$I = 3$ Three-Pion Scattering Amplitude from Lattice QCD

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We analyze the spectrum of two- and three-pion states of maximal isospin obtained recently for isosymmetric QCD with pion mass $M \approx 200$ MeV in Hörz and Hanlon, [Phys. Rev. Lett. **123**, 142002 (2019)]. Using the relativistic three-particle quantization condition, we find $\sim 2\sigma$ evidence for a nonzero value for the contact part of the $3\pi^+$ $(I = 3)$ scattering amplitude. We also compare our results to leading-order chiral perturbation theory. We find good agreement at threshold and some tension in the energy dependent part of the $3\pi^+$ scattering amplitude. We also find that the $2\pi^+$ $(I = 2)$ spectrum is fit well by an s-wave phase shift that incorporates the expected Adler zero.

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Introduction.—Lattice QCD (LQCD) provides a powerful (if indirect) tool for *ab initio* calculations of strong-interaction scattering amplitudes. The formalism for determining two-particle amplitudes is well understood [1–12], and there has been enormous progress in its implementation in recent years [13–32] (see Ref. [33] for a review). The present frontier is the determination of three-particle scattering amplitudes and related decay amplitudes. LQCD calculations promise access to three-particle scattering processes that are difficult or impossible to access experimentally. Examples of important applications are understanding properties of resonances with significant three-particle branching ratios (including the Roper resonance [34], and many of the X, Y, and Z resonances [35]), determining the three-nucleon interaction (important for large nuclei and neutron star properties), predicting weak decays to three particles (e.g., $K \to 3\pi$), and calculating the 3π contribution to the hadronic-vacuum polarization that enters into the prediction of muonic $g - 2$ [36].

Three-particle amplitudes are determined using LQCD by calculating the energies of two- and three-particle states in a finite volume [37,38]. The challenges to carrying this out are twofold. On the one hand, the calculation of spectral levels becomes more challenging as the number of particles increases. On the other, one must develop a theoretical formalism relating the spectrum to scattering amplitudes. Significant progress has recently been achieved in both directions, with energies well above the three-particle threshold being successfully measured, and a formalism for three identical (pseudo)scalar particles available. The formalism has been developed and implemented following three approaches: generic relativistic effective field theory (RFT) [39–45], nonrelativistic effective field theory [46–49], and (relativistic) finite volume unitarity (FVU) [50,51] (see, also, Refs. [52,53] and Ref. [54] for a review). To date, only the RFT formalism has been explicitly worked out including higher partial waves. The application to LQCD results has, so far, been restricted to the energy of the three-particle ground state, either using the threshold expansion [55–57], or, more recently, the FVU approach for $3\pi^+$ [51].

Recently, precise results were presented for the spectrum of $2\pi^+$ and $3\pi^+$ states in $O(a)$-improved isosymmetric QCD with pions having close to physical mass, $M \approx 200$ MeV [58]. These were obtained in a cubic box of length L with $ML \approx 4.2$, for several values of the total momentum $\vec{P} = (2\pi/L)\vec{d}$ with $\vec{d} \in \mathbb{Z}^3$, and for several irreducible representations (irreps) of the corresponding symmetry groups. Isospin symmetry ensures that G parity is exactly conserved and, thus, that the $2\pi^+$ and $3\pi^+$ sectors are decoupled. In total, sixteen $2\pi^+$ levels and eleven $3\pi^+$ levels were obtained below the respective inelastic thresholds at $E_2^* = 4M$ and $E^* = 5M$, Here, E_2^* and $E^* = \sqrt{E^2 - \vec{P}^2}$ are the corresponding center-of-mass energies, with E the total three-particle energy.

The purpose of this Letter is to perform a global analysis of the spectra of Ref. [58] using the RFT formalism and determine the underlying $3\pi^+$ interaction. This breaks new ground for an analysis of the three-particle spectrum in several ways: we use multiple excited states, in both trivial and nontrivial irreps, including results from moving frames. Therefore, this analysis serves as a testing ground for the utility of the three-particle formalism in an almost physical example. An additional appealing feature is that the size of the $3\pi^+$ interaction can be calculated using chiral perturbation theory (χPT). We present the leading order (LO) prediction here.

After this Letter was made public, an independent study of the results of Ref. [58], using the FVU approach, appeared [59].

