

Emergence of the $\pi(1300)$ Resonance from Lattice QCD

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The mass of the lightest hadron in nature, the pion, is one seventh of that of the nucleon and one tenth of the mass of its first excited state, the $\pi(1300)$. This enormous energy difference opens an interesting window into the confinement of quarks and the structure of the lightest hadrons. In this Letter, we provide the first calculation of resonance parameters of the $\pi(1300)$ from lattice quantum chromodynamics (QCD). For this purpose, recently derived state-of-the-art tools are adapted and applied both in the construction of three-hadron operators and for mapping finite-volume spectra to infinite-volume amplitudes, subsequently analytically continuing these to complex energies. For our heavy pion mass ensembles, we find a clear signal of the resonance. Making a simple assumption of vanishing pion mass dependence for the three-body force, but incorporating constraints from Chiral Perturbation Theory for all the two-body channels, enables a robust extrapolation to the physical point. Applying model averaging, we extract a pole position of $M_{\pi(1300)} = (1169 \pm 46) - i(62^{+168}_{-62})$ MeV supporting values from phenomenology.

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Introduction—The strong interaction of quarks and gluons as fundamental particles of nature is fascinating and contradicts our daily experience: they behave as individual particles at large energies but only confined into so-called hadrons at low energies. The theory describing this

interaction is called quantum chromodynamics (QCD). Unraveling the spectrum of QCD is at the core of many theoretical endeavors and is also driving large experimental efforts; for recent reviews, see Refs. [1–4]. For example, investigations of states with strange or heavy charm and bottom quarks have been investigated, for instance, with the LHCb experiment at the Large Hadron Collider (LHC) or with the Beijing Spectrometer III (BES III) at the Beijing Electron–Positron Collider II (BEPC II), see, e.g., Ref. [5] or the upcoming/proposed experiments such as AMBER at LHC [6], SIS100 at GSI/FAIR [7], Klong at JLAB [8], STCF [9,10], or CEPC [11].

In the hadron spectrum, the pion, the lightest hadron with a mass of one seventh of the proton, is identified as a Goldstone boson of the spontaneously broken chiral symmetry and, therefore, plays a pivotal role in our understanding of quark-gluon interactions. However, it turns out that its first excited state, listed as $\pi(1300)$ and observed by Ananeva and collaborators in 1981 [12] in diffractive dissociation on nuclei, is much less understood. It is currently assumed to

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have a mass of 1300 ± 100 MeV and a width of 200–600 MeV [13]. However, even the existence of the $\pi(1300)$ as a hadronic resonance might be debatable. While strong evidence for it was found by CLEO [14], an “elusive $\pi(1300)$ ” bump disappeared at low t' in COMPASS [15] resulting in no entry for it in the particle data group (PDG) [13]. If it exists, it is about ten times heavier than the pion, almost mass degenerate with the other members of the first excited pseudoscalar octet, $\eta(1295)$ and $K(1460)$ [16], and as heavy as the excited $N(1440)$ state of the nucleon, which is only 1.5 times heavier than the proton. Unraveling this pattern is, therefore, fundamental to understanding the emergence of the hadron spectrum. In addition, the $\pi(1300)$ is special because its $J^{PC} = 0^{-+}$ quantum numbers allow for a decay to three pions without any centrifugal barrier. Indeed, all pions are in relative S -wave enhancing three-body effects, which distinguishes this resonance from the previously studied ω [17] and a_1 [18] resonances. The S -wave system contains the emblematic $f_0(500)$ resonance [19] in a subchannel and enhances the elusive three-body effects through the strong $\pi\pi$ decays of this broad isobar to recombine with the S -wave spectator pion, making the $\pi(1300)$ a unique testing ground for few-body studies.

The $\pi(1300)$ is important for several fields. First, while it is primarily a $q\bar{q}$ state, it may contain significant $q\bar{q}g$ hybrid components [20,21]. Second, its poorly constrained properties contribute to dominant uncertainties in QCD sum-rule determinations of light-quark masses [22,23]. Third, in $\tau \rightarrow 3\pi\nu_\tau$ decays, the large width of $\pi(1300)$ can enhance charge-parity (CP)-violating effects in extensions of the standard model [24].

