Two-Flavor Simulations of ρ(770) and the Role of the KK[over ¯] Channel

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Two-flavor Simulations of the $\rho(770)$ and the Role of the $K\bar{K}$ Channel

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The $\rho(770)$ meson is the most extensively studied resonance in lattice QCD simulations in two ($N_f = 2$) and three ($N_f = 2+1$) flavor formulations. We analyze $N_f = 2$ lattice scattering data using unitarized Chiral Perturbation Theory, allowing not only for the extrapolation in mass but also in flavor, $N_f = 2 \rightarrow N_f = 2+1$. The flavor extrapolation requires information from a global fit to $\pi\pi$ and πK phase shifts from experiment. While the chiral extrapolation of $N_f = 2$ lattice data leads to masses of the $\rho(770)$ meson far below the experimental one, we find that the missing $K\bar{K}$ channel is able to explain this discrepancy.

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Introduction and Method. With advances in algorithms and increasing computational resources it has become feasible to extract phase shifts from lattice-QCD simulations. The Lüscher formalism relates the discrete energy eigenvalues of the QCD Hamiltonian simulated in a finite box to phase shifts, up to contributions that are exponentially suppressed with the box size [1, 2]. Moving frames, twisted boundary conditions or asymmetric boxes are means to extract more eigenvalues from the same volume [3–11]. This allows to scan the amplitude at several energies over the resonance region, which is a prerequisite for the reliable extraction of resonance masses and widths. An energy-dependent fit to extracted phase shifts is required, but it is also possible to short-circuit the Lüscher equation and fit amplitude parameters directly to energy eigenvalues [7].

More complicated multi-channel analyses have been carried out recently [12–14] that require in most cases a parameterization in energy to relate different eigenvalues and thus to compensate for missing information needed to describe such systems at a given energy. Introducing an optical potential absorbs degrees of freedom without the need of explicit parameterization, applicable to multi-channel but also multi-particle systems [15, 16].

Yet, the simplest hadronic system containing a resonance, $I = 1$ elastic $\pi\pi$ scattering via the $\rho(770)$ resonance, continues to be subject of recent lattice QCD simulations providing a more and more accurate determination of the amplitude and a test ground to benchmark new techniques. Phase shifts for the $I = 1$ $\pi\pi$ interaction were extracted in calculations with two mass-degenerate light flavors ($N_f = 2$) [17–24] and ones that include the strange quark flavor ($N_f = 2+1$) [13, 25–29]. For three flavors, the ρ meson was analyzed and extrapolated using unitarized Chiral Perturbation Theory (UCHPT) [30–34] in Refs. [30–32] and using CHPT with vector fields in Refs. [35, 36]. Finite-volume effects were studied in Refs. [37–39]. The first extrapolation of $N_f = 2+1$ lattice phase shifts was recently performed in Ref. [40]. See Refs. [41, 42] for the chiral extrapolation of partially quenched lattice results.

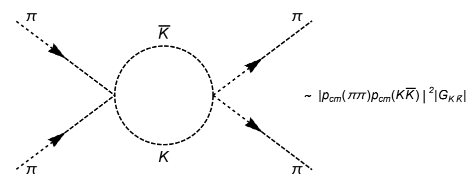

FIG. 1. Insertion of a $K\bar{K}$ intermediate state in $\pi\pi$ scattering, iterated in the present approach to provide coupled-channel unitarity.

A recent lattice QCD study from the GWU group [24] noted that the ρ mass extracted from $N_f = 2$ simulations is lighter than its physical value. This is also supported by an independent calculation from the RQCD Collaboration [22] very close to the physical mass, that finds an even lighter mass for the ρ, albeit with larger error bars.

