, we summarize the most important formulas for the freed-isobar PWD (see appendix F.1.1) and for the corresponding RMF (see appendix F.1.2). More detailed explanations of the freed-isobar analysis can be found in refs. [39, 42, 125].

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#### F.1.1 Freed-Isobar Partial-Wave Decomposition

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As already discussed in chapter 8, the goal of the freed-isobar PWD is to determine the dynamic amplitudes of selected isobars from data by parameterizing them using piecewise constant functions, i.e.

$$\mathcal{D}_\xi^{\text{free}}(m_{h^-h^+}) = \sum_i \mathfrak{D}_\xi^{\text{free}}(m_{h^-h^+}^i) \Theta(m_{h^-h^+}; m_{h^-h^+}^i). \quad (\text{F.1})$$

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Here,  $m_{h^-h^+}$  is the invariant mass of the isobar system, i.e.  $m_{K^-\pi^+}$  or  $m_{\pi^-\pi^+}$ , the window functions  $\Theta(m_{h^-h^+}; m_{h^-h^+}^i)$  are one within the bin  $i$  around  $m_{h^-h^+}^i$  and zero everywhere else, and  $\mathfrak{D}_\xi^{\text{free}}(m_{h^-h^+}^i)$  are the values of the dynamic amplitude  $\mathcal{D}_\xi^{\text{free}}(m_{h^-h^+})$  within the bin  $i$  around  $m_{h^-h^+}^i$ , which are free parameters.

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Using equation (F.1) as parameterization for the dynamic amplitudes of the isobar yields for decay amplitudes defined in equation (5.9)

$$\begin{aligned} \tilde{\Psi}_a(\tau, m_{K\pi\pi}) &= \sum_{\lambda_\xi} \alpha_{X \rightarrow \xi b L} \sqrt{\frac{2L+1}{4\pi}} \left[ {}^\varepsilon D_{M\lambda_\xi}^J(\phi_{\text{GI}}, \theta_{\text{GI}}, 0) \right]^* F_L(m_{K\pi\pi})(L, 0; J_\xi, \lambda_\xi | J, \lambda_\xi) \\ &\times \sum_i \mathfrak{D}_\xi^{\text{free}}(m_{h^-h^+}^i) \Theta(m_{h^-h^+}; m_{h^-h^+}^i) \\ &\times \alpha_\xi \sqrt{\frac{2J_\xi+1}{4\pi}} \left[ D_{\lambda_\xi 0}^{J_\xi}(\phi_{\text{HF}}, \theta_{\text{HF}}, 0) \right]^* F_{J_\xi}(m_{h^-h^+}). \end{aligned} \quad (\text{F.2})$$

6450 One should note that  $m_{h^-h^+}$  is included in  $\tau$ . Exchanging the sums  $\sum_{\lambda_\xi}$  and  $\sum_i$ , F.2 can be  
 6451 interpreted as a sum,

$$\tilde{\Psi}_a(\tau, m_{K\pi\pi}) = \sum_i \tilde{\Psi}_{a,i}(\tau, m_{K\pi\pi}), \quad (\text{F.3})$$

6452 over individual decay amplitudes for each  $m_{h^-h^+}$  bin

$$\begin{aligned} \tilde{\Psi}_a(\tau, m_{K\pi\pi}; m_{h^-h^+}^i) &\equiv \tilde{\Psi}_{a,i}(\tau, m_{K\pi\pi}) \\ &\equiv \sum_{\lambda_\xi} \alpha_{X \rightarrow \xi b L} \sqrt{\frac{2L+1}{4\pi}} \left[ \varepsilon D_{M\lambda_\xi}^J(\phi_{GJ}, \theta_{GJ}, 0) \right]^* F_L(m_{K\pi\pi})(L, 0; J_\xi, \lambda_\xi | J, \lambda_\xi) \\ &\quad \times \mathcal{D}_\xi^{\text{free}}(m_{h^-h^+}^i) \Theta(m_{h^-h^+}; m_{h^-h^+}^i) \\ &\quad \times \alpha_\xi \sqrt{\frac{2J_\xi+1}{4\pi}} \left[ D_{\lambda_\xi 0}^{J_\xi}(\phi_{HF}, \theta_{HF}, 0) \right]^* F_{J_\xi}(m_{h^-h^+}). \end{aligned} \quad (\text{F.4})$$

6453 The  $\tilde{\Psi}_a(\tau, m_{K\pi\pi}; m_{h^-h^+}^i)$  encode the dependence of the decay amplitude on the angles of the  
 6454  $X^- \rightarrow \xi^0 b^-$  and the  $\xi^0 \rightarrow h^- h^+$  decays, where  $h^- h^+$  is either  $K^- \pi^+$  or  $\pi^- \pi^+$ . In addition,  
 6455  $\tilde{\Psi}_a(\tau, m_{K\pi\pi}; m_{h^-h^+}^i)$  includes the centrifugal barrier factors  $F_L(m_{K\pi\pi})$  and  $F_{J_\xi}(m_{h^-h^+})$ . The  $m_{h^-h^+}$   
 6456 dependence given by the dynamic amplitude  $\mathcal{D}_\xi(m_{h^-h^+})$  of the isobar resonance, which is model  
 6457 dependent, is removed from  $\tilde{\Psi}_a(\tau, m_{K\pi\pi}; m_{h^-h^+}^i)$ .

6458 The same normalization scheme given in equation (5.10) as for the conventional decay amplitudes  
 6459 is applied, which yields the so-called freed decay amplitudes

$$\Psi_a(\tau, m_{K\pi\pi}; m_{h^-h^+}^i) \equiv \frac{\tilde{\Psi}_a(\tau, m_{K\pi\pi}; m_{h^-h^+}^i)}{\mathcal{D}_\xi^{\text{free}}(m_{h^-h^+}^i) \alpha_{X \rightarrow \xi b L} \alpha_\xi \sqrt{\mathfrak{R}_a(m_{K\pi\pi}; m_{h^-h^+}^i)}}. \quad (\text{F.5})$$

6460 Here, also the unknown value of the dynamic amplitude  $\mathcal{D}_\xi^{\text{free}}(m_{h^-h^+}^i)$  within the  $m_{h^-h^+}$  bin  $i$  is  
 6461 removed, in addition to the unknown couplings  $\alpha_{X \rightarrow \xi b L}$  and  $\alpha_\xi$ . The freed wave-normalization  
 6462 integral reads

$$\mathfrak{R}_a(m_{K\pi\pi}; m_{h^-h^+}^i) = \int_{(m_{K\pi\pi}, t')} d\tilde{m}_{K\pi\pi} d\tilde{t}' \int d\Phi_3(\tau) \left| \frac{\tilde{\Psi}_a(\tau, \tilde{m}_{K\pi\pi}; m_{h^-h^+}^i)}{\mathcal{D}_\xi^{\text{free}}(m_{h^-h^+}^i) \alpha_{X \rightarrow \xi b L} \alpha_\xi} \right|^2. \quad (\text{F.6})$$

6463 One should note that due to the window function in  $\tilde{\Psi}_a(\tau, m_{K\pi\pi}; m_{h^-h^+}^i)$ , the integral  $\int d\Phi_3(\tau)$ ,  
 6464 which also includes integration over  $m_{h^-h^+}$  as  $m_{h^-h^+}$  is included in  $\tau$ , does not run over the full  
 6465  $K^- \pi^- \pi^+$  phase space, but only over the range of the  $m_{h^-h^+}$  bin  $i$ .

6466 Analogously to the definition of the transition amplitudes in the conventional PWD, we combine  
 6467 all terms that appear in the model intensity [cf. equation (5.14)], except for the known freed  
 6468 decay amplitudes, to the so-called freed-isobar amplitudes

$$\begin{aligned}
 \mathfrak{T}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i) &\equiv \mathcal{T}_{a,i}^z(m_{K\pi\pi}, t') \\
 &= \mathcal{T}_a^z(m_{K\pi\pi}, t') / \sqrt{\mathfrak{N}_a(m_{K\pi\pi})} \\
 &\equiv \sqrt{\frac{\mathcal{L}}{(2\pi\mathfrak{F})^2}} \sqrt{m_{K\pi\pi}} \left\{ \sum_{k \in \mathbb{S}_a} \mathcal{P}_{k,a}^z(m_{K\pi\pi}, t') \mathcal{D}_k(m_{K\pi\pi}) \alpha_{k \rightarrow \xi bL} \right\} \alpha_\xi \\
 &\quad \times \sqrt{\mathfrak{N}_a(m_{K\pi\pi}; m_{h^-h^+}^i)} \\
 &\quad \times \mathfrak{D}_\xi^{\text{free}}(m_{h^-h^+}^i).
 \end{aligned} \tag{F.7}$$

6469 One should note that in contrast to the transition amplitude  $\mathcal{T}_a^z(m_{K\pi\pi}, t')$  defined in equation (5.15),  
 6470  $\mathfrak{T}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)$  also includes the dynamic amplitude  $\mathfrak{D}_\xi^{\text{free}}(m_{h^-h^+}^i)$  of the isobar resonance  
 6471 and hence also depends on  $m_{h^-h^+}$ . This means that at fixed  $(m_{K\pi\pi}, t')$ ,  $\mathfrak{T}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)$   
 6472 mainly<sup>[a]</sup> encodes the  $m_{h^-h^+}$  dependence of the dynamic amplitude of the isobar resonance  
 6473 times an  $(m_{K\pi\pi}, t')$  dependent scale and phase.