Theoretically, there is little known about the $\pi(1300)$ from first principles, which makes such a computation highly desirable and important. The theoretical method of choice is lattice QCD (LQCD), which allows for a non-perturbative computation of the properties of such states from first principles. LQCD is formulated in Euclidean space-time such that unstable states can be accessed only after a mapping of LQCD spectra to scattering amplitudes, possible for two- or three-hadron systems (see reviews [25–27], recent status updates [28–30], and related works [31–50]). The finite-volume framework for three-body decays has been formulated [51–53], but so far only the a_1 [18] and the ω [17] mesons have been investigated directly from the lattice. For the first time, we go beyond the postdiction of well-established resonances and carry out exploratory spectroscopy on the lattice. The $\pi(1300)$ has so far only been investigated without treating it as a resonant state [54,55]; for a review, see Ref. [56]. In this Letter, we go beyond this by performing the first investigation of the $\pi(1300)$ using the full three-body finite-volume formalism. We also study it at two values of the pion mass, which allows us, using effective field theories, to obtain a first theoretical determination of its pole position at the physical point. For the schematic overview of the methodology,

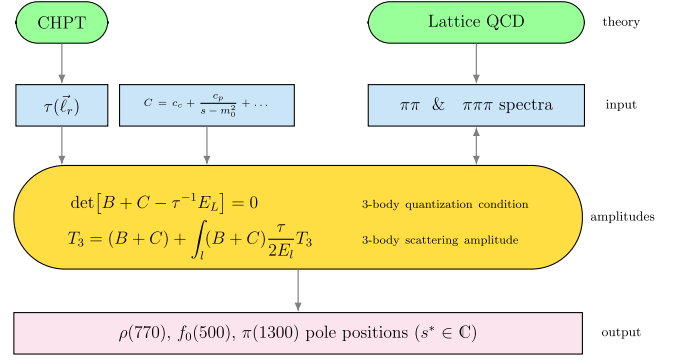


FIG. 1. Workflow of the pole position determination for two- and three-body systems from lattice QCD. Finite-volume spectra are determined from the lattice, while information about short range two- or three-body forces is augmented by chiral perturbation theory (CHPT).

see Fig. 1 and the subsequent section; for further theoretical works, see Refs. [57–61].

Lattice QCD spectrum—LQCD is formulated in a finite volume $L^3 \times T$ in space-time discretized with a lattice spacing, denoted a . Monte Carlo simulations are performed to generate so-called gauge ensembles. In this Letter, we use four such ensembles with $N_f = 2 + 1$ dynamical quark flavors at a single value of the lattice spacing $a = 0.07746(18)$ fm generated by the Chinese LQCD (CLQCD) collaboration; see Ref. [62] for details. The four ensembles (denoted as F32P21, F48P21, F32P30, and F48P30) feature two values of the pion mass $M_\pi \approx 305$ MeV (P30) and $M_\pi \approx 208$ MeV (P21), as well as two spatial volumes with $L = 32$ (F32) and $L = 48$ (F48), respectively. In addition, we have $T = 2L$ for the temporal extent, apart from ensemble F32P30, where $T = 3L$.

The discrete finite-volume spectra are extracted by diagonalizing a correlator matrix $C_{ij}(t) = \langle O_i(t) O_j(0) \rangle - \langle O_i \rangle \langle O_j \rangle$. Its elements are Euclidean two-point correlators of operators O_i . By solving a generalized eigenvalue problem (GEVP) [63–66], so-called principal correlators $\lambda_n(t)$ are determined, which decay as $\lambda_n(t) \sim \exp(-E_n t)$ for large enough t values, such that aE_n can be estimated. Details of the applied analysis procedure, including a discussion of the removal of so-called thermal pollutions, can be found in Supplemental Material [67]. Because of the breaking of the rotational symmetry, the operators O_i are constructed in irreducible representations (irreps) of the cubic group. It has been observed in the literature (for a review, see, e.g., Ref. [3]) that the inclusion of multiparticle operators in $C(t)$ is essential for a reliable determination of the relevant lattice energy levels. Thus, we use the publicly available OpTion package [68] to construct all relevant single- and multiparticle operators in the two-pion ($I = 0, 1, 2$) and three-pion ($I = 1$) channels. In the three- π channel, for instance, we work in the A_1^- irrep with isospin $I = 1$ and appropriate relative momenta including