Formalism and implementation.—All approaches to determining three-particle scattering amplitudes using LQCD proceed in two steps, which we outline here. In the first step, one uses a quantization condition (QC), which predicts the finite-volume spectrum in terms of an intermediate infinite-volume three-particle scattering quantity. In the RFT approach, the QC for identical, spinless particles with a G-parity-like Z_2 symmetry takes the form (up to corrections of $\mathcal{O}(1\%)$ that are exponentially suppressed in ML) [39]

$$\det\,[F_3(E,\vec{P},L)^{-1} + \mathcal{K}_{\mathrm{df},3}(E^*)] = 0. \tag{1}$$

Here, F_3 and $\mathcal{K}_{\mathrm{df},3}$ are matrices in a space describing three on-shell particles in finite volume. They have indices of angular momentum of the interacting pair, ℓ, m, and finite-volume momentum of the spectator particle, k. F_3 depends on the two-particle scattering amplitude and on known geometric functions, while $\mathcal{K}_{\mathrm{df},3}$ is the three-particle scattering quantity referred to above. It is quasilocal, real, and free of singularities related to three-particle threshold (and so “divergence-free”, i.e., df), thus, playing a similar role to the two-particle K matrix $\mathcal{K}_2$ in two-particle scattering. It is, however, unphysical, as it depends on an ultraviolet (UV) cutoff. Given prior knowledge of $\mathcal{K}_2$, and a parametrization of $\mathcal{K}_{\mathrm{df},3}$, the energies of finite-volume states are determined by the vanishing of the determinant in Eq. (1). The parameters in $\mathcal{K}_{\mathrm{df},3}$ are then adjusted to fit to the numerically determined spectrum. Examples on how to numerically solve Eq. (1) have been presented in Refs. [42,44,45].

The second step requires solving infinite-volume integral equations in order to relate $\mathcal{K}_{\mathrm{df},3}$ to the three-particle scattering amplitude $\mathcal{M}_3$. In fact, as explained below, it is a divergence-free version of the latter, denoted $\mathcal{M}_{\mathrm{df},3}$, that is most useful. The equations relating $\mathcal{K}_{\mathrm{df},3}$ to $\mathcal{M}_{\mathrm{df},3}$ were derived in Ref. [40], and solved in Ref. [42].

The parametrizations we use for $\mathcal{K}_2$ and $\mathcal{K}_{\mathrm{df},3}$ are based on an expansion about two- and three-particle thresholds. For $\mathcal{K}_2$, this leads to the standard effective range expansion (ERE), recalled below. At linear order in this expansion only s-wave interactions are nonvanishing, with d-wave interactions first entering at quadratic order (p-wave interactions are forbidden by Bose symmetry). For $\mathcal{K}_{\mathrm{df},3}$, the expansion is in powers of $\Delta = (E^{*2} - 9M^2)/(9M^2)$, and was developed in Refs. [42,44] based on the Lorentz and particle-interchange invariance of $\mathcal{K}_{\mathrm{df},3}$. Through linear order in Δ, $\mathcal{K}_{\mathrm{df},3}$ is given by

$$\mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso},0}_{\mathrm{df},3} + \mathcal{K}^{\mathrm{iso},1}_{\mathrm{df},3}\Delta, \tag{2}$$

where $\mathcal{K}^{\mathrm{iso},0}_{\mathrm{df},3}$ and $\mathcal{K}^{\mathrm{iso},1}_{\mathrm{df},3}$ are constants. There is no dependence on the momenta of the three particles at this order; this corresponds to a contact interaction, and leads to the designation “isotropic” (iso). Momentum dependence first enters at $\mathcal{O}(\Delta^2)$.

In our main analysis, we keep only the s-wave two-particle interaction and the isotropic terms in Eq. (2). With these approximations, the QC of Eq. (1) reduces to a finite matrix equation that can be solved by straightforward numerical methods. Previous implementations have considered only the three-particle rest frame, $\vec{P} = 0$ [42,44,45] (see, also, Ref. [48,51]). Here, we have extended the implementation to moving frames, so that we can use all the results obtained by Ref. [58].

In the Supplemental Material [60], we provide further details of the implementation for a general frame, as well as additional details concerning the fits and error estimates described in the remainder of this Letter.

