Three-Body Dynamics of the $a_1(1260)$ Resonance from Lattice QCD

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Resonant hadronic systems often exhibit a complicated decay pattern in which three-body dynamics play a relevant or even dominant role. In this work we focus on the $a_1(1260)$ resonance. For the first time, the pole position and branching ratios of a three-body resonance are calculated from lattice QCD using one-, two-, and three-meson interpolators and a three-body finite-volume formalism extended to spin and coupled channels. This marks a new milestone for *ab initio* studies of ordinary resonances along with hybrid and exotic hadrons involving three-body dynamics.

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Introduction.—Many unresolved questions in the excited spectrum of strongly interacting particles are related to the hadronic three-body problem [1]. Some examples of interest include: axial mesons like the $I^G(J^{PC}) = 1^-(1^{++})a_1(1260)$ or exotic mesons, such as the $J^{PC} = 1^{-+}\ \pi_1(1600)$ claimed by the COMPASS Collaboration [2] by analyzing three-pion final states; this and other exotic mesons searched for in the GlueX experiment [3]; the Roper resonance $N(1440)1/2^+$ with its unusually large branching ratio to the $\pi\pi N$ channel and a very nonstandard line shape [4–7]; heavy mesons like the $X(3872)$ with large branching ratio to $D\bar{D}\pi$ states [8,9]. Furthermore, multineutron forces are crucial for the equation of state of a neutron star [10]. Recent advances in lattice QCD (LQCD) on few-nucleon systems [11,12] complement dedicated experimental programs, e.g., at the FRIB facility [13].

Lattice QCD provides information about the structure and interactions of hadrons as they emerge from quark-gluon dynamics. For scattering this information is extracted indirectly by accessing the energy of the multihadron states in finite volume. The connection to infinite-volume scattering amplitudes is provided by *quantization conditions*. In the two-hadron sector this technique is already a precision tool for extracting phase shifts and resonance information [14–18]. Moving to the three-hadron sector new challenges emerge, both in terms of determining precisely the energy of three-particle states from QCD and in developing the necessary quantization conditions.

Three-hadron LQCD calculations have been performed mostly for pion and kaon systems at maximal isospin [19–26]. Through the use of a large basis of one-, two-, and three-meson interpolators, these calculations provide reliable access to the energies of three-particle states and, using recently developed quantization conditions, infinite-volume amplitudes can be accessed [27–75]. Among these approaches we highlight relativistic field theory (RFT) [33,34], nonrelativistic effective field theory (NREFT) [39,40], and finite volume unitarity (FVU) [51,52]. For reviews see Refs. [76–78].

So far, no resonant three-body pole position has been studied with LQCD data using any finite-volume methodology. In this Letter we take on this challenge, calculating the excited-state spectrum of the $a_1(1260)$ in LQCD and subsequently mapping it to the infinite volume. This enables, for the first time, the determination of resonance pole position and branching ratios for a three-body resonance from first principles.

The $a_1(1260)$ decays exclusively to three pions [1,2] and can be measured cleanly in τ decays [79,80] allowing for its three-body decay channels to be determined. The resonance is wide [1] indicating strong and nontrivial three-body effects which make it a prime candidate to study three-body dynamics. This is reflected in an increased interest in the dynamics and the structure of the $a_1(1260)$ [81–95] including pioneering calculations [96,97]. Of these approaches, Refs. [87,93] use frameworks that manifestly incorporate three-body unitarity which is the linchpin of the FVU formalism [51] and a prerequisite for the mapping between finite and infinite volume.

We generalize the FVU formalism to include two-particle subsystems with spin, to map the LQCD spectrum to the resonance pole of the $a_1(1260)$. Furthermore, the dominant decay of the $a_1(1260)$ into $\pi\rho$ occurs in two channels (S and D waves) which requires an upgrade of the formalism to coupled channels. Finally, the challenge of analytic continuation of three-body amplitudes to complex pole positions is also resolved in this study and we deliver the first three-body unitary pole determination of the a_1 from experiment.

By calculating the excited LQCD spectrum, mapping it to the infinite-volume coupled-channel amplitude, and finally determining the $a_1(1260)$ pole and branching ratios we demonstrate that detailed calculations of three-body resonances from first principles QCD have become possible. This paves the way for the *ab initio* understanding of a wide class of resonance phenomena, including hybrid and exotic hadrons, that lie at the heart of nonperturbative QCD.