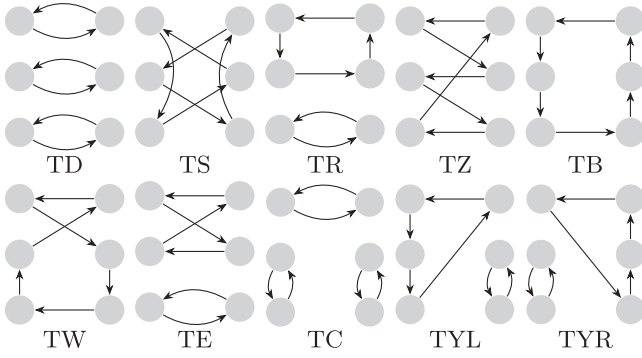


FIG. 2. Diagram topologies for $I = 1$ $\pi\pi\pi \rightarrow \pi\pi\pi$. All diagrams with the same source and sink are permutations and recombinations of these topologies. The other topologies can be found in Supplemental Material [67].

three- π , $\rho\pi$, $\sigma\pi$ and single- π operators. The list of all operators is compiled in Supplemental Material [67].

For the contractions of the correlator matrix, we apply distillation [69], with example contraction topologies shown in Fig. 2. The other topologies and implementation details can be found in Supplemental Material [67]. We note in passing that there are several hundred contractions needed in the three-pion sector, factorially more than in the two-particle channels.

The extracted lattice energy levels are shown in Fig. 3 in lattice units (lower x axis) and in units of M_π (upper x axis)

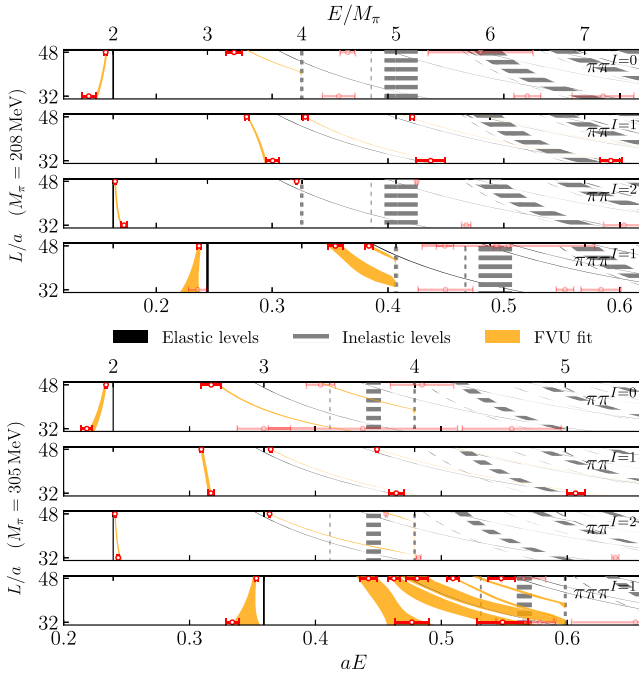


FIG. 3. Finite-volume spectra for $I = 0, 1, 2\pi\pi$ and $I = 1\pi\pi\pi$ for heavy and light pion mass. Red points represent the interacting lattice energy levels, the faded ones of which are not included in the analysis. Solid bands are the noninteracting elastic levels, and dashed bands depict the inelastic levels. The orange bands are the solutions from the overall best fit.

as the red circles for the different ensembles and channels. In the two-pion sector, for $I = 0, 1$ the lowest aE_n is below the $2M_\pi$ threshold, indicating attractive interaction, while aE_n above this threshold is consistent with a small repulsive interaction in the $I = 2$ channel, as expected. In the three-pion sector, a volume-independent ground-state level consistent with the pion mass is observed for both M_π values, but omitted in the figure. Above the 3π threshold, simple identification of levels with states is not possible. We note, however, that there is a visible aggregation of states for $\pi\pi\pi(I = 1)$ with $M_\pi \approx 305$ MeV around and above the $4M_\pi$, indicating strong attraction possibly due to the presence of a resonance. This hypothesis will be tested below.