χPT prediction for $\mathcal{K}_{\mathrm{df},3}$ and $\mathcal{M}_{\mathrm{df},3}$.—$\mathcal{M}_{\mathrm{df},3}$ and $\mathcal{K}_{\mathrm{df},3}$ have not previously been calculated in χPT, so here, we present the LO result. The LO Lagrangian in the isosymmetric two-flavor theory is [61,62]

$$\mathcal{L}_\chi = \frac{F^2}{4}\mathrm{tr}(\partial_\mu U \partial^\mu U^\dagger) + \frac{M^2F^2}{4}\mathrm{tr}(U + U^\dagger), \quad \text{with}$$
$$U = e^{i\phi/F} \quad \text{and} \quad \phi = \begin{pmatrix} \pi^0 & \sqrt{2}\pi^+ \\ \sqrt{2}\pi^- & -\pi^0 \end{pmatrix}. \tag{3}$$

Here, F is the decay constant in the chiral limit, normalized such that $F_\pi = 92.4$ MeV. We note that, at this order, $F = F_\pi$. Expanding in powers of the pion fields, $\mathcal{L} = \mathcal{L}_{2\pi} + \mathcal{L}_{4\pi} + \mathcal{L}_{6\pi} + \cdots$, we need only the 4π and 6π vertices.

From $\mathcal{L}_{4\pi}$, we obtain the standard LO result for the $2\pi^+$ scattering amplitude [63],

$$\mathcal{M}_2 = \frac{2M^2 - E_2^{*2}}{F^2}, \tag{4}$$

which displays the well-known Adler zero below threshold at $E_2^{*2} = 2M^2$ [64]. Given the ERE parametrization of the s-wave phase shift,

$$q\cot\delta_0(q) = -\frac{1}{a_0} + \frac{rq^2}{2} + Pr^3q^4 + \cdots, \tag{5}$$

where $q^2 = E_2^{*2}/4 - M^2$, one can infer from Eq. (4) the LO results for the scattering length and effective range

$$Ma_0 = \frac{M^2}{16\pi F^2} \quad \text{and} \quad M^2ra_0 = 3. \tag{6}$$

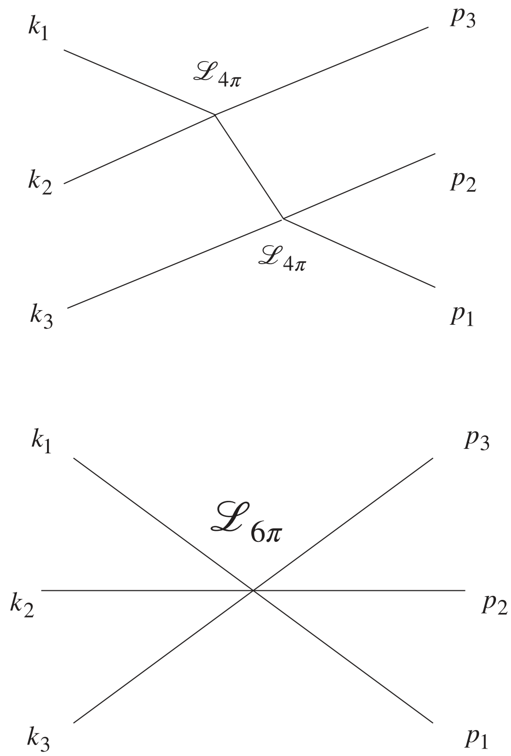

FIG. 1. LO contributions to the three-particle scattering amplitude $\mathcal{M}_3$. Momentum assignments must be symmetrized.

The $3\pi^+$ amplitude $\mathcal{M}_3$ is given at LO by the diagrams of Fig. 1. As is well known, $\mathcal{M}_3$ diverges for certain external momenta, as the propagator in Fig. 1(a) can go on shell. This motivated the introduction of a divergence-free amplitude in Ref. [39]

$$\mathcal{M}_{\rm df,3} \equiv \mathcal{M}_3 - \mathcal{D}, \tag{7}$$

$$\mathcal{D} = \mathcal{S}\left\{-\mathcal{M}_2(s_{12})\frac{1}{b^2 - M^2}\mathcal{M}_2(s'_{12})\right\} + O(\mathcal{M}_2^3), \tag{8}$$

where $s_{12} = (p_1 + p_2)^2$, $s'_{12} = (k_1 + k_2)^2$, $b = p_1 + p_2 - k_3$, and $\mathcal{S}$ indicates symmetrization over momentum assignments. $\mathcal{D}$ is defined to have the same divergences as $\mathcal{M}_3$, so that their difference is finite. At LO in χPT, only the LO term in $\mathcal{D}$ contributes, and we find

$$\begin{aligned} M^2\mathcal{M}_{\rm df,3} &= \frac{M^4}{F^4}(18 + 27\Delta) \\ &= (16\pi M a_0)^2(18 + 27\Delta), \end{aligned} \tag{9}$$

a result that is real and isotropic. As a side result, we have also calculated the related threshold amplitude that enters into the $1/L$ expansion of the three-particle energy [65], finding $\mathcal{M}_{3,\rm th} = 27M^2/F^4$.