6474 In order to determine the freed-isobar amplitudes  $\{\mathfrak{T}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)\}$  from data, they are param-  
 6475 eterized by complex-valued piecewise functions, which are constant within each  $(m_{K\pi\pi}, t', m_{h^-h^+})$   
 6476 cell. We used the same binning in  $m_{K\pi\pi}$  and  $t'$  as used in the conventional PWD (see chap-  
 6477 ter 5). The bin widths in  $m_{h^-h^+}$  are given by the window functions  $\Theta(m_{h^-h^+}; m_{h^-h^+}^i)$  and listed in  
 6478 appendix F.2.

6479 In the conventional PWD, formulating  $\mathcal{T}_a^z(m_{K\pi\pi}, t')$  as piecewise constant functions in  $(m_{K\pi\pi}, t')$   
 6480 allowed us to analyze our data independently in  $(m_{K\pi\pi}, t')$  cells, because amplitudes from  
 6481 different  $(m_{K\pi\pi}, t')$  cells do not interfere. Here, the amplitudes of partial waves with isobars in  
 6482 different subsystems interfere at fixed  $m_{h^-h^+}$ . For example, amplitudes of partial waves with  
 6483  $K^- \pi^+$  isobar interfere at fixed  $m_{K^- \pi^+}$  with the amplitudes of partial waves with  $\pi^- \pi^+$  isobar at  
 6484 all  $m_{\pi^- \pi^+}$ , because fixing  $m_{K^- \pi^+}$  does not fix  $m_{\pi^- \pi^+}$ . Hence, the freed PWD cannot be performed  
 6485 independently in  $m_{h^-h^+}$  bins, but the full  $m_{h^-h^+}$  range of a given  $(m_{K\pi\pi}, t')$  cell has to be fit  
 6486 simultaneously in one PWD fit.

6487 The sum over the  $m_{h^-h^+}$  bins  $i$  and the sum over the partial waves  $a$  in the model intensity can be  
 6488 merged to one sum that runs over  $(a, i)$ , such that the model intensity of the freed isobar PWD  
 6489 reads<sup>[b]</sup>

$$\mathcal{I}^{\text{free}}(\tau, m_{K\pi\pi}, t') = \sum_z \left| \sum_{a,i} \mathcal{T}_{a,i}^z(m_{K\pi\pi}, t') \Psi_{a,i}(\tau, m_{K\pi\pi}) \right|^2. \tag{F.8}$$

<sup>[a]</sup> The wave-normalization integral  $\mathfrak{N}_a(m_{K\pi\pi}; m_{h^-h^+}^i)$  introduces only a smooth  $m_{h^-h^+}$  dependence in the freed-isobar amplitudes, e.g. the centrifugal-barrier factor  $F_{J_\xi}(m_{h^-h^+}^i)$  is included in  $\mathfrak{N}_a(m_{K\pi\pi}; m_{h^-h^+}^i)$ , because  $F_{J_\xi}(m_{h^-h^+}^i)$  is appearing in the corresponding freed decay amplitude.

<sup>[b]</sup> As discussed below, we freed only a single wave per freed-isobar PWD fit. Hence there is only one wave  $a$  where we additionally sum over  $i$ .

6490  $\mathcal{I}^{\text{free}}(\tau, m_{K\pi\pi}, t')$  has the same structure as  $\mathcal{I}(\tau, m_{K\pi\pi}, t')$  in the conventional PWD [see equa-  
 6491 tion (5.16)]. Therefore, the same likelihood formalism is used for the freed-isobar PWD as used  
 6492 for the conventional PWD and described section 5.1. However, because there is one freed-isobar  
 6493 amplitude per  $m_{h^-h^+}$  bin of each freed partial wave, the number of free parameters is drastically  
 6494 increased in the freed-isobar PWD.

6495 Given the limited size of our  $K^-\pi^-\pi^+$  sample, compared to e.g. the COMPASS  $\pi^-\pi^-\pi^+$  sample,  
 6496 we could not free the dynamic amplitudes of isobars in multiple partial waves in a single fit.  
 6497 Still, in order to perform proof-of-principle tests of the freed-isobar approach, we performed  
 6498 four independent freed-isobar PWDs, in which we studied the  $[\pi\pi]_P$  (see section 8.1),  $[K\pi]_P$  (see  
 6499 section 8.2),  $[K\pi]_D$  (see section 8.3), and  $[K\pi]_S$  (see section 8.4) amplitudes.

6500 In order to keep the number of free parameters at a manageable size, which still can be determined  
 6501 with our  $K^-\pi^-\pi^+$  sample of limited size, we used a spin-density matrix with rank=1 for this  
 6502 proof-of-principle tests of the freed-isobar PWD. Also, we did not perform Bootstrapping of the  
 6503 freed-isobar PWDs to keep the computational costs low, i.e. we used the maximum-likelihood  
 6504 estimates for the freed-isobar amplitudes and the corresponding covariance matrix in the RMFs  
 6505 discussed in appendix F.1.2.

## 6506 F.1.2 Resonance-Model Fit of Freed-Isobar Amplitudes

6507 In order to study the resonances appearing in the isobar subsystems and to measure their masses  
 6508 and widths, we performed RMFs of the extracted freed-isobar amplitudes. To this end, the  $m_{h^-h^+}$   
 6509 dependence of the freed-isobar amplitudes is modeled.

6510 The freed-isobar amplitudes are modeled using only resonance components. Analogously to  
 6511 equation (6.6), the corresponding modeled amplitudes read

$$\hat{\mathcal{Z}}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i) = \sqrt{\mathfrak{N}_a(m_{K\pi\pi}; m_{h^-h^+}^i) m_{K\pi\pi}} \mathcal{P}_P(m_{K\pi\pi}, t') \sum_{k \in \mathbb{S}_a} {}^k C_a^z(m_{K\pi\pi}, t') \mathcal{D}_k(m_{h^-h^+}^i; \zeta_k). \quad (\text{F.9})$$

6512 We used relativistic Breit-Wigner amplitudes according to equation (5.39) for the dynamic  
 6513 amplitudes  $\mathcal{D}_k(m_{h^-h^+}^i; \zeta_k)$  (see tables F.3 and F.4). Analogously to the  $t'$  dependence in the  
 6514 conventional RMF, the  $m_{K\pi\pi}$  and  $t'$  dependence is not explicitly modeled here, but the coupling  
 6515 amplitudes  ${}^k C_a^z(m_{K\pi\pi}, t')$  are modeled by piecewise constant functions in  $m_{K\pi\pi}$  and  $t'$ , i.e. there is  
 6516 an independent complex-valued parameter for each  $(m_{K\pi\pi}, t')$  cell for each coupling amplitude.

6517 In the  $\chi^2$  optimization, the modeled amplitude  $\hat{\mathfrak{T}}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)$  is directly compared to the  
 6518 measured amplitude  $\mathfrak{T}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)$ . To this end, the real-valued vector  $\vec{\mu}$  of the freed-isobar  
 6519 amplitudes is constructed. Its elements,

$$\mu_i(m_{K\pi\pi}, t') = \begin{cases} \Re\left(\mathfrak{T}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)\right) & , \text{ if } i \text{ is even} \\ \Im\left(\mathfrak{T}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)\right) & , \text{ if } i \text{ is odd,} \end{cases} \quad (\text{F.10})$$

6520 represent different  $m_{h^-h^+}$  bins.<sup>[c]</sup> Analogously, the corresponding RMF model quantities read

$$\hat{\mu}_i(m_{K\pi\pi}, t') = \begin{cases} \Re\left(\hat{\mathfrak{T}}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)\right) & , \text{ if } i \text{ is even} \\ \Im\left(\hat{\mathfrak{T}}_a^z(m_{K\pi\pi}, t'; m_{h^-h^+}^i)\right) & , \text{ if } i \text{ is odd} \end{cases} . \quad (\text{F.11})$$