From LQCD spectra to scattering amplitudes—The lattice spectra provide the first-principle information on the two- and three-body interactions. Practically, this information can be accessed through the so-called quantization condition, for which we employ the state-of-the-art finite-volume unitarity (FVU) three-body quantization conditions [70]; see Refs. [17,18,35,38,71–73] for applications. As such it determines the finite-volume spectrum (fixed irrep, A_1^-) given two- and three-body short range interaction terms K and C as roots of

$$\det[(B + C) - \tau^{-1}E_L] = 0, \quad \tau = (\tilde{K}^{-1} - \Sigma^{\text{FV}})^{-1}, \quad (1)$$

with matrices of dimension corresponding to isospin(I_2) $\times$ helicity(λ) $\times$ spectator – momentum($\mathbf{p} \in (2\pi)/L\mathbb{Z}^3$) space. For the quantum number $I^G(J^{PC}) = 1^-(0^{++})$ in the center of mass system, this yields the following basis $\{\sigma(-\mathbf{p})\pi(\mathbf{p}), \rho(\lambda = -1, -\mathbf{p})\pi(\mathbf{p}), \rho(\lambda = 0, -\mathbf{p})\pi(\mathbf{p}), \rho(\lambda = +1, -\mathbf{p})\pi(\mathbf{p}), G(-\mathbf{p})\pi(\mathbf{p})\}$. Here, σ , ρ , and G serve as placeholders for two-pion subsystems of isospin $I_2 = 0, 1, 2$, respectively. Matrices Σ^{FV} , B , and E_L only depend on momenta and masses, representing all possible on-shell configurations of three pions, while the two- or three-body forces ($\tilde{K}^{-1}/C$) contain the physical information about a particular channel [17,18,74]. We note that the roots of τ^{-1} determine the two-body energy eigenvalues in the pertinent isospin channel.

In the two-body sector, each finite-volume energy eigenvalue determines one value of $\tilde{K}^{-1}$ (neglecting higher partial waves, below inelastic channels). However, in a three-particle system, one particle (spectator) can take certain momentum away, necessitating a detailed understanding of the functional behavior of C and K^{-1} . Little is known about the form of the three-body force for this system, forcing us to pick a generic form for a transition $\alpha \xrightarrow{C} \beta$ in the orbital angular momentum basis [75],

$$c^{\alpha\beta} = c_c^{\alpha\beta} + \frac{c_p^{\alpha\beta}}{s - m_0^2}, \quad \alpha = \beta \in \{\sigma\pi, \rho\pi\}, \quad (2)$$

where s is the total three-body energy squared, and only the phenomenologically most relevant channels are turned on.

In contrast to this, for the relevant two-body subsystem, we can take advantage of many existing theoretical studies and relate its dynamics directly to phase shifts as

$$\begin{aligned}\tilde{K}_{I_2}^{-1}(\sigma) &= K_{I_2}^{-1}(\sigma) + \text{Re}\Sigma_{I_2}^{\text{IV}}(\sigma), \\ K_{I_2}^{-1}(\sigma) &= \begin{cases} -\frac{p(\sigma)\cot\delta_{I_2}^{I_2}(\sigma)}{16\pi\sqrt{\sigma}}, & \text{for } I_2 = 0, 2, \\ -\frac{p^3(\sigma)\cot\delta_{I_2}^{I_2}(\sigma)}{12\pi\sqrt{\sigma}}, & \text{for } I_2 = 1. \end{cases} \quad (3)\end{aligned}$$

Here, σ , p , and Σ^{IV} denote two-body invariant mass squared, two-body center-of-mass momentum and two-body self-energy integral, respectively. For explicit (now standard) formulas, see Refs. [17,74]. To parametrize the phase shifts, we adopt a well-tested [76–78] modified inverse amplitude method (mIAM) approach [79] that synthesizes S -matrix theory and chiral perturbation theory (CHPT). The amplitude behaves correctly (including Adler zero) deep below the two-body threshold, which is needed for the three-body formalism. However, at some very low σ , it is unrealistic, mitigated here by $K_{I_2}^{-1}(\sigma) \mapsto K_{I_2}^{-1}(\sigma_{\text{MP}})e^{-\sigma+\sigma_{\text{MP}}}$, effectively turning the interaction smoothly to zero below the matching point σ_{MP} . The latter, together with the largest spectator momentum $|l_{\text{max}}|$ and the largest self-energy $|k_{\text{max}}|$, represents all necessary cutoffs of the three-body formalism. The procedure outlined above is depicted graphically in Fig. 1.