In this letter, we discuss the hypothesis that the problem is tied to the missing strange quark, or, formulated in terms of hadrons as degrees of freedom, the absence of the $K\bar{K}$ channel. At first sight, the $K\bar{K}$ channel does not seem to play a role; indeed, from the observed small inelasticity in the ρ channel [43] and the small $K\bar{K}$ phase shifts obtained in analyses [13, 44, 45], it has been conjectured that the ρ effectively decouples from the $K\bar{K}$ channel. Yet, consider the insertion of an intermediate $K\bar{K}$ state in the rescattering of two pions as displayed in Fig. 1. The p-wave dictates the behavior close to the thresholds according to $p_{\rm cm}^2(\pi\pi)p_{\rm cm}^2(K\bar{K})$ where $p_{\rm cm}$ are the momenta in the center of mass. Additionally, there is a kaon loop $G_{K\bar{K}}$ including dispersive parts [24]. The combined contribution exhibits a maximum close to the ρ mass. The full, unknown interaction differs, of course, from this expression, but by a function that varies only slowly with energy. In other words, while the effects from real kaons are suppressed through the centrifugal barrier, virtual kaons can indeed contribute to the $\pi\pi$ amplitude at the ρ position, effectively shifting its mass. However, a substantial shift of the ρ mass might induce a significant effect of the $K\bar{K}$ channel above threshold. Therefore, results have to be checked with available constraints on $K\bar{K}$ phase shifts and inelasticities from experiment and $N_f = 2+1$ lattice QCD simulations (see discussions below and in supplemental material [46]).

In the present work, we use UCHPT to extrapolate $N_f = 2$ lattice results to the physical pion mass, but also to three flavors to study the role of the strange quark. Phase shifts from $N_f = 2+1$ simulations allow for direct extrapolation to the physical point and will be subject of future studies. The discussed mechanism of virtual or real intermediate $K\bar{K}$ states is taken into account by choosing an SU(3) formulation in which $K\bar{K}$ states are re-summed to all orders through unitarity in coupled channels. In the inverse amplitude formulation and taking into account NLO contact interactions, this model has been formulated in Ref. [44]. We replace here the cut-off with dimensional regularization [24]. Also, there is a minor modification in $I = 0$ πK, $\pi\eta$ scattering [45] at high energies. For the extrapolation of f_π, the M_π dependence of Refs. [31, 47], summarized in Ref. [48], is used. The workflow to extrapolate to the physical point is as follows (see also App. B of Ref. [24] for a similar procedure):

1. To fit the lattice phase shifts, the $K\bar{K}$ channel is removed from the coupled-channel $\pi\pi/K\bar{K}$ system. The low-energy constants (LECs in the definition of Ref. [24]) appear in two distinct linear combinations in the $I = L = 1$ $\pi\pi \to \pi\pi$ transition, $\hat{l}_1 = 2L_4 + L_5$, $\hat{l}_2 = 2L_1 - L_2 + L_3$, which are the two fit parameters used (not to be confused with SU(2) CHPT LECs).

2. $N_f = 2$ lattice phase shifts are fitted including the known correlation between energy and phase shift (the error bars in the $(W, \delta(W))$ plane are effectively inclined); in case of Refs. [22, 24], the covariance of energy eigenvalues is included in the fit. Data to be included in the fit are chosen in the maximal range around the resonance position, in which the fit passes Pearson's χ^2 test at a 90% upper confidence limit.

3. The result is extrapolated to the physical pion mass $M_\pi = 138$ MeV and then the channel transitions $\pi\pi \to K\bar{K}$ and $K\bar{K} \to K\bar{K}$ are switched on. The combinations of LECs appearing in these transitions are different from those of $\pi\pi \to \pi\pi$ and taken from a global fit to experimental $\pi\pi$ and πK phase shift data similar to that of Ref. [45].

4. The solution is given by LECs and their uncertainties at the physical point. To translate the results to the commonly used notation, all phase shifts are fitted with the usual Breit-Wigner (BW) parameterization in terms of g and m_ρ (see, e.g., Ref. [24]) although they could be quoted in terms of pole positions and residues which becomes increasingly popular [40, 49, 50].

Results. Available $N_f = 2$ phase shift data [17, 19, 20, 22, 24] are analyzed. The data of Ref. [21] are not considered since they are superseded by those of Ref. [24]. Results of Ref. [19] for larger pion masses are not analyzed, because they are beyond the expected applicability of the chiral extrapolation.

The extrapolations for the different $N_f = 2$ simulations are shown in Fig. 2. For each simulation, the left picture shows the lattice phase shifts and fit (only best fit shown). Phases included in the fit, according to the discussed criterion, are highlighted. As for consistency of the performed fits, the 68% confidence ellipses in $\hat{l}_1, \hat{l}_2$ from RQCD [22], GWU [24] ($m_\pi = 227$ MeV and $m_\pi = 315$ MeV), Lang et al. [20], and CP-PACS [17] all have a common overlap; the ellipse from QCDSF [18] is very slightly off, while the one from ETMC [19] is clearly incompatible (see supplemental material for a picture [46]).