The last step is to relate $\mathcal{M}_{\rm df,3}$ to $\mathcal{K}_{\rm df,3}$. We find these quantities to be equal at LO

$$\mathcal{K}_{\rm df,3} = \mathcal{M}_{\rm df,3}[1 + \mathcal{O}(M^2/F^2)], \tag{10}$$

so that $\mathcal{K}_{\rm df,3}$ is also given by Eq. (9). This implies that $\mathcal{K}_{\rm df,3}$ is scheme independent at LO in χPT. We can also quantify the expected size of the corrections, finding them to range between 10% and 50%, with the larger error applying to the term linear in Δ.

Fitting the two-particle spectrum.—Determining the two-particle phase shift is an essential step, as it enters into the three-particle QC. In particular, we need a parametrization valid below threshold, as the two-particle momentum in the three-particle QC takes values in the range $q^2/M^2 \in [-1, 3]$. We extract information on the s-wave phase shift using a form of the two-particle QC that holds in all frames for those irreps that couple to $J = 0$. We use the bootstrap samples provided in Ref. [58] to determine statistical errors, so that correlations are accounted for properly.

We use a parametrization of the phase shift (adapted from that of Ref. [66]; see, also, Ref. [67]) that includes the Adler zero predicted by χPT, as well as the kinematical factor E_2^*

$$\frac{q}{M}\cot\delta_0(q) = \frac{E_2^* M}{E_2^{*2} - 2z_2^2}\left(B_0 + B_1\frac{q^2}{M^2} + B_2\frac{q^4}{M^4} + \cdots\right). \tag{11}$$

We either set $z_2^2 = M^2$, the LO value, or leave it as a free parameter. B_0 and B_1 are related in a simple way to a_0 and r. Previous lattice studies have used the ERE, Eq. (5) (see, e.g., Refs. [68–70]), but this has the disadvantage, due to the Adler zero, of having a radius of convergence of $|q^2| = |M^2 - z_2^2/2| \approx M^2/2$. In particular, the ERE gives results for $-1 < q^2/M^2 < 0$ that are substantially different

TABLE I. Fits of the two-particle spectrum to the Adler-zero form of $q\cot\delta_0$, Eq. (11).

Fit	B_0	B_1	B_2	z_2^2/M^2	χ^2/d.o.f.	Ma_0	M^2ra_0
1	−11.2(7)	−2.1(3)	⋯	1 (fixed)	12.13/(11-2)	0.089(6)	2.63(8)
2	−10.4(9)	−3.7(1.0)	0.5(3)	1 (fixed)	9.75/(11-3)	0.096(8)	2.3(3)
3	−11.7(1.8)	−2.0(4)	⋯	0.94(22)	12.06/(11-3)	0.091(9)	2.4(9)

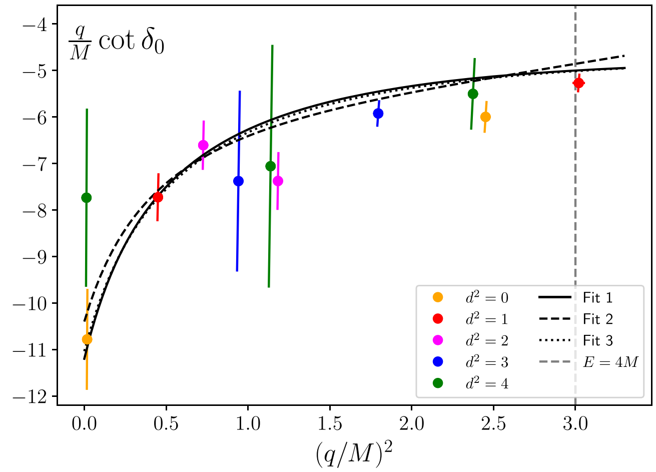

FIG. 2. Values of $q\cot\delta_0$ obtained from the two-particle spectrum of Ref. [58] using the two-particle QC, together with various fits.