LQCD spectrum.—We extract the finite-volume spectrum in the $a_1(1260)$ sector with total momentum $\boldsymbol{P} = (0,0,0)$ using an ensemble with $N_f = 2$ dynamical fermions, with masses tuned such that the pion mass is 224 MeV. The lattice spacing $a = 0.1215$ fm is determined using Wilson flow parameter t_0 [98]. This ensemble has been used multiple times [22,25,99–102] to successfully study two- and three-meson scattering, thus, we will only review the most important calculation details and new features relevant for the $a_1(1260)$. Computationally expensive quark propagators are estimated with LapH smearing [103], calculated using an optimized inverter [104]. Having access to the so-called perambulators makes it straightforward to construct a large basis of operators for use in the variational method [105–107], which removes excited state contamination and allows extraction of the excited state spectrum.

Performing the calculation in a cubic volume reduces the rotational symmetry group $SO(3)$ to the group O_h. States on the lattice thus cannot be classified by their angular momentum quantum number. Instead, they are classified by the irreducible representations (irreps) of O_h. For the $a_1(1260)$ the irrep of interest is T_{1g} which subduces onto the continuum quantum numbers $J^P = 1^+$. Aside from ensuring that our operators have the correct angular momentum content we must also construct them to have total isospin $I = 1$ to match the $a_1(1260)$. The last major consideration for constructing our operator basis is to ensure sufficient overlap with the lowest-lying states of the spectrum. In that regard we utilize both a single-meson

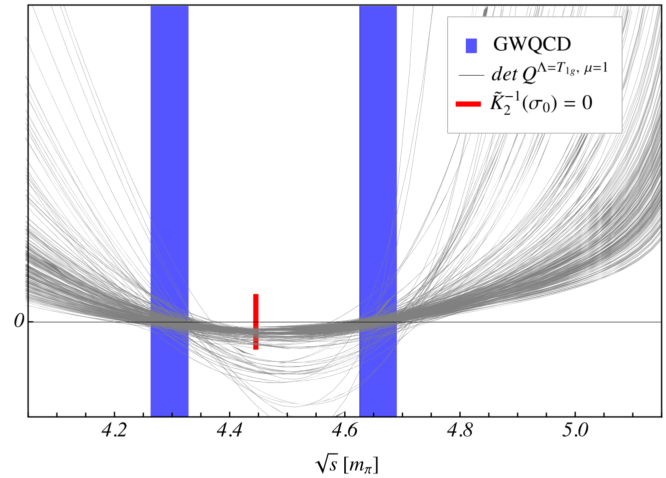

FIG. 1. Right-hand side of the quantization condition (5) (gray) refitted to the correlated LQCD energy eigenvalues (blue bars indicating 1-σ uncertainties). The red bar shows the position of the ground level in the case of vanishing interactions.

$\bar{q}q$ operator and multimeson operators for each of the most prominent decay channels of the $a_1(1260)$, $\rho\pi, \sigma\pi$, and $\pi\pi\pi$. Further details of the operator construction can be found in supplement A [108].

The most challenging aspect of the calculation is ensuring the operator basis is sufficient to extract the states below the inelastic scattering threshold. For this ensemble and symmetry channel, there are only two such states, yet 11 operators were required to stabilize the fit of the first excited state. We find that the stability of the excited state relies heavily on the inclusion of a three-pion operator where two of the pions have back-to-back momenta $(2\pi/L)(1,1,0)$, despite the expected noninteracting energy of such a three-pion state lying far above the inelastic threshold. In addition, we also ensure stability under the variation of fit range and variational parameters. The obtained energy eigenvalues are depicted in Fig. 1, see supplement C [108] for numerical values.

Quantization condition.—The $a_1(1260)$ couples to three-pion states in the $I^G(J^{PC}) = 1^-(1^{++})$ channel that can be decomposed as $\pi\rho$ in S and D waves, $\pi f_0(500)$ and $\pi(\pi\pi)_{I=2}$ in P waves and other channels. Phenomenologically $(\pi\rho)_S$ is dominant [124] with the branching ratios into other channels quite uncertain [1].