Analysis and results—When applying the three-body quantization to finite-volume spectra, certain choices [e.g., parametrization in Eq. (2), or cutoffs] need to be made. To assess the systematics associated with this, we have tested ~ 2000 different scenarios, all of which are described in Supplemental Material [67]. We found that varying cutoffs from $\sigma_{\text{MP}} = 1M_\pi^2$, $|l_{\text{max}}| = \sqrt{3}[(2\pi)/(aL)]$, $|k_{\text{max}}| = \sqrt{3} \cdot 5^2[(2\pi)/(aL)]$ does not have any significant impact on our fit/final results. This leaves us with 47 main fits with their quality shown in Fig. 4. The quality of the overall best

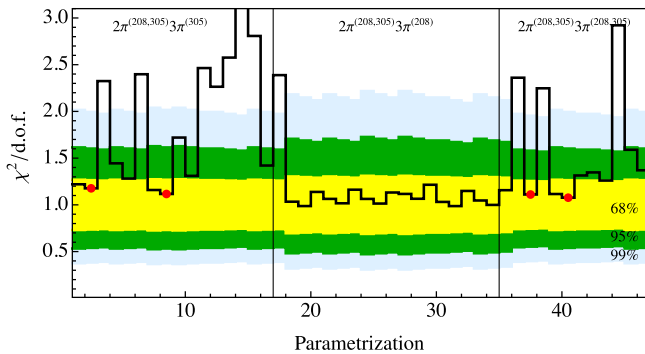


FIG. 4. Quality of the 47 central fit results. The used LQCD input is marked as $2\pi^{(M_\pi)}$ and $3\pi^{(M_\pi)}$, respectively. The 68%, 95%, and 99% confidence intervals around $\mathbb{E}[\chi^2]$ of the χ^2 distribution are shown by the shaded bands; dots mark our best fits, used to determine the pole positions in Fig. 5.

fit ($\chi^2/d.o.f. = 1.08$, see parameter table in Supplemental Material [67]) is contrasted with the available finite-volume spectra in Fig. 3.

We observe that, when only light pion mass three-body input (F32/48P21) is considered, nearly all types of parametrizations of C lead to excellent fit quality within the 68% confidence interval of the χ^2 distribution. The likely reason for this is that there are only very few energy levels below the relevant threshold (see Fig. 3). Besides this, we consistently observe that a slightly better $\chi^2/d.o.f.$ is obtained for mIAM3. We, therefore, only use mIAM3 fits in the following to avoid overcounting similar models.

The parameters obtained in the fit to the finite-volume spectra are used in an infinite-volume three-body formalism (IVU) [17,73,74,80,81], allowing us to extract universal parameters of hadron resonances; see Fig. 1 for the general workflow. This requires solving an integral equation, accomplished efficiently using the complex contour method. For details and comparisons between methods, see Refs. [74,82,83]. We note that integrating over the momentum of the spectator up to a certain cutoff defines the maximal energy range up to which the amplitude fulfills unitarity, i.e., $\sqrt{s_{\text{max}}} = \sqrt{\sigma + l_{\text{max}}^2} + \sqrt{M_\pi^2 + l_{\text{max}}^2}|_{\sigma=4M_\pi^2}$. On the other hand, for a fixed s , larger cutoff values can lead to $\sigma \ll \sigma_{\text{MP}}$, rendering the two-body input unrealistic. We observe that our cutoff choice maximizes the range of applicability of the methodology.

For the fits to light pion mass data only, we observe that only a few of the fits lead to a $\pi(1300)$ pole. This, but also a very sparse finite-volume spectrum in Fig. 3, indicates that $\pi(1300)$ is weakly pion mass dependent with a pole expected at $M_{\pi(1300)} \approx 1300/208 \gtrsim 6M_\pi$ —well outside of the energy range that can be tackled by current lattice and finite-volume methods. Luckily, this is not the case for the heavy pion mass $M_{\pi(1300)} \approx 1300/305 \approx 4.2M_\pi$, such that all fits in 68%, 95%, and 99% confidence intervals around the observed χ_{obs}^2 indeed lead to a $\pi(1300)$ pole. Interestingly, these fits include also those with no explicit pole term in the parametrization of the three-body force, thus generating a $\pi(1300)$ pole dynamically.