6521 We fit the freed-isobar amplitudes from all four  $t'$  bins and from a chosen range in  $m_{K\pi\pi}$  (see  
 6522 table F.3) simultaneously in one RMF. With the above definitions, the corresponding  $\chi^2$  function  
 6523 reads

$$\chi_{\text{freed}}^2 = \sum_{t', m_{K\pi\pi}} \sum_{i, j} \Delta\mu_i(m_{K\pi\pi}, t') \text{Prec}[\mu_i(m_{K\pi\pi}, t'), \mu_j(m_{K\pi\pi}, t')] \Delta\mu_j(m_{K\pi\pi}, t'). \quad (\text{F.12})$$

6524 Here,

$$\Delta\mu_i(m_{K\pi\pi}, t') = \mu_i(m_{K\pi\pi}, t') - \hat{\mu}_i(m_{K\pi\pi}, t') \quad (\text{F.13})$$

6525 is the residual between the measured freed-isobar amplitude and the corresponding RMF model  
 6526 quantity, and  $\text{Prec}[\mu_i, \mu_j]$  is the precision matrix, i.e. the inverse of the covariance matrix of the  
 6527 freed-isobar amplitudes as obtained from the freed-isobar PWD.<sup>[d]</sup>

## 6528 F.2 Bin Widths used in the Freed-Isobar Partial-Wave 6529 Decomposition

6530 Table F.1 lists the bin widths in two-body mass  $m_{h^-h^+}$  of the piecewise constant freed-isobar  
 6531 amplitudes in the various two-body mass ranges as used in the freed-isobar analysis discussed  
 6532 in chapter 8. The lowest and highest  $m_{h^-h^+}$  bins are chosen wider than the bin width given in  
 6533 table F.1, so that the analyzed range corresponds to the full  $m_{h^-h^+}$  range. The lower border of the  
 6534 lowest  $m_{h^-h^+}$  bin is given by the sum of the masses of the two final-state particles in the isobar

<sup>[c]</sup> We dropped the partial wave label  $a$  and the coherent sector label  $z$  for  $\mu_i$ , because we freed only one partial wave per freed-isobar fit, and because we used a rank=1 model in the freed PWDs.

<sup>[d]</sup> We used the maximum-likelihood estimates for the freed-isobar amplitudes and the corresponding covariance matrix. As the real and imaginary parts of the freed-isobar amplitudes are the free parameters in the PWD fits, error propagation is not necessary to obtain the corresponding covariance matrix, in contrast to the covariance matrix of the spin-density matrix elements. Hence, Bootstrapping is not essential for the freed-isobar PWDs.

6535 system, i.e.  $m_{K^-\pi^+/\pi^-\pi^+}^{\min} = m_{K^-/\pi^-} + m_{\pi^+}$ , rounded down to a precision of three decimal digits.  
 6536 The upper border of the highest  $m_{h^-h^+}$  bin is given by the upper border of the analyzed  $m_{K\pi\pi}$   
 6537 range minus the mass of the bachelor particle, i.e.  $m_{K^-\pi^+/\pi^-\pi^+}^{\max} = 3 \text{ GeV}/c^2 - m_{\pi^-/K^-}$ , rounded up  
 6538 to a precision of three decimal digits. This rounding ensures that the bins cover the full analyzed  
 6539 two-body mass range including numerical effects. For example, the first bin for the  $[\pi\pi]_P$  isobar  
 6540 amplitude (see table F.2a) ranges from 0.279 to 0.320  $\text{GeV}/c^2$  and the last bin ranges from 2.440  
 6541 to 2.506  $\text{GeV}/c^2$ .

### 6542 F.3 Isobar Resonances included in the Resonance-Model Fits

6543 In order to study the resonance content of the measured freed-isobar amplitudes we performed  
 6544 independent RMFs of the  $[\pi\pi]_P$ ,  $[K\pi]_P$ , and  $[K\pi]_D$  isobar amplitudes. Table F.3 lists the  
 6545 resonance components and fit ranges used in these RMFs. The lower limits for the  $m_{\pi^-\pi^+}$  and  
 6546  $m_{K^-\pi^+}$  fit ranges are given by the corresponding phase-space border. The upper limits are chosen  
 6547 to include only the  $m_{\pi^-\pi^+}$  or  $m_{K^-\pi^+}$  range of the corresponding ground state isobar resonance.  
 6548 Table F.4 lists the mass and width parameter limits and start parameter ranges of the resonance  
 6549 components included in these RMFs.

Table F.1: Bin widths of the piecewise constant freed-isobar amplitudes in the various two-body mass ranges for (a) the  $[\pi\pi]_P$ , (b) the  $[K\pi]_P$ , (c) the  $[K\pi]_D$ , and (d) the  $[K\pi]_S$  isobar amplitudes as used in the freed-isobar analyses discussed in chapter 8. Note that the lowest and highest  $m_{h^-h^+}$  bins are wider than the given bin width (see text).

(a)  $[\pi\pi]_P$

$m_{\pi^-\pi^+}$ Range	$m_{\pi^-\pi^+}$ Bin Width
0.279 to 0.640 GeV/ $c^2$	40 MeV/ $c^2$
0.640 to 0.920 GeV/ $c^2$	20 MeV/ $c^2$
0.920 to 2.506 GeV/ $c^2$	40 MeV/ $c^2$

(b)  $[K\pi]_P$

$m_{K^-\pi^+}$ Range	$m_{K^-\pi^+}$ Bin Width
0.633 to 0.800 GeV/ $c^2$	20 MeV/ $c^2$
0.800 to 1.000 GeV/ $c^2$	10 MeV/ $c^2$
1.000 to 1.720 GeV/ $c^2$	20 MeV/ $c^2$
1.720 to 2.861 GeV/ $c^2$	40 MeV/ $c^2$

(c)  $[K\pi]_D$

$m_{K^-\pi^+}$ Range	$m_{K^-\pi^+}$ Bin Width
0.633 to 1.120 GeV/ $c^2$	40 MeV/ $c^2$
1.120 to 1.720 GeV/ $c^2$	20 MeV/ $c^2$
1.720 to 2.861 GeV/ $c^2$	40 MeV/ $c^2$

(d)  $[K\pi]_S$

$m_{K^-\pi^+}$ Range	$m_{K^-\pi^+}$ Bin Width
0.633 to 2.861 GeV/ $c^2$	40 MeV/ $c^2$

Table F.3: Model components and fit ranges of the RMFs to the freed-isobar amplitudes. The first column lists the freed-isobar amplitude. The second column lists the isobar resonance components included in the RMF model. They are specified in table F.4. The next double-column lists the  $m_{\pi^- \pi^+}$  or  $m_{K^- \pi^+}$  range in which the data from this partial wave are considered in the RMF. The last double-column lists the  $m_{K\pi\pi}$  range in which the data from this partial wave is considered in the RMF.

Isobar Amplitude	Resonance	$m_{\pi^- \pi^+ / K^- \pi^+}$ Range [GeV/ $c^2$ ]		$m_{K\pi\pi}$ Range [GeV/ $c^2$ ]	
$[\pi\pi]_P$	$\rho(770)$	0.279	1.000	1.1	2.5
$[K\pi]_P$	$K^*(892)$	0.633	1.100	1.1	2.5
$[K\pi]_D$	$K_2^*(1430)$	0.633	1.600	1.4	3.0

Table F.4: Resonance components included in the RMFs of the freed-isobar amplitudes (given in the first column). Furthermore, we list the fit-parameter limits and start-parameter ranges (see text) for the mass and width parameters. The last column gives the decay mode that we assumed for the dynamic width of the resonance in equation (5.40), where the first two letter give the daughter particles and last letter gives the angular orbital momentum between the daughter particles.