Since the isoscalar $\pi\pi$ interaction weakens at heavier pion mass [101,109,110], for now we restrict the discussion to the $\pi\rho$ channels. In that, and following the unitary three-body formalism [93,125], the $\pi(p_1)\pi(p_2)\pi(p_3) \to \pi(p_1')\pi(p_2')\pi(p_3')$ scattering amplitude can be rewritten in terms of a two-pion spin-1 cluster, carrying a helicity index $\lambda^{(\prime)} \in \{-1,0,1\}$, and a third pion (spectator). For $s \coloneqq (p_1+p_2+p_3)^2 \eqqcolon P^2$, $\sigma_l \coloneqq (P-l)^2$ and $E_l \coloneqq \sqrt{\boldsymbol{l}^2 + m_\pi^2}$ this yields

$$\langle p_1' p_2' p_3' | T_3(s) | p_1 p_2 p_3 \rangle = \aleph \sum_{\substack{\lambda,\lambda' \\ m,n}} \hat{v}_{\lambda'}(\boldsymbol{p}'_{\bar{n}}, \boldsymbol{p}'_{\bar{\bar{n}}}) (\tau(\sigma_{p'_n}) T^c_{\lambda'\lambda}(s, \boldsymbol{p}'_n, \boldsymbol{p}_m) + 2E_{p_n} (2\pi)^3 \delta^3(\boldsymbol{p}'_n - \boldsymbol{p}_m)) \tau(\sigma_{p_m}) \hat{v}_\lambda(\boldsymbol{p}_{\bar{m}}, \boldsymbol{p}_{\bar{\bar{m}}}),$$

$$T^c_{\lambda'\lambda}(s, \boldsymbol{p}', \boldsymbol{p}) = B_{\lambda'\lambda}(s, \boldsymbol{p}', \boldsymbol{p}) + C_{\lambda'\lambda}(s, \boldsymbol{p}', \boldsymbol{p}) + \int \frac{d^3\boldsymbol{l}}{(2\pi)^3 2E_l} (B_{\lambda'\lambda''}(s, \boldsymbol{p}', \boldsymbol{l}) + C_{\lambda'\lambda''}(s, \boldsymbol{p}', \boldsymbol{l})) \tau(\sigma_l) T^c_{\lambda''\lambda}(s, \boldsymbol{l}, \boldsymbol{p}) \quad (1)$$

where $\aleph$ is an isospin combinatorial factor, and in each occurrence $\bar{x} \in \{1,2,3\} \backslash \{x\}$ and $\bar{\bar{x}} \in \{1,2,3\} \backslash \{x, \bar{x}\}$. The coupling of the spin-1 system to the asymptotic states is facilitated via $\hat{v}(p,q)_\lambda = -i\epsilon^\mu_\lambda (p+q)(p_\mu - q_\mu)$ for the usual helicity state vectors ϵ, provided for convenience in supplement B [108]. The $\pi\rho$ interaction kernel projected to $I = 1$ consists of (1) the one-pion-exchange term

$$B_{\lambda'\lambda}(s, \boldsymbol{p}', \boldsymbol{p}) = \frac{\hat{v}^*_{\lambda'}(P - p - p', p) \hat{v}_\lambda(P - p - p', p')}{2E_{\boldsymbol{p}'+\boldsymbol{p}}(\sqrt{s} - E_{\boldsymbol{p}} - E_{\boldsymbol{p}'} - E_{\boldsymbol{p}'+\boldsymbol{p}})}, \quad (2)$$

which is a consequence of three-body unitarity [125]; and (2) a short-range three-body force generically parametrized by a Laurent series in the JLS basis, denoting total, relative and intrinsic angular momentum, respectively. For ($\ell^{(\prime)} \in \{S, D\}$),

$$C_{\ell'\ell}(s, \boldsymbol{p}', \boldsymbol{p}) = \sum_{i=-1}^{\infty} c^{(i)}_{\ell'\ell}(\boldsymbol{p}', \boldsymbol{p}) \left(\frac{s - m^2_{a_1}}{m^2_\pi} \right)^i, \quad (3)$$

including first-order poles to account for resonances. The projection to helicity basis follows standard procedure [111], recapitulated in supplement B [108].