Taking into account fits in the 68% confidence interval around $\mathbb{E}[\chi^2]$ of the χ^2 distribution, which include heavy three-body input (red dots in Fig. 4), we extract pole positions depicted in Fig. 5, including the pole positions of the two-pion resonances in the isovector and isoscalar subsystems. Extrapolating to the physical point in the two-body sector is achieved by setting M_π to its physical value as dictated by CHPT. In the three-body case, the simplest ansatz (see above) is to use parameters obtained from fits to the heavy pion mass data, assuming negligible pion mass dependence of all terms in Eq. (2) evaluated in physical/lattice units. Results of individual fits and a model average of those using the Akaike information criterion [84] are depicted in Fig. 5. The model average result constitutes our

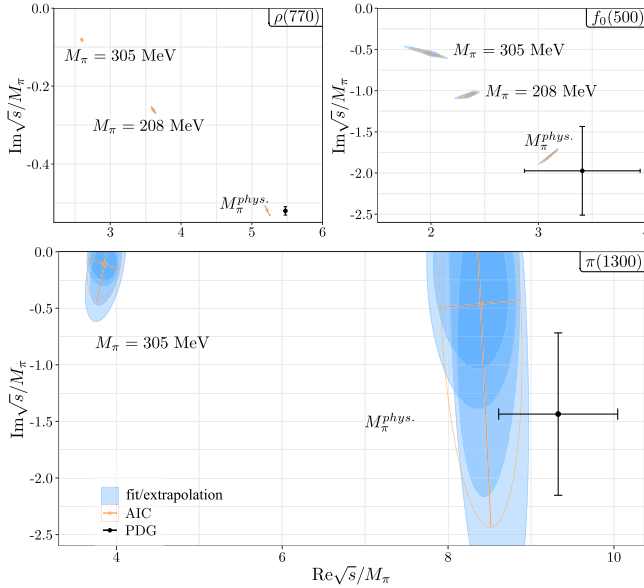


FIG. 5. Pole positions on the second Riemann sheet of the two- and three-hadron systems with total energy $E \in \mathbb{C}$, respectively, to $\rho(770)$, $f_0(500)$, $\pi(1300)$ states. Shaded areas represent results from individual fits in the 68% confidence interval around the observed χ^2_{obs} . Orange crosses depict the AIC model-averaged results. PDG results are provided by the black crosses for comparison.

principal finding,

$$\begin{aligned} M_{\pi(1300)} &= (1169 \pm 46) - i(62 \pm 169) \text{ MeV}, \\ M_{\rho(770)} &= (727 \pm 3) - i(72 \pm 1) \text{ MeV}, \\ M_{f_0(500)} &= (433 \pm 7) - i(250 \pm 7) \text{ MeV}. \end{aligned} \quad (4)$$

Our results for the two-body resonances agree quite well with the PDG values [13], except for $\text{Re} M_{\rho(770)}$. Since our result for $\text{Re} M_{\rho(770)}$ is consistent with previous lattice studies on these but also other ensembles [17,76], we attribute this discrepancy to finite lattice spacing effects, discussed in Ref. [85] using the same lattice configurations. The agreement in all other results indicates (a similar observation was made recently in [46]) that the three-body data actually constrain the two-body sector, for which larger uncertainties would be expected otherwise.

Regarding the main goal and novel result of this Letter—the prediction of the parameters of the excited state of the pion from QCD—we observe agreement with the PDG values within 1σ uncertainties. We emphasize that, for all extracted pole positions $\text{Im} M_{\pi(1300)} < 0$, while the extracted errors are unconstrained due to the simplistic Gaussian statistics employed here.

Conclusion—We have determined the resonance parameter of the $\pi(1300)$ from QCD through a lattice calculation of finite-volume spectra including one-, two-, and three-hadron operators, and by utilizing state-of-the-art

three-particle quantization conditions. Our light pion three-body spectra do not provide sufficient input for a reliable extraction of resonance parameters. At the heavier pion mass, all fits lead to a scattering amplitude featuring a resonance, effectively ruling out the no-resonance scenario. With these results and the simplest possible ansatz for the quark-mass dependence of the three-body force, the resonance parameters at the physical point are extracted and found to be comparable with PDG values.

Various sources of systematics have been tested, such as different parametrizations of the two-/three-body input or cutoff dependencies, which only mildly affect our main conclusions. Still, in the future, it would be interesting to map out the quark-mass dependence in more detail, for example, at even heavier pion mass values. Additionally, providing line shapes and Dalitz plots would be of great interest for comparing them to phenomenological studies of multihadron.

Software QUDA [86–88] is used to solve the perambulators, as performed in Refs. [89,90].

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Data availability—The data that support the findings of this article are openly available [91].

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