Isobar Amplitude	Resonance	Parameter	Limits [MeV/ $c^2$ ]		Start Ranges [MeV/ $c^2$ ]		Decay
$[\pi\pi]_P$	$\rho(770)$	$m_0$	600	900	765	780	$\pi \pi P$
		$\Gamma_0$	80	600	140	150	
$[K\pi]_P$	$K^*(892)$	$m_0$	700	1100	850	950	$K \pi P$
		$\Gamma_0$	10	600	40	60	
$[K\pi]_D$	$K_2^*(1430)$	$m_0$	1300	1500	1425	1435	$K \pi D$
		$\Gamma_0$	80	600	105	115	



## G Systematic Studies

### G.1 Partial-Wave Decomposition

#### G.1.1 The Information-Field-Theory Model

In section 5.7.2, we describe a study in which we selected a wave set for the PWD using a method based on information field theory (IFT) in order to suppress insignificant waves and to impose continuity of the wave set in  $m_{K\pi\pi}$ . This IFT wave-set selection is an alternative to the regularization methods presented in sections 5.2.2 and 5.2.3. In the IFT wave-set selection, the four  $t'$  bins were treated independently, as in the main analysis. IFT is a Bayesian probability theory. Therefore, the quantity we determined in each  $t'$  bin is the probability distribution of the transition amplitudes  $\{\mathcal{T}_a^z(m_{K\pi\pi})\}$  in all  $m_{K\pi\pi}$  bins given the measured  $K^-\pi^-\pi^+$  sample  $\{\nu\}$ . Using Bayes formula this posterior probability reads<sup>[a]</sup>

$$P(\{\mathcal{T}_a^z(m_{K\pi\pi})\} | \{\nu\}) = \frac{P(\{\nu\} | \{\mathcal{T}_a^z(m_{K\pi\pi})\})}{P(\{\nu\})} P_0(\{\mathcal{T}_a^z(m_{K\pi\pi})\}). \quad (\text{G.1})$$

Here,  $P(\{\nu\})$  is the evidence. The probability  $P(\{\nu\} | \{\mathcal{T}_a^z(m_{K\pi\pi})\})$  of the measured  $K^-\pi^-\pi^+$  sample given the transition amplitudes incorporates the information from the data. It is given by the product over the likelihoods  $\mathcal{L}_{\text{PWD}}(\{\mathcal{T}_a^z(m_{K\pi\pi})\}; \{\nu\}_{m_{K\pi\pi}})$  defined in equation (5.33) of all  $m_{K\pi\pi}$  bins:

$$P(\{\nu\} | \{\mathcal{T}_a^z(m_{K\pi\pi})\}) = \prod_{m_{K\pi\pi}} \mathcal{L}_{\text{PWD}}(\{\mathcal{T}_a^z(m_{K\pi\pi})\}; \{\nu\}_{m_{K\pi\pi}}). \quad (\text{G.2})$$

We considered only the  $K^-\pi^-\pi^+$  sample from the 2008 diffraction data set, because handling of multiple data sets was not easily implementable in the IFT framework and thus not feasible in the IFT systematic study.

The prior probability  $P_0(\{\mathcal{T}_a^z(m_{K\pi\pi})\})$  encodes the prior knowledge about the transition amplitudes. Here, we implemented our knowledge about the continuity of the transition amplitudes as a function of  $m_{K\pi\pi}$  and the condition to suppress insignificant waves. We formulated independent prior terms for the transition amplitudes of each wave  $a$ , i.e.

$$P_0(\{\mathcal{T}_a^z(m_{K\pi\pi})\}) = \prod_a P_a(\vec{\mathcal{T}}_a^z). \quad (\text{G.3})$$

<sup>[a]</sup> We drop the  $t'$  dependence here for simplicity since we treated the four  $t'$  bins independently.

6572 Here,  $\vec{\mathcal{T}}_a^z$  is the vector of the 100 transition amplitudes in the 100  $m_{K\pi\pi}$  bins of wave  $a$  in the  
6573 coherent sector  $z$ ,<sup>[b]</sup> i.e. the  $k$ th component of this vector is<sup>[c]</sup>

$$[\vec{\mathcal{T}}_a^z]_k = \mathcal{T}_a^z(m_{K\pi\pi,k}), \quad (\text{G.4})$$

6574 where  $m_{K\pi\pi,k}$  is the mass at the position of the  $k$ th  $m_{K\pi\pi}$  bin. As in the main analysis, we used a  
6575 rank=1 PWD model for the wave-set selection fits in the IFT study. We drop the sector label  $z$   
6576 from now on, because each transition amplitude is uniquely labeled by the wave label  $a$ .

6577 In the prior, the correlation between transition amplitudes of wave  $a$  at different  $m_{K\pi\pi}$  locations  
6578 is represented by the covariance matrix:

$$[C_a]_{kl} = \mathfrak{C}_a(m_{K\pi\pi,k}, m_{K\pi\pi,l}). \quad (\text{G.5})$$

6579 Here,  $\mathfrak{C}_a(m_{K\pi\pi,k}, m_{K\pi\pi,l})$  is the two-point correlation function.

6580 In order to formulate the prior probability, we perform the Fourier transformation,

$$\vec{\mathcal{T}}'_a = \mathcal{F} \{ \vec{\mathcal{T}}_a \}, \text{ with } [\vec{\mathcal{T}}'_a]_i = \mathcal{T}'_a(\omega_i), \quad (\text{G.6})$$

6581 of the transition amplitudes from the  $m_{K\pi\pi}$  space of mass bins to the corresponding Fourier space  
6582  $\vec{\omega}$ . The corresponding probability  $P'_a(\vec{\mathcal{T}}'_a)$  of the Fourier-transformed transition amplitudes has  
6583 the covariance matrix  $C'_a$ . Assuming statistical homogeneity for the transition amplitudes, i.e.

$$\mathfrak{C}_a(m_{K\pi\pi,i}, m_{K\pi\pi,j}) = \mathfrak{C}_a(m_{K\pi\pi,i} - m_{K\pi\pi,j}), \quad (\text{G.7})$$

6584 the covariance matrix in the Fourier space,

$$\mathfrak{C}_a(\omega_i, \omega_j) = [C'_a]_{ij} = \delta_{ij} \left( [\vec{\sigma}_a]_i \right)^2, \quad (\text{G.8})$$

6585 is diagonal [184]. This means that the Fourier-transformed transition amplitudes are independent.  
6586 Hence, they can be expressed in terms of uncorrelated random variables  $\vec{\xi}_a$ , which have a standard  
6587 deviation of one, i.e.

$$[\vec{\mathcal{T}}'_a]_i = [\vec{\sigma}_a]_i [\xi_a]_i \quad (\text{G.9})$$

6588 The form of the prior probability in terms of  $\vec{\xi}_a$  still has to be chosen. The  $\vec{\xi}_a$  represent the  
6589 Fourier-transformed transition amplitudes. Asymptotically, their probability distribution becomes  
6590 a Gaussian distribution under certain conditions (see Theorem 4.4.2 in ref. [185]). Thus, we used  
6591 a Gaussian standard distribution,

$$P_0(\vec{\xi}_a) = \mathcal{N}(\vec{\xi}_a; \mathbf{0}, \mathbb{1}), \quad (\text{G.10})$$

<sup>[b]</sup> In this study, we used an equidistant binning in the full  $m_{K\pi\pi}$  range with a bin width of 20 MeV/ $c^2$ , because using different  $m_{K\pi\pi}$  bin widths as done in the main analysis could not easily be implemented in the IFT framework.

<sup>[c]</sup> In this section, we use the notation of a vector or matrix in rectangular bracket with the index in the subscript to indicate a single element of the vector or matrix that corresponds to the given index.

6592 as prior probability for  $\vec{\xi}_a$ .<sup>[d]</sup> This prior probability has a standard deviation of one, as required  
 6593 by the construction of  $\vec{\xi}_a$ , and a mean of zero in order to suppress insignificant waves.

6594 However, the standard deviations  $[\vec{\sigma}_a]_i$  that correspond to the frequency  $\omega_i$  in Fourier space  
 6595 need to be constrained. Since we assume continuity of the transition amplitudes in  $m_{K\pi\pi}$ , high  
 6596 frequencies, which correspond to fluctuations of the transition amplitudes from bin to bin, are  
 6597 less probable in the prior compared to low frequencies. Thus,  $[\vec{\sigma}_a]_i$  should be smaller for larger  
 6598  $\omega_i$ . Based on previous experiences from ref. [127], we used a power-law spectrum in order to  
 6599 suppress high frequencies, which reads

$$[\vec{\sigma}_a]_i = \alpha_a \cdot |\omega_i|^{-\beta_a} \quad \text{for } i \neq 0. \quad (\text{G.11})$$

6600 As equation (G.11) diverges for  $\omega_0 = 0$ , we used a constant  $\gamma_a$  for the zeroth component of the  
 6601 standard deviation, i.e.

$$[\vec{\sigma}_a]_0 = \alpha_a \cdot \gamma_a. \quad (\text{G.12})$$

6602 Here,  $\alpha_a$ ,  $\beta_a$ , and  $\gamma_a$  are three additional free hyperparameters per partial wave  $a$ , which we  
 6603 introduced in our formulation of the prior probability. In contrast to the Cauchy regularization in  
 6604 equation (5.55) and the continuity term in equation (5.57), which each have only one parameter  
 6605 common to all partial waves; in the IFT study the usage of independent parameters for each wave  
 6606 introduces additional adaptability in the wave-set selection. However, a much larger number of  
 6607 hyperparameters needs to be determined. Instead of choosing the hyperparameters, we inferred  
 6608 them from data using hyperpriors to constrain them. For  $\beta_a$ , we used a Gaussian hyperprior,  
 6609 i.e.

$$P_0(\beta_a) = \mathcal{N}(\beta_a; \mu_\beta, \sigma_\beta), \quad (\text{G.13})$$

6610 with  $\mu_\beta = 0.9$  and  $\sigma_\beta = 0.01$  common to all waves. These parameters were chosen based on  
 6611 recommendations from ref. [127]. The parameters  $\alpha_a$  set the scales of the standard deviations  
 6612 of the Fourier-transformed transition amplitudes and thus relate to the scales of the transition  
 6613 amplitudes. As discussed in section 5.2.2, the overall scale of the transition amplitudes spans up  
 6614 to five orders of magnitude. To take this into account, we assumed a log-Gaussian hyperprior for  
 6615  $\alpha_a$ , i.e.

$$P_0(\ln \alpha_a) = \mathcal{N}(\ln \alpha_a; \mu_{\ln \alpha}, \sigma_{\ln \alpha}), \quad (\text{G.14})$$

6616 with  $\mu_{\ln \alpha} = -1$ . and  $\sigma_{\ln \alpha} = 0.1$  common to all waves. We fixed the parameter  $\gamma_a$  to a value of  
 6617 1.0 for all waves. These parameters were chosen based on recommendations from ref. [127].  
 6618 Tests using a free  $\gamma_a$  with a log-Gaussian hyperprior did not yield improved fit results, but the fits  
 6619 were much more unstable.