The right pictures of Fig. 2 show the $N_f = 2$ chiral extrapolation to the physical mass (blue dashed line/light blue area). Then, without changing that extrapolated result, the UCHPT prediction for the missing strange quark is included in terms of the $K\bar{K}$ channel (solid red line). Experimental data [43, 51] are post-dicted.

In the following discussion of results, we exclude the data from Aoki *et al.*/PACS-CS [17] (2 measured phase shifts fitted with 2 parameters) and Feng *et al.*/ETMC [19] because the uncertainties are very large, even when simultaneously fitting data from two different pion masses. As Fig. 2 reveals, the $N_f = 2$ extrapolations all lead to a ρ mass lighter than experiment. This is particularly clear for the results of Refs. [20, 22, 24] where the computed ρ mass is lighter than the experimental one even before extrapolating to physical quark mass, so that the extrapolation cannot be responsible for this discrepancy.

Switching on the $K\bar{K}$ channel shows significant effects and increases the ρ mass, leading in all but the excluded cases to a much improved post-diction of the experimental data. For the lattice data by Bali *et al.*/RQCD [22], taking the covariances of energy eigenvalues into account narrows the band of uncertainties by about 30%. The phase shifts of Ref. [24] are the most accurate ones, leading to a narrow band in the final result. In fact, the lattice data uncertainties are so small that beyond the region of $\pm 2\Gamma$ around the resonance mass, the fit does not pass the mentioned χ^2 test and therefore data are not included. In any case, we have also fitted all phase shifts and found that the best fits for the two pion masses barely change. As the fits of the two pion masses of Ref. [24] are consistent, a common fit has been carried out in Ref. [24] leading to the most constraining results on the $\hat{l}_i$ and the chiral and flavor extrapolations. As for the simulation by Göckeler *et al.*/QCDSF [18] we have also included the data from $M_\pi = 390$ MeV in a combined fit, which significantly reduces uncertainties. The best fit barely changes when fitting only the $M_\pi = 240$, 250 MeV phases. The highest data point by Lang *et al.* [20] needed to be removed to fulfill the mentioned χ^2 test. Including this