The spin-1 propagator ensures two-body unitarity in all subchannels and is expressed in terms of an n-times subtracted self-energy Σ_n and a K-matrix-like quantity $\tilde{K}_n$,

$$\begin{aligned} \tau^{-1}_{\lambda'\lambda}(\sigma_p) &= \delta_{\lambda'\lambda} \tilde{K}^{-1}_n(s, \boldsymbol{p}) - \Sigma_{n,\lambda'\lambda}(s, \boldsymbol{p}), \\ \tilde{K}^{-1}_n(s, \boldsymbol{p}) &= \sum_{i=0}^{n-1} a_i \sigma^i_p \text{ and } \Sigma_{n,\lambda'\lambda}(s, \boldsymbol{p}) \\ &= \int \frac{d^3k}{(2\pi)^3} \frac{\sigma^n_p}{(4E^2_k)^n} \frac{\hat{v}^*_{\lambda'}(P - p - k, k) \hat{v}_\lambda(P - p - k, k)}{2E_k(\sigma_p - 4E^2_k + i\epsilon)}. \end{aligned} \quad (4)$$

We found that $n = 2$ is sufficient to render the self-energy term convergent without destroying analytic properties of the amplitude in Eq. (1). The finite-volume version of Eq. (4) captures the power-law finite-volume effects, see Ref. [126] for exponentially suppressed t and u channel contributions.

Putting an interacting multihadron system into a cubic box of size L restricts the momentum space $\mathbb{R}^3 \to \mathcal{S}_L \coloneqq (2\pi/L)\mathbb{Z}^3$. This means that the integral equation (1) becomes an algebraic one via $\int d^3\boldsymbol{k}/(2\pi)^3 \to 1/L^3 \sum_{\boldsymbol{k} \in \mathcal{S}_L}$, the solutions of which are singular if and only if mesons are on shell. Thus, the positions of singularities in $s < 5m_\pi$ are equivalent to the energy eigenvalues up to $e^{-m_\pi L}$ terms, determined from

$$0 = \det[B(s) + C(s) - E_L(\tilde{K}^{-1}_2(s) - \Sigma^L_2(s))]_{\substack{(\lambda'\lambda) \\ (\boldsymbol{p}'\boldsymbol{p})}}, \quad (5)$$

which defines the generalized FVU quantization condition. Here $E_L \coloneqq 2E_p L^3$, while the explicit expression for the finite-volume Σ^L_2 is provided in supplement B [108]. The major novelty induced by the ρ spin lies in the nondiagonal $\Sigma_{\lambda'\lambda}$ corresponding to in-flight mixing of ρ helicities.

We note that the determinant is taken over helicity ($\lambda \in \{-1, 0, +1\}$) and spectator momentum spaces ($\boldsymbol{p} \in \mathcal{S}_L$). Finding the energies associated with a particular row μ of irrep Λ of the symmetry group G can be done in the standard fashion by block diagonalizing the quantization condition and examining the determinant only for the relevant block [72,127]. In practice this is accomplished by first converting from the helicity basis to canonical state vectors, $|\boldsymbol{p}\lambda\rangle \to \langle \boldsymbol{p}m|$, then block diagonalizing, $|\boldsymbol{p}m\rangle \to \langle \Lambda\mu|$.

Fits.—The quantization condition in Eq. (5) contains the volume-independent, regular quantities C and $\tilde{K}^{-1}_2$. We fix the parameters of the latter by using the two-pion finite-volume spectrum [100–102], matching the isovector amplitude $T^{I=\ell=1}_{22} = \hat{v}\tau\hat{v}$ to the one determined in Ref. [109]. We obtain $a_0 = -0.1577\ m^2_\pi$, $a_1 = 0.0133$.

The three-body force in Eq. (3) is inherently cutoff dependent with respect to the spectator momentum in Eq. (5). This cutoff needs to be held fixed when connecting finite and infinite-volume quantities. We take $|\boldsymbol{p}| \leq 2\pi/L|(1,1,0)| \approx 2.69\ m_\pi$. Finally, exploring various possibilities we found that truncating the general expansion (3) according to

$$C_{\ell'\ell}(s, \boldsymbol{p}', \boldsymbol{p}) = g_{\ell'} \left(\frac{|\boldsymbol{p}'|}{m_\pi} \right)^{\ell'} \frac{m^2_\pi}{s - m^2_{a_1}} g_\ell \left(\frac{|\boldsymbol{p}|}{m_\pi} \right)^\ell + c\delta_{\ell'0}\delta_{\ell0}, \quad (6)$$

yields a sufficient parametrization of the three-body spectrum. We emphasize that with only two three-body levels (as expected for the given $m_\pi L \approx 3.3$) the fit parameters will be poorly constrained.