<sup>[d]</sup> Note that  $\vec{\xi}_a$  is actually a vector of complex-valued components. We used independent Gaussian priors for the real part and the imaginary part of these components. This can be done, because in the Fourier space the individual components are independent assuming statistical homogeneity, because the Fourier transformation is a linear operation and hence acts individually on the real part and the imaginary part of the transition amplitudes, and because we do not assume any correlation between the real part and the imaginary part of the transition amplitudes in the prior probability.

6620 In summary, we formulated the prior probability in terms of the Fourier-transformed transition  
 6621 amplitudes as a standard Gaussian distribution in  $\vec{\xi}_a$  centered around zero. As the prior is centered  
 6622 around zero, it suppresses insignificant waves. The standard deviation of the Fourier-transformed  
 6623 transition amplitudes and thereby the strength of the suppression of the corresponding waves is  
 6624 individually adjusted for each wave to the data, because we modeled the standard deviations by a  
 6625 power-law spectrum with individual hyperparameters for each wave. Therefore, the bias from  
 6626 regularization and imposing continuity in the prior probability is potentially reduced compared  
 6627 to the Cauchy and continuity terms used in the main analysis.

6628 The final posterior probability of the IFT wave-set selection in a given  $t'$  bin reads:

$$P(\{\mathcal{T}_a(m_{K\pi\pi})\}, \{\ln \alpha_a\}, \{\beta_a\} | \{v\}) = \frac{P(\{v\} | \{\mathcal{T}_a^z(m_{K\pi\pi})\})}{P(\{v\})} \prod_a P_0(\vec{\xi}_a) P_0(\ln \alpha_a) P_0(\beta_a) J_a. \quad (\text{G.15})$$

6629 Using equations (G.6), (G.9), (G.11), and (G.12), the transition amplitudes,<sup>[e]</sup>

$$\vec{\mathcal{T}}_a = \mathcal{F}^{-1} \{ \vec{\sigma}_a(\ln \alpha_a, \beta_a) \cdot \vec{\xi}_a \}, \quad (\text{G.16})$$

6630 of the  $N_{\text{waves}}$  partial waves can be expressed in terms of the free parameters of the IFT model,  
 6631 i.e. the number of waves times the number of  $m_{K\pi\pi}$  bins parameters  $[\vec{\xi}_a]_i$ , which represent the  
 6632 Fourier coefficients; the  $N_{\text{waves}}$  parameters  $\ln \alpha_a$ , which give a scale to the standard deviations of  
 6633 the transition amplitudes in the Fourier space; and the  $N_{\text{waves}}$  parameters  $\beta_a$ , which represent the  
 6634 slope of the power-law spectrum. The Jacobian term  $J_a$  appears in equation (G.15) arises from  
 6635 this variable transformation.

6636 We used the Python software NIFTy [129] to implement the posterior probability in equa-  
 6637 tion (G.15). NIFTy allows us to formulate the posterior probability as a generative model, i.e. to  
 6638 construct the transition amplitudes according to equation (G.16) from the free parameters  $\{\vec{\xi}_a\}$ ,  
 6639  $\{\ln \alpha_a\}$ , and  $\{\beta_a\}$  in a bottom-up approach. The Jacobian  $J_a$  from the variable transformation and  
 6640 the prior probabilities are calculated automatically.

6641 Given the complexity of the model and the computational expensive evaluation of the likelihood  
 6642 function in equation (G.2), a full study of the posterior probability distribution in equation (G.15)  
 6643 was not feasible. Thus, we performed a maximum-a-posteriori fit to determine the IFT estimates  
 6644 for the transition amplitudes, i.e. we optimized the free parameters of the IFT model such that  
 6645 they minimize equation (G.15).<sup>[f]</sup> In addition, it was sufficient to perform only a maximum-a-  
 6646 posteriori fit, because we used the result of the IFT wave-set selection only to determine whether  
 6647 a wave significantly contributes to the data and should be included in the wave set.

<sup>[e]</sup> Here, we use the short-hand notation  $[\vec{\sigma}_a(\ln \alpha_a, \beta_a) \cdot \vec{\xi}_a]_i = [\vec{\sigma}_a(\ln \alpha_a, \beta_a)]_i \cdot [\vec{\xi}_a]_i$  for the vector that is Fourier back-transformed.

<sup>[f]</sup> As the evidence  $P(\{v\})$  does not depend on the fit parameters, it was neglected in the maximum a posteriori fits.

6648 **G.1.2 Summary of Systematic Studies of the Partial-Wave Decomposition**

6649 In this section, we show a comparison of the results from systematic studies and from the  
 6650 main analysis for all partial waves that are discussed in this work. Figure G.1 shows the  $t'$ -  
 6651 summed intensity spectra of the partial waves that are included in the 10-wave RMF discussed in  
 6652 section 6.2. Figure G.2 shows further waves that are not affected by the leakage effect. Figure G.3  
 6653 shows the  $t'$ -summed intensity spectra of partial waves that are affected by the leakage effect.