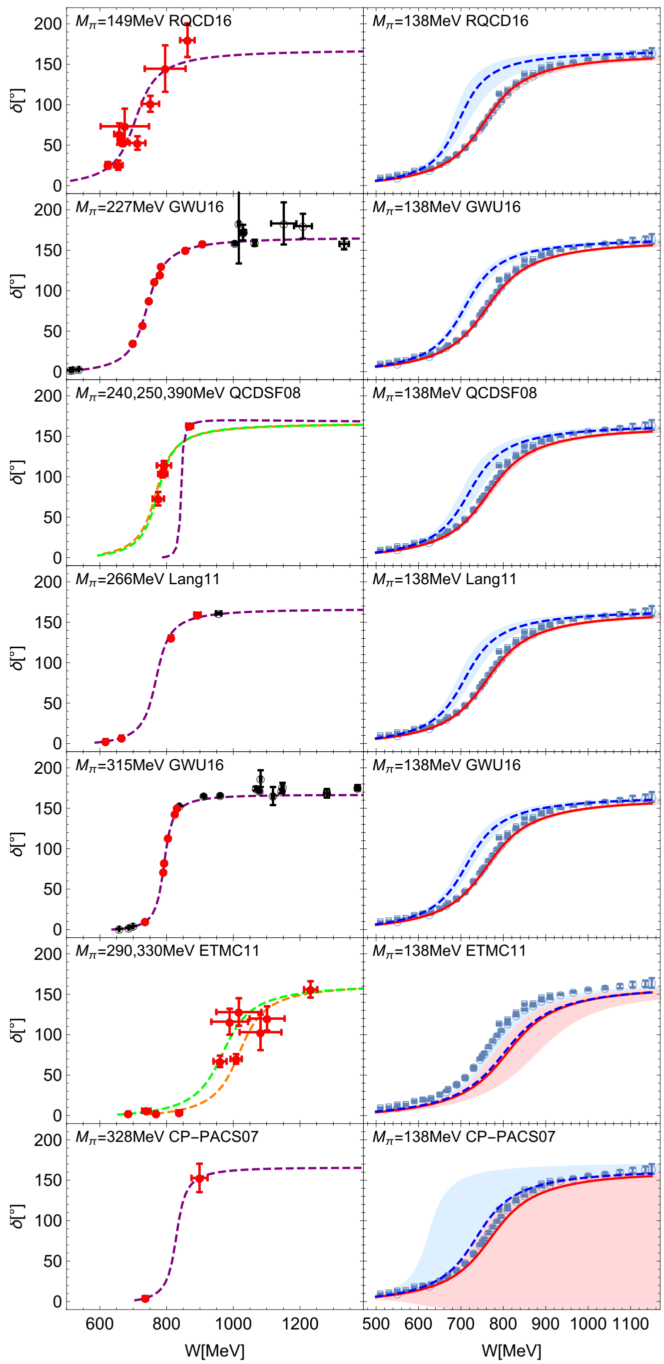

FIG. 2. Results for the $N_f = 2$ lattice simulations (ordered by pion mass) of Bali *et al.*/RQCD [22], Guo *et al.*/GWU [24], Göckeler *et al.*/QCDSF [18], Lang *et al.* [20], Feng *et al.*/ETMC [19], Aoki *et al.*/CP-PACS [17]. For each result, the left picture shows the lattice data and fit, the right figure shows the $N_f = 2$ chiral extrapolation (blue dashed line/light blue area). Without changing this result, the $K\bar{K}$ channel is then included to predict the effect from the missing strange quark (red solid line/light read area). Experimental data (blue circles from [51], squares from [43]) are then postdicted. For inherent model uncertainties, see text.

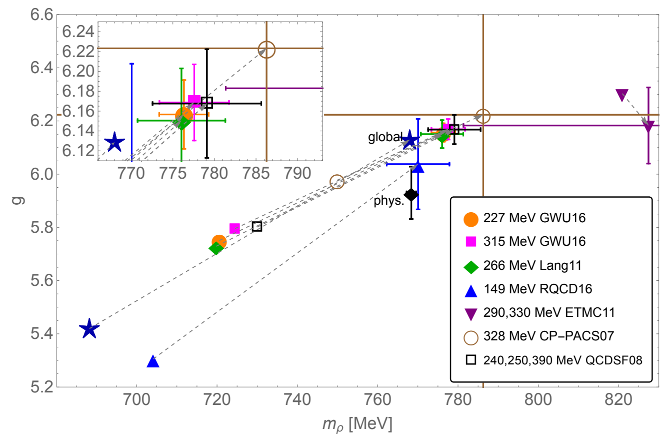

FIG. 3. Effect of the $K\bar{K}$ channel in the (m_ρ, g) plane indicated with arrows, after chiral extrapolation to the physical pion mass. See Fig. 2 for the labeling of the extrapolations. Only statistical uncertainties are shown, and only for the case after including $K\bar{K}$. See text for further explanations and supplemental material [46] for the effect of the chiral extrapolation.

point barely changes the central result (red line) but only leads to smaller uncertainties. The solution is also stable when removing the second-highest point and keep the highest.

For all fits, we have also checked that the inelasticity from the $K\bar{K}$ channel does not become larger than the observed total inelasticity [43] up to $W \sim 1.15$ GeV. The $\omega\pi$ contribution to the latter has been evaluated in Ref. [52] (see also Ref. [35]). Our $K\bar{K}$ inelasticity is rather of similar size as the $K\bar{K}$ inelasticity derived in Ref. [52] from the Roy-Steiner solution of Ref. [53]. The inelasticity is in any case smaller than the bound quoted in Ref. [54]. Yet, 4π channels are omitted in the current work because the fitted lattice phase shifts are situated below finite-volume thresholds, except for the highest energy of Ref. [22] (omitting this point does not change the best fit). The 4π channels are effectively absorbed in the LECs in the lattice fits, but introduce some uncertainty in the chiral extrapolation.

In the supplemental material [46], the inelasticity is shown with experiment [43] and also with the $N_f = 2+1$ lattice simulation of Ref. [13] at $M_\pi = 236$ MeV. Inelasticities are well predicted and the small $K\bar{K}$ phase shift has even the same size and sign as in Ref. [13].