To assess statistical uncertainty, we perform fits of $\{m_{a_1}, g_S, g_D, c\}$ to resampled energy eigenvalues, each time picking a random starting value $5m_\pi < m_{a_1} < 12m_\pi$. The result is depicted in Fig. 1 using a subset of all considered samples (2000). The distribution of parameters and correlations, along with χ^2 distributions are provided in supplement C [108]. We find the largest correlations in (m_{a_1}, g_D) and (g_S, c), meaning that the bare mass m_{a_1} can be easily renormalized by the D-wave a_1 self-energy which is proportional to g_D^2; indeed, the latter is almost real in the considered energy region and therefore strongly correlated with the real m_{a_1} parameter. As a sanity check, when adiabatically tuning down the $\pi\pi$ interaction, the ground level indeed approaches the energy at which $\tilde{K}_2^{-1} = 0$ (red bar in Fig. 1), as the ρ becomes infinitely narrow and stable at the corresponding invariant mass.

Analytic continuation and poles.—To extract the physical resonance parameters, i.e., the pole position and branching ratios of the $a_1(1260)$, we turn back to the infinite-volume scattering amplitude in Eq. (1). With all parameters fixed from the lattice, $T^c_{\ell'\ell}$ is calculated in the JLS basis [93,128]. The integration over spectator momenta is performed on a complex contour, avoiding singularities for both real and complex-valued $\sqrt{s}$. See supplement D [108] for technical details and the projection $T^c_{\lambda'\lambda} \to T^c_{\ell'\ell}$.

For each of the obtained parameter sets, we search for singularities of $T^c_{\ell'\ell}$ on the second Riemann sheet. The resulting pole positions are depicted in blue in Fig. 2. As expected from the previous discussion of parameter correlation a precise determination of the a_1 pole position requires more input. Surprisingly, the distribution of poles is indeed finite with a stronger concentration around heavier a_1. This is apparent as the darker blue regions indicate higher sample density.

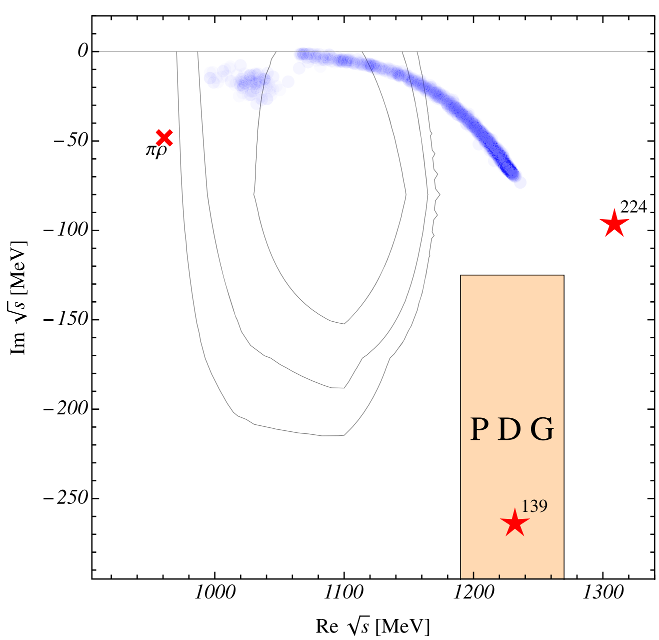

FIG. 2. The a_1 pole positions from FVU (darker blue indicates higher sample density). The PDG result [1] and its uncertainties are included as the orange rectangle. The $\pi\rho$ branch point is indicated by the red cross and a naive chiral extrapolation with red stars (from $m_\pi = 139$ MeV to $m_\pi = 224$ MeV). The crude two-body Breit-Wigner–Lüscher approximation is indicated with black contours.