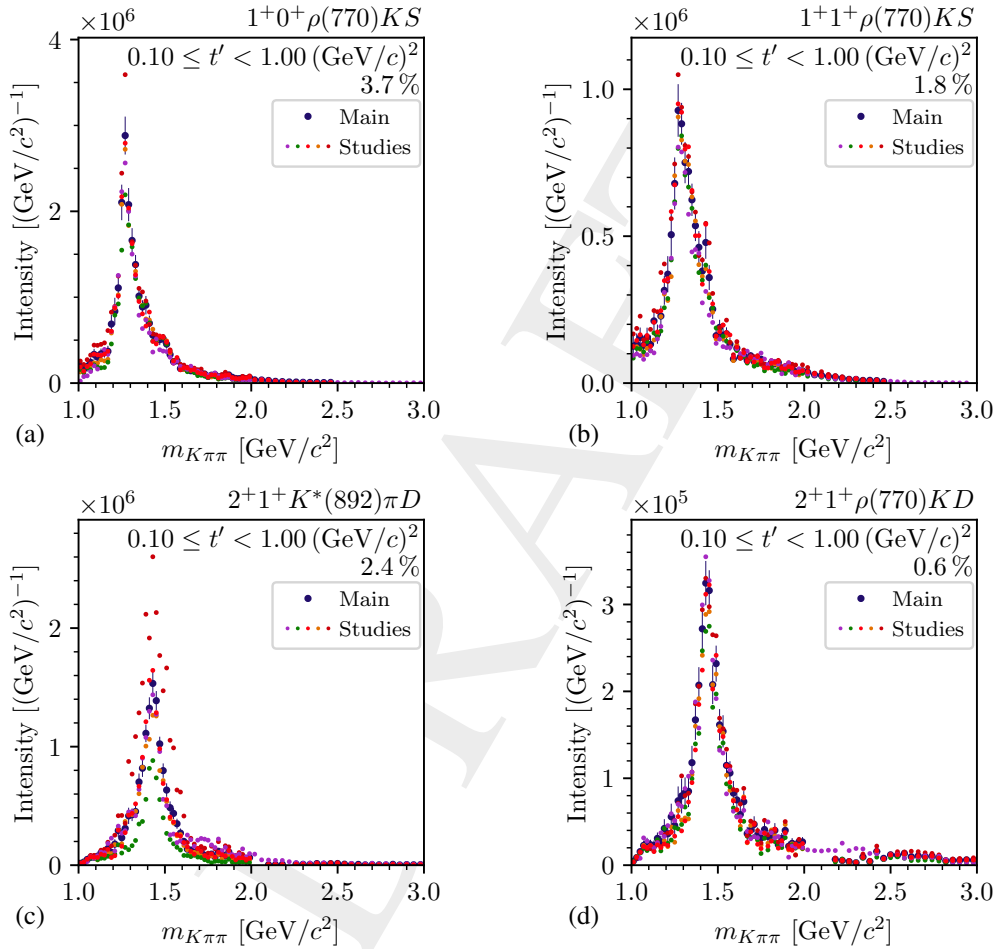


Figure G.1: Comparison of the results from various systematic studies and from the main analysis for partial waves that are included in the 10-wave RMF discussed in section 6.2. The large blue data points show the Bootstrapping estimates from the main analysis. The small differently-colored data points show the maximum-likelihood estimates from the various systematic studies. The violet data points show the study using the wave set constructed from the IFT wave-set selection fits (see section 5.7.2). The light red data points show the study without the  $3^+ 1^+ K^*(892)\pi D$  wave in the range  $m_{K\pi\pi} < 1.7 \text{ GeV}/c^2$  (see section 5.9). The green, red, and orange data points show the studies with a weaker RICH threshold of  $\mathcal{T}_R = 1.05$ , with a more restrictive RICH threshold of  $\mathcal{T}_R = 1.30$ , and with a more restrictive momentum limit of  $40 \text{ GeV}/c$  for final-state particle identification; respectively (see section 5.7.1). We do not show uncertainties for the maximum-likelihood estimates from the systematic studies (see section 5.7).

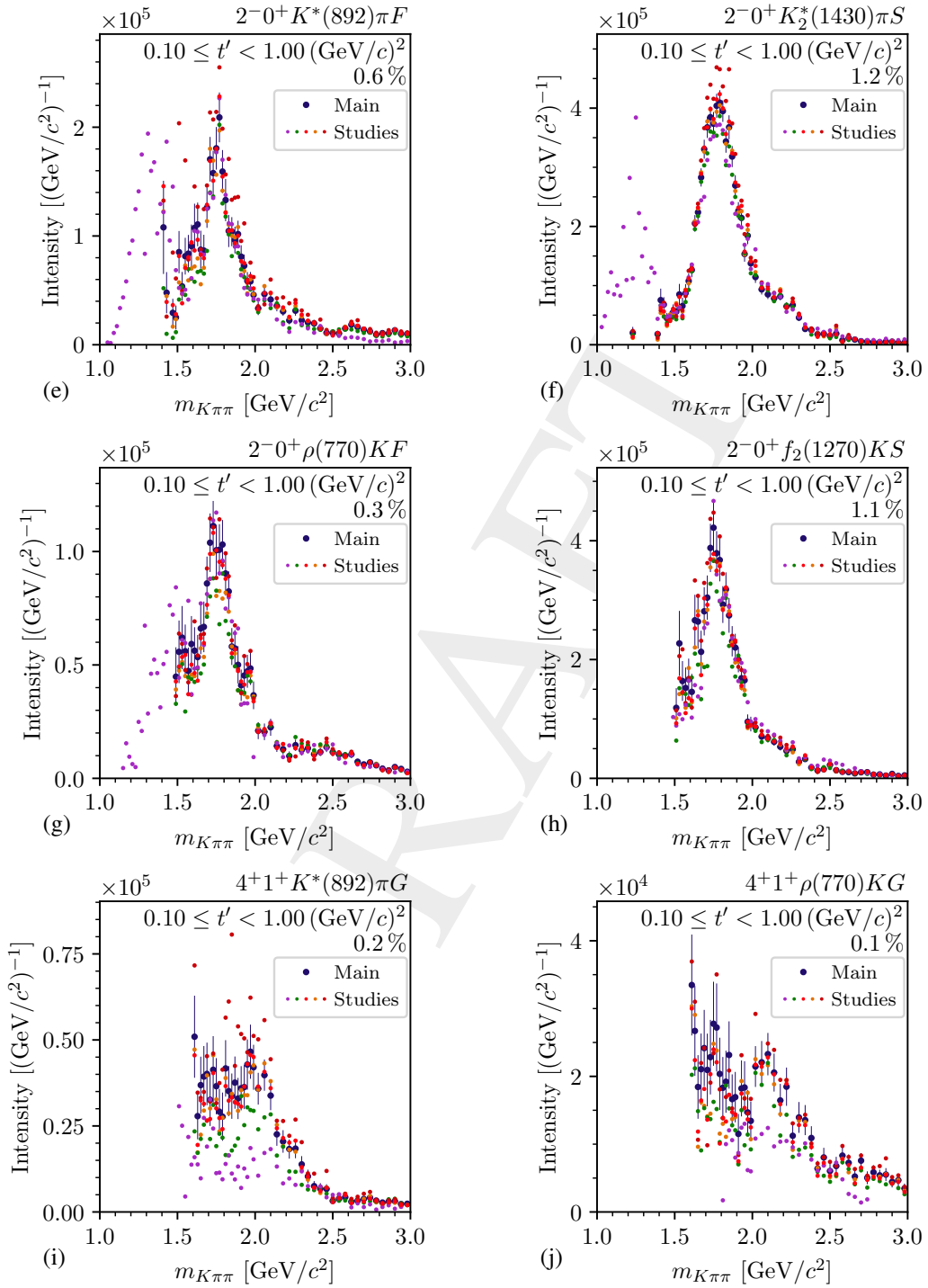


Figure G.1: Continued

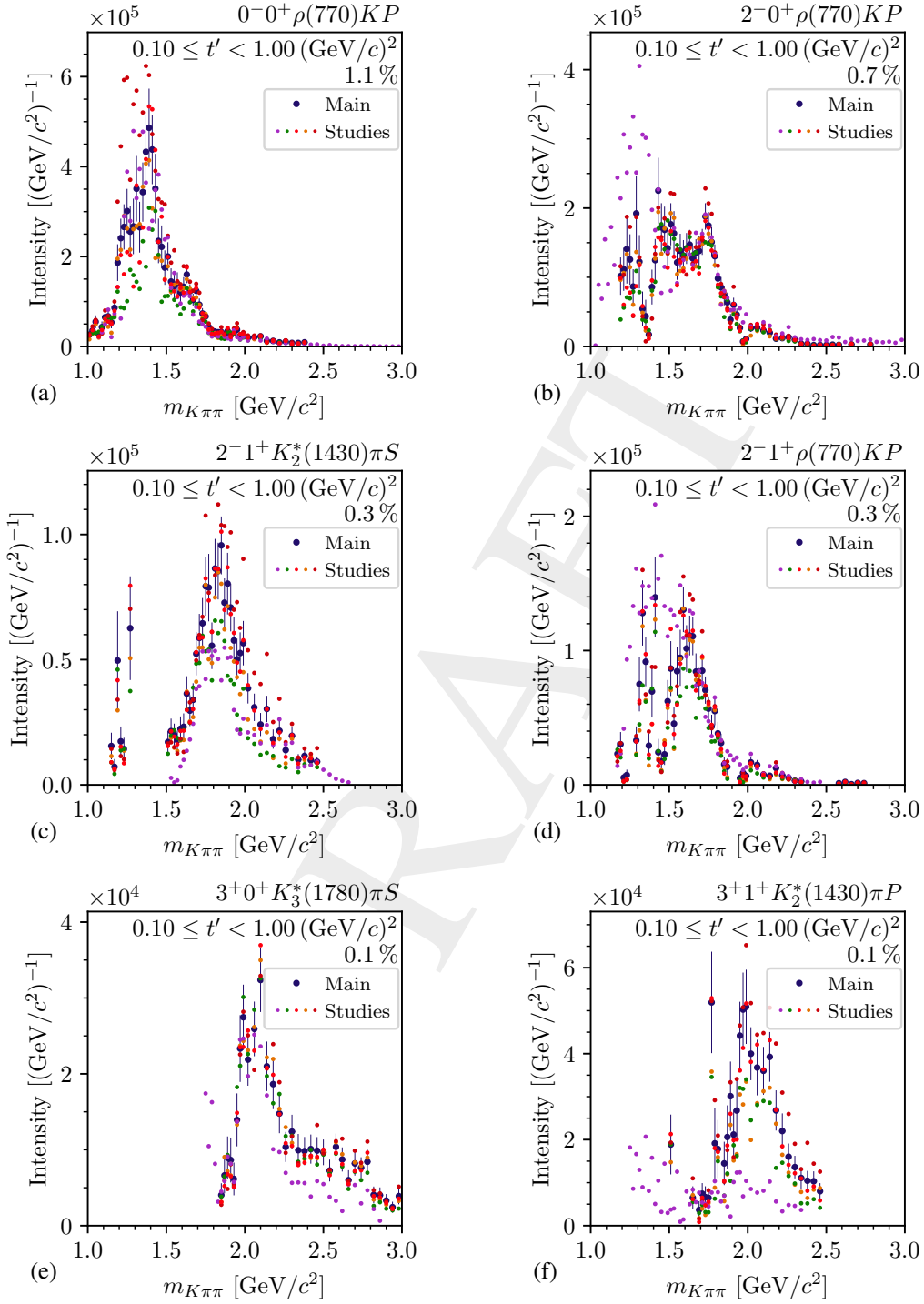


Figure G.2: Same as figure G.1 but for the partial waves that are not included in the 10-wave RMF and not affected by the leakage effect.