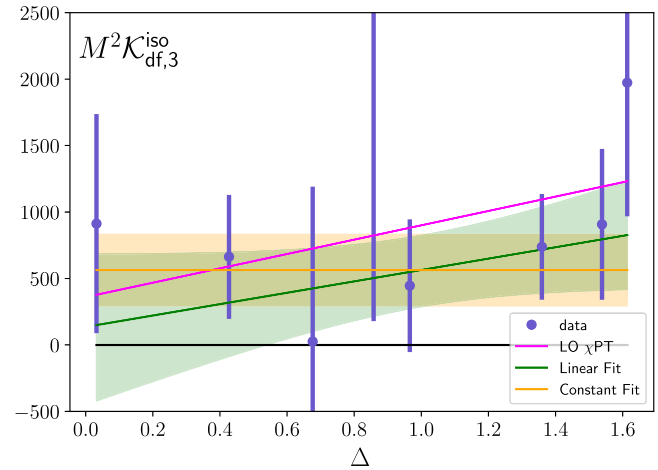

FIG. 3. Results for $M^2\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$ from individual three-particle levels, using method 1, together with constant and linear fits, and the LO prediction of χPT.

from the Adler-zero form. This is related to the fact that in (11), B_1 and B_2 are both of next-to-leading order (NLO) in χPT, in contrast to the ERE form where r and P are both nonzero at LO, as can be seen from the explicit χPT expressions given in Ref. [68]. The formal radius of convergence of our expression (11) is $|q^2| = M^2$, due to the left-hand cut, but following common practice, we ignore this and use it up to $q^2/M^2 = 3$. We find that fitting with the restriction $|q^2|/M^2 < 1$ has only a small impact on the resulting parameters. We have also checked that fits using the ERE form provide a worse description of the data.

The results of several fits are listed in Table I and shown in Fig. 2. All fits give reasonable values of χ^2 divided by the number of degrees of freedom, $\chi^2/\mathrm{d.o.f.}$, and yield values for $M^2 r a_0$ close to the predicted LO value of 3. Using the value of F obtained from the same lattice configurations in Ref. [71,72], the LO chiral prediction from Eq. (6) is $Ma_0 = 0.0938(12)$, and this is also in good agreement with the results of the fits. Overall, we conclude that the spectrum from Ref. [58] confirms the expectations from χPT. We choose the minimal fit 1 as our standard choice since B_2 is poorly determined (fit 2) and the Adler-zero position is consistent with the LO result if allowed to float (fit 3).

We have performed a similar fit to the five energy levels from Ref. [58] which are sensitive only to the d-wave amplitude. Despite very small shifts from the free energies, we find a 3σ signal for the d-wave scattering length, $(Ma_2)^5 = 0.0006(2)$. The smallness of this result is qualitatively consistent with the fact that this is a NLO effect in χPT, and justifies our neglect of d waves in the three-particle analysis.

Fitting the three-particle spectrum.—Now, we use the three-particle spectrum to determine $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$. Eight levels are sensitive to $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$, while three are in irreps only sensitive to two-particle interactions. Since all levels are correlated, a global fit to two- and three-particle spectra is needed to properly estimate errors.

Before presenting the global fits, however, we use an approach ("method 1") that allows a separate determination of $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$ for each of the eight levels sensitive to this parameter. Within each bootstrap sample, we fit the two-particle levels to the fit 1 Adler-zero form described above, and then adjust $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$ so that the three-particle QC reproduces the energy of the level under consideration. The results are shown in Fig. 3. The values of $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$ are all positive, and a constant fit yields $M^2\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}} = 560(270)$ with $\chi^2/\mathrm{d.o.f.} = 8.5/7$. The LO χPT result (given by $M^2\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}} = 360 + 540\Delta$, taking Ma_0 from fit 1) is reasonably consistent with the linear fit, as shown. This indicates that a significant result for $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$ of the expected size may be obtainable.

This fit does not include three-particle energy levels in irreps sensitive only to δ_0. These, however, can be used as a consistency check. We find good agreement between the data and the energies predicted by the QC.

TABLE II. Global fits to the two- and three-particle spectrum using the two- and three-particle QCs.