Putting our results into perspective: (1) We compare them to an approximate procedure employed earlier [96], assuming a stable ρ-meson. In that, using Lüscher's method [129,130] the finite-volume spectrum is mapped to phase-shifts. Subsequently, a simple Breit-Wigner parametrization is used to determine the pole positions. The resulting confidence regions are depicted by the black (un-shaded) contours in Fig. 2. It appears that this Breit-Wigner approach has only small overlap with the full FVU at lower masses, demonstrating the need for using the full three-body quantization condition. (2) We depict the current Particle Data Group (PDG) values [1] as $\sqrt{s} \approx M - i\Gamma/2$ in Fig. 2. The real part of the PDG mass overlaps with our predictions, but the PDG width is at least twice as large. This is expected since the pion mass in our case is heavier than the physical one, resulting in a reduced phase space for resonance decay. (3) We perform a qualitative chiral extrapolation of fits to experimental data [93]. The corresponding pole determination at the physical point is the first of its kind with a three-body unitary amplitude. Then, we increase the pion mass appearing in the loops and the ρ mass, but we cannot modify other parameters because there is no model for their mass dependence. (see supplement D [108] for technical details). With this incomplete extrapolation, we obtain the second red star in Fig. 2 ("224"). It confirms the expectation of the a_1 becoming heavier and narrower. Although this does not lead to an overlap with the pole region from LQCD, as expected, it does demonstrate that quark mass effects can be as large as the observed discrepancy. Pole extractions from future lattice data at different pion masses will allow to directly map out the chiral trajectory.

Finally, one can ask whether an explicit singularity in our parametrization leads to a bias towards the existence of an $a_1(1260)$. Removing that pole and allowing for one more term in the Laurent expansion, i.e., setting $C_{\ell'\ell} \coloneqq (c + c's)\delta_{\ell'0}\delta_{\ell 0}$, one obtains fits that all lead to a pole in the $\pi\rho$ amplitude. While those poles are concentrated close to the real axis at $\sqrt{s} \approx 1.04$ GeV, i.e., too light and too narrow, the exercise shows that a_1 poles are dynamically generated as demanded by LQCD data even if no explicit singularities are present in the parametrization of C.

The pole residues of the amplitude factorize [93], $\mathrm{Res}(T^c_{\ell'\ell}(\sqrt{s})) = \tilde{g}_{\ell'}\tilde{g}_{\ell}$ in terms of couplings $\tilde{g}_S$ and $\tilde{g}_D$, analogously to the usual branching ratios but independent of background terms [1]. Their 1-σ regions are shown in Fig. 3 as a function of real spectator momentum. Clearly there are systematics attached (e.g., the missing $\pi\sigma$ channel) to this first determination of the resonance coupling, which can be addressed once the LQCD dataset is increased. We expect these effects to be small [131].

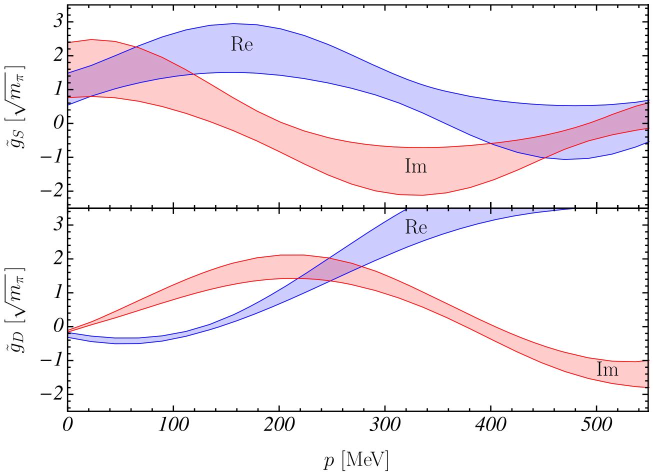

FIG. 3. The 1-σ confidence regions for the couplings $\tilde{g}_S$ and $\tilde{g}_D$ defined by pole residues (see text).

The calculation of pole position and residues for a three-body unitary amplitude is another novelty of this work.

Summary.—In this Letter we have presented the first determination of the resonance parameters of the axial a_1 resonance from QCD. For that, three milestones had to be reached. First, the finite-volume spectrum for a resonant three-hadron system was determined including three-meson operators in a lattice QCD calculation. Second, a three-body quantization condition including subsystems with spin and coupled channels was derived and applied to the finite-volume spectrum. Finally, the corresponding unitary three-body scattering amplitude was solved and analytically continued to the complex plane to determine the pole positions and branching ratios. We explored various forms of the short-range three-body force. In our main solution we found an overlap of the mass of the a_1 with the phenomenological range, but substantially lower width.

This study paves the way for understanding exotic and hybrid resonances for which three-body dynamics are critical. For the $a_1(1260)$ resonance, further extending the lattice calculation will have many benefits. Additional data at this pion mass will resolve the sub-dominant channels like $\pi\sigma$, and lead to a more precise pole position of the $a_1(1260)$. Results at other pion masses will help complete the picture of the a_1, its chiral trajectory, and its properties from first principles.

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