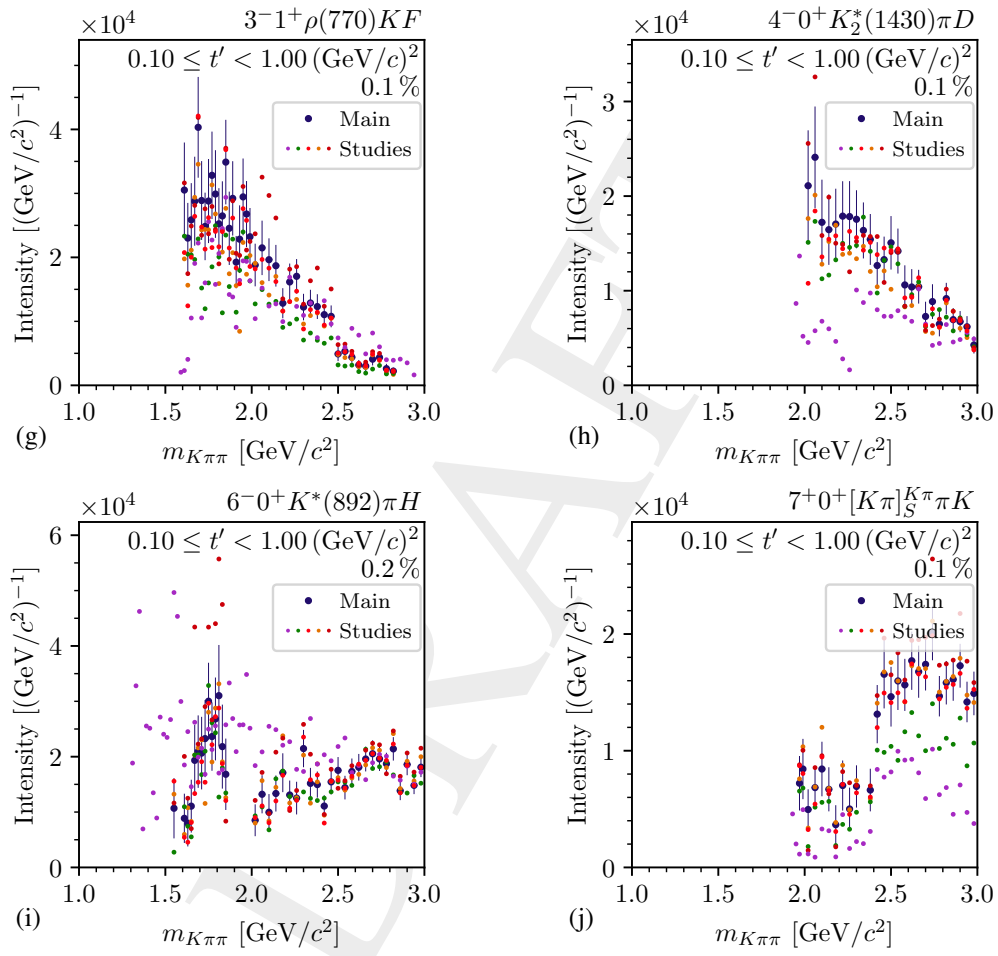


Figure G.2: Continued



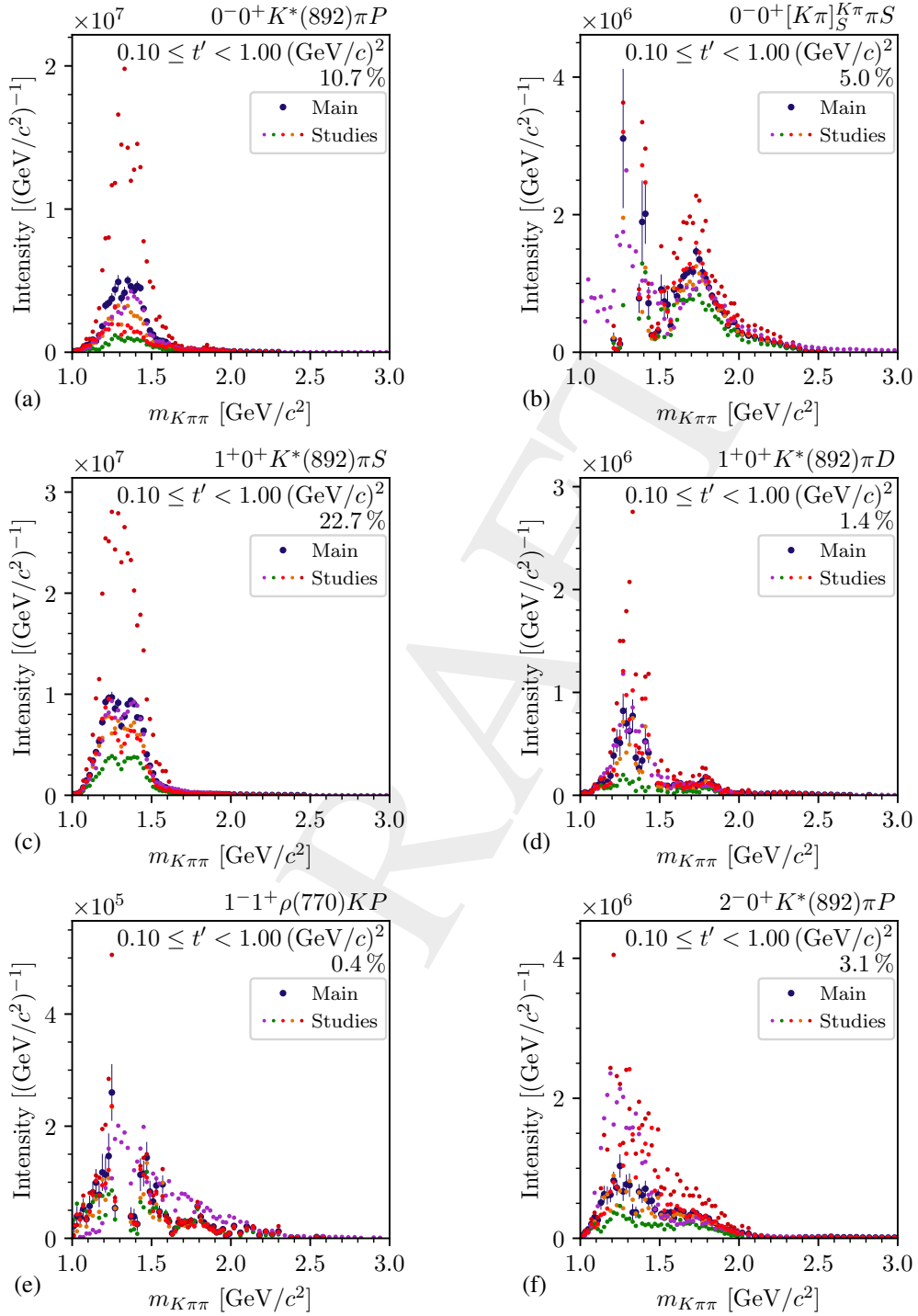


Figure G.3: Same as figure G.1 but for the partial waves that are affected by the leakage effect.