Fit	B_0	B_1	z_2^2/M^2	$M^2\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},0}$	$M^2\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}$	$\chi^2/\mathrm{d.o.f.}$	Ma_0	$M^2 r a_0$
4	−11.1(7)	−2.3(3)	1 (fixed)	270(160)	⋯	27.06/(22-3)	0.090(6)	2.59(8)
5	−11.1(7)	−2.4(3)	1 (fixed)	550(330)	−280(290)	26.04/(22-4)	0.090(5)	2.57(8)

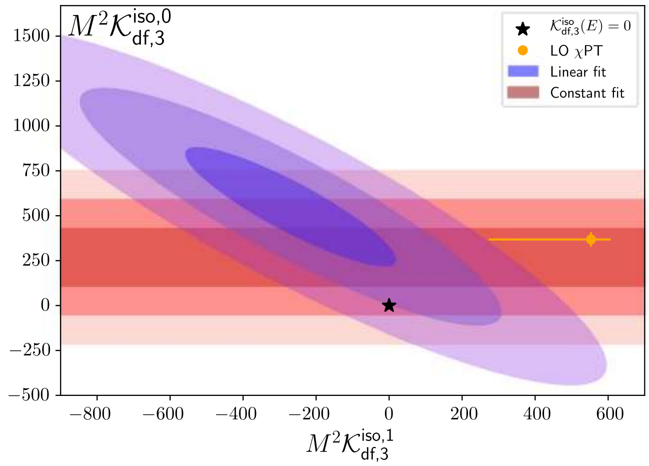

FIG. 4. One, two, and three-sigma confidence intervals for $M^2\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$ for the two different global fits (4 and 5).

To establish the true significance of the results for $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$ we perform global fits to the eleven two-particle and eleven three-particle levels that depend on δ_0 and/or $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$. We do so both for constant and linear $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$. The results are collected in Table II. Fit 4 finds a value for $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$ that has around 1.8σ statistical significance and also gives values for B_0 and B_1 that are consistent with those from fits 1–3 above and with the LO χPT predictions. The p value of the fit is $p = 0.103$.

In fit 5, we try a linear ansatz for $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$, and find that the current dataset of Ref. [58] is insufficient for a separate extraction of both constant and linear terms. We note, however, that, even in this fit, the scenario $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3} = 0$ is excluded at $\sim 2\sigma$.

In Fig. 4, we present a summary of the errors resulting from the global fits. We also include the value from LO χPT, along with an estimate of the NLO corrections. As can be seen, the constant term agrees well with the prediction, whereas the larger disagreement for the linear term is only of marginal significance given the large uncertainty in the χPT prediction.

One concern with our global fits is that we are using the forms for $\mathcal{K}_2$ and $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$ beyond their radii of convergence. For $\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}$, we do not know the radius of convergence, but a reasonable estimate is that one should use levels only with $|\Delta| < 1$. To check the importance of this issue, we have repeated the global fits imposing $q^2/M^2 < 1$ and $\Delta < 1$, so that the fit includes only five $2\pi^+$ and five $3\pi^+$ levels. We find fit parameters that are consistent with those in Table II, but with much larger errors. For example, the result from the equivalent of fit 4 gives $M^2\mathcal{K}^{\mathrm{iso},0}_{\mathrm{df},3} = 610(350)$.

We close by commenting on sources of systematic errors. The results of Ref. [58] are subject to discretization errors, but these are of $O(a^2)$, and likely small compared to the statistical errors from [58]. The quantization condition itself neglects exponentially suppressed corrections, but these are numerically small ($e^{-ML} \sim 1\%$) compared to our final statistical error. Errors from truncation of the threshold expansion for $\mathcal{K}_2$ and $\mathcal{K}_{\mathrm{df},3}$ are also present but harder to estimate.

Conclusions.—We have presented statistical evidence for a nonzero $3\pi^+$ contact interaction, obtained by analyzing the spectrum of three pion states in isosymmetric QCD with $M \approx 200$ MeV obtained in Ref. [58]. This illustrates the utility of the three-particle quantization condition. It also emphasizes the need for a relativistic formalism, since most of the spectral levels used here are in the relativistic regime. It gives an example where lattice methods can provide results for scattering quantities that are not directly accessible to experiment.

We expect that forthcoming generalizations to the formalism (to incorporate nondegenerate particles with spin, etc.), combined with advances in the methods of lattice QCD (to allow the accurate determination of the spectrum in an increasing array of systems), will allow generalization of the present results to resonant three-particle systems in the next few years.

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