The predicted $\pi\pi$ scattering lengths are close to the $\mathcal{O}(p^4)$ CHPT value but some are just outside the 1-σ range of the experimental result, while effective ranges are of similar size as the $\mathcal{O}(p^6)$ CHPT value [55] as quoted in the supplemental material [46].

In Fig. 3 we show the effect of the $K\bar{K}$ channel in the (m_ρ, g) plane. Remember that (m_ρ, g) emerge from Breit-Wigner fits to the UCHPT solutions. This is also the case for the experimental point, indicated as "phys.". The comparability of all shown (m_ρ, g) with other values in the literature is therefore limited but in practice quite accurate.

To keep the figure simple, no error bars are shown for the chirally extrapolated results; see previous remark on consistency of the fits. Once the $K\bar{K}$ channel is switched on, Fig. 3 shows that g and m_ρ are slightly over-extrapolated. A possible reason is model deficiency. On one hand, problems could originate from the formulation: we include NLO contact terms [44] but not the one-loop contributions at NLO as in Ref. [31]. On the other hand, the LECs entering the $\pi\pi \to K\bar{K}$ and $K\bar{K} \to K\bar{K}$ transitions are not fully determined from the fit of $N_f = 2$ lattice data and therefore taken from a global fit to experimental $\pi\pi$ and πK phase shifts in different isospin and angular momentum, similar to that of Ref. [45]. That global fit compromises between different data sets, leading to a slightly wider ρ resonance. In Fig. 3, a Breit-Wigner fit to that solution is indicated as "global" with a star. Indeed, the value for g is slightly too large. In any case, it is instructive to remove here the $K\bar{K}$ channel. As Fig. 3 shows (star at $m_\rho \approx 690$ MeV), the result (again, deduced only from experimental information) exhibits the same trend as the $N_f = 2$ lattice data, i.e., a lighter and narrower ρ.

Inherent model uncertainties from the $2 \to 2+1$ flavor extrapolation can be roughly estimated as in Ref. [24] by inserting the fitted $\hat{l}_1$, $\hat{l}_2$ in the $\pi\pi \to K\bar{K}$ and $K\bar{K} \to K\bar{K}$ transitions, instead of taking them from the global fit to experimental data. As a result, instead of over-extrapolating in m_ρ and g, these quantities are now mostly under-extrapolated. The observed differences translate into model/systematic uncertainties of comparable size as the statistical uncertainties shown in Fig. 3 (see supplemental material for values [46]).

As part of the ρ mass shift originates from the regularized $K\bar{K}$ propagator [24], we also test the dependence of the results on the value of the subtraction constant, changing it from the default value $a = -1.28$ [24] to $a = -0.8$ and $a = -1.7$. The global fits to experimental phase shifts visibly deteriorate for these extreme values, e.g., for πK scattering, but barely change in the ρ channel as experimental phase-shift data are more precise. Following the described workflow, we find changes of the final results of less than 10 MeV in m_ρ and less than 0.08 in g.

In conclusion, the present results demonstrate the relevance of the $K\bar{K}$ channel, that can explain the systematically small lattice ρ masses at the physical point after the chiral SU(2) extrapolation. From the discussion, it becomes clear that a full one-loop calculation [31, 56] for confirmation and further improvement of the present results is desirable. A rough estimate for neglected changes in the $\pi\pi \to \pi\pi$ transition when including the strange quark can be obtained by using the SU(2)-SU(3) matching relations for LECs [47], resulting in very small changes, of less than 1 MeV, in the ρ masses.

Summary: All accessible phase shift data on the ρ meson from $N_f = 2$ lattice QCD simulations are analyzed using the inverse amplitude method including NLO terms from Chiral Perturbation Theory. The $N_f = 2$ fits are extrapolated to the physical pion mass, and the $K\bar{K}$ channel is subsequently switched on without further changing the fit parameters. For this step, combinations of SU(3) low-energy constants, that are not accessible through the $N_f = 2$ lattice data, are taken from a global fit to experimental meson-meson phase shifts. The $K\bar{K}$ channel improves the extrapolations of the ρ mass significantly except when the lattice data have large uncertainties.

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