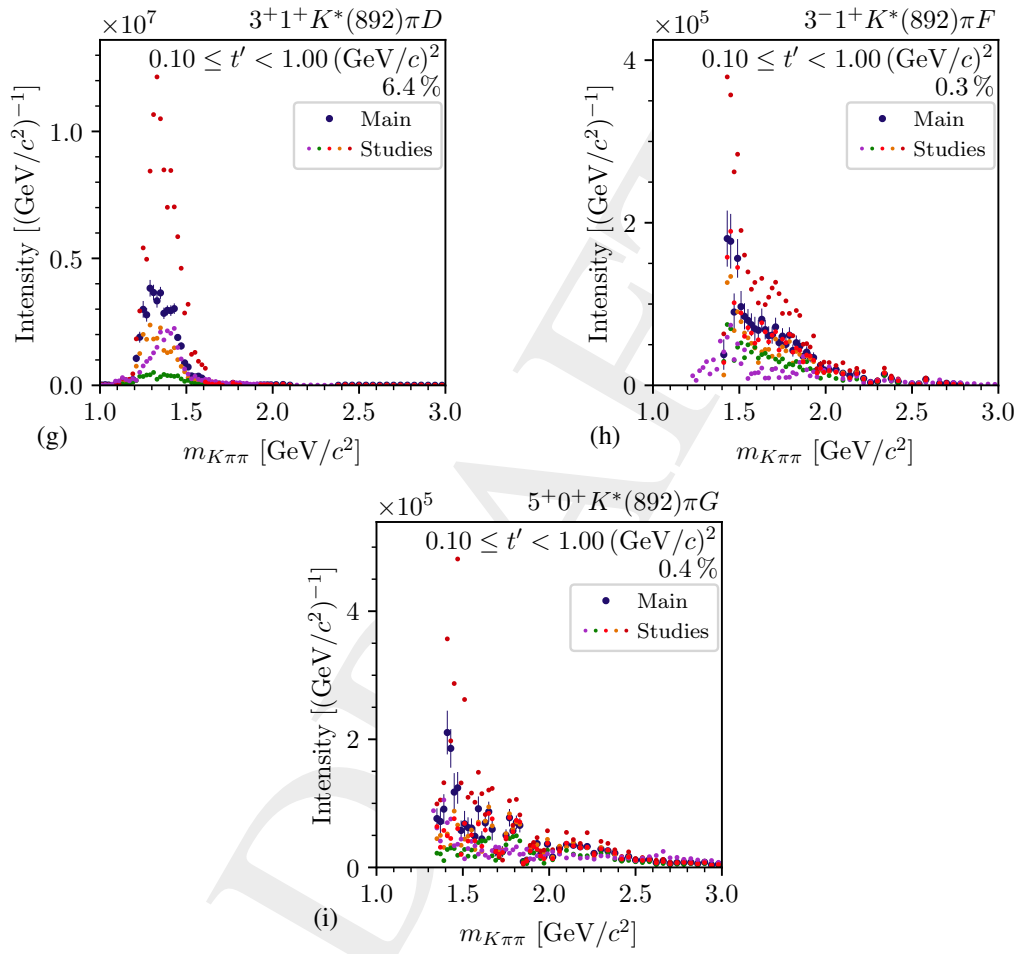


Figure G.3: Continued

## H Software Stack

Table H.1: List of the most important software frameworks used in this analysis. The first column gives the name, the second column a short description of the framework. The third column lists the most important sections for which this framework was used. The last column gives the reference to the framework.

Name	Description	See	Ref.
CORAL	COMPASS software for event reconstruction from raw detector data	2.2	[53]
PHAST	Software for event selection used for the preselection	4.1	[186]
Antok	Software for event selection and to create plots of kinematic distributions used for the final $K^- \pi^- \pi^+$ event selection	4.1	[187]
CEDAR Helper	Library for the CEDAR likelihood approach and the corresponding calibration tools	3.1	[188]
RPD Helper	Library to use the information from the recoil-proton detector	4.1	[189]
COMGEANT	COMPASS detector simulation software based on Geant3	C.2	[190]
ROOTPWA	Toolkit for partial-wave analysis of multi-particle final states used for all PWDs, which uses the NLOpt package [85] to perform the negative log-likelihood minimization	5, 8	[191]
ROOTPWAtools	Collection of additional tools for PWDs using ROOTPWA	5, 8	[192]
sfitter	Toolkit for resonance-model fits used for all RMFs, which uses iminuit [143] to perform the $\chi^2$ minimization	6, 8	[193]
batchelor	Toolkit for job submission on computing clusters	4.1, 5, 6, 8	[194]
modernplotting	Software to create plots for high-energy physics; based on matplotlib [195]	all	[196]
RPWAplotting	Software to create plots of partial-wave analysis results; based on modernplotting	5, 6, 8	[197]



## 6655 Glossary

6656 **Numbers** | **A** | **B** | **C** | **D** | **E** | **F** | **G** | **H** | **I** | **K** | **L** | **M** | **N** | **O** | **P** | **R** | **S** | **T** | **W**

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## Own Contributions

7633

7634 My analysis of the reaction  $K^- + p \rightarrow K^- \pi^- \pi^+ + p$  at COMPASS is based on a previous  
7635 unpublished COMPASS analysis by P. Jasinski [44], where a first event selection and a PWD  
7636 were performed using only a subset of the COMPASS data. My analysis also relies on the  
7637 experience gained in the COMPASS  $\pi^- \pi^- \pi^+$  analysis [11, 38–41, 80].

7638 I extended, improved, and fine-tuned the existing event selection for the  $K^- \pi^- \pi^+$  sample in many  
7639 regards. For example, I performed a preselection for events with three charged final-state particles,  
7640 which is used in many other COMPASS analyses [43, 62, 65, 66]. Especially noteworthy, I  
7641 developed, implemented, and verified a novel approach for beam-particle identification using  
7642 the full information from both CEDAR detectors, based on first ideas from C. Bicker. To this  
7643 end, I formulated a coordinate transformation, which is the heart of this approach and which  
7644 allowed me to calibrate the employed likelihood function without relying on pure beam-kaon  
7645 and beam-pion calibration samples. Compared to the previously used approach, I doubled the  
7646 efficiency for beam-kaon identification and thereby doubled the size of the  $K^- \pi^- \pi^+$  sample. In  
7647 addition, I increased the  $K^- \pi^- \pi^+$  sample size by almost another factor of two, compared to the  
7648 existing COMPASS  $K^- \pi^- \pi^+$  sample [44], by using the full COMPASS data set, which consists  
7649 of data from two data taking campaigns (2008 and 2009) with slightly different experimental  
7650 acceptances, which I had to take into account.

7651 Based on this  $K^- \pi^- \pi^+$  sample, I performed a partial-wave decomposition (PWD). I made  
7652 significant contributions to the PWD software framework ROOTPWA [191]. For the first time  
7653 for the  $K^- \pi^- \pi^+$  sample, I applied model-selection techniques to determine an optimal wave  
7654 set. In close collaboration with F. Kaspar, who worked on the wave-set selection for  $\pi^- \pi^- \pi^+$ , I  
7655 extended the wave-set selection approach developed in previous COMPASS analyses [67, 108]  
7656 by taking into account acceptance effects and by imposing continuity in  $m_{K\pi\pi}$ . Furthermore, I  
7657 applied, for the first time at COMPASS, Bootstrapping techniques starting at the event-sample  
7658 level to propagate uncertainties up to the PWD level. In addition, I developed and implemented in  
7659 ROOTPWA an approach to simultaneously fit multiple data samples with different experimental  
7660 acceptances. To this end, I generated large data samples using the COMPASS detector Monte  
7661 Carlo simulation.

7662 During the analysis, I observed analysis artifacts in some partial waves. I could trace back the  
7663 origin of these artifacts to the leakage effect, which is caused by the limited kinematic range of  
7664 the final-state particle identification. I established three independent approaches to identify the  
7665 leakage artifacts and I showed that the non-leakage waves are free of these artifacts so that they  
7666 can be interpreted reliably in terms of physics signals.

7667 A first resonance-model fit (RMF) to the results of the PWD, which was based on an approach  
7668 similar to the one used in the COMPASS  $\pi^-\pi^-\pi^+$  analysis [40, 41], failed. I identified the  
7669 incoherent background contributions to be the main reason for this failure. Then, I developed an  
7670 ansatz that effectively handles these incoherent background processes at the stage of the PWD  
7671 and explicitly models them at the stage of the RMF. Using this ansatz, I developed a RMF model  
7672 with 10 partial waves. Based on this model, I performed fits in which I studied 7 strange mesons  
7673 in detail. To this end, I developed a new software for RMFs [193]. Furthermore, I performed  
7674 a first set of systematic studies, and I performed extensive pseudodata studies to validate my  
7675 analysis ansatz. In addition, I extended this model to study 7 further strange mesons. Finally,  
7676 I performed first tests of studying resonances appearing the  $K^-\pi^+$  and  $\pi^-\pi^+$  subsystems of the  
7677  $K^-\pi^-\pi^+$  final state, which required further extensions of my RMF software [193]. The physics  
7678 results presented in this thesis are summarized in figure 9.1.

7679 In addition to the work described in this thesis, I was involved in other COMPASS analyses of  
7680 bachelor and master students [61, 65, 198, 199]. I also contributed to the COMPASS data taking  
7681 campaigns in the years 2016, 2017, 2018, and 2021.

7682 I presented various aspects of my analysis in regular meetings within the COMPASS collaboration.  
7683 Furthermore, I presented my analysis and other COMPASS results at various national and  
7684 international workshops and conferences. I published some of these results in the corresponding  
7685 proceedings [200–202]. Finally, I had the honor to be invited to give a plenary talk on news from  
7686 the light and strange meson sector at the 19th HADRON conference [203].

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$$\frac{1}{x^2} \rightarrow +\infty^{+\infty}$$

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DRAFT