

Finite-volume spectrum of $\pi^+\pi^+$ and $\pi^+\pi^+\pi^+$ systems

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The finite-volume spectrum of the $\pi^+\pi^+$ and $\pi^+\pi^+\pi^+$ systems is deduced using a previously derived 3-body quantization condition. The results agree perfectly with the available lattice data from NPLQCD collaboration ($L = 2.5$ fm and $m_\pi \in \{291, 352, 491, 591\}$ MeV). Statistical uncertainties are estimated and extrapolations to physical pion mass are performed.

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Introduction Rapid computational and algorithmic advances of Lattice QCD occurred over the recent years, allowing to gain new insights into the structure and interaction patterns of hadrons. Performed in a finite volume, such *ab-initio* calculations result in a discrete eigenvalue spectrum. The latter is related to the infinite volume one by the virtue of the quantization condition.

Lüscher’s method [1, 2] is such a condition for 2-body systems with generalizations to, e.g., higher spins and multi-channel systems [3–8]. However, many open questions of modern hadron physics (e.g. the existence of spin-exotics or the Roper-puzzle) are related to systems with three particles. First Lattice QCD calculations have already been performed [9–12]. The corresponding 3-body quantization condition has been explored thoroughly in last years [13–21] including some numerical investigations [20–23]. However, an analysis of physical systems has not yet been performed.

In this work we present a first data-driven simultaneous analysis of finite-volume spectrum of 2- and 3-body systems ($\pi^+\pi^+$ and $\pi^+\pi^+\pi^+$) using the quantization condition derived in Ref. [20]. The importance of this channel is twofold: 1) The ground state level is available from the NPLQCD Collaboration [24, 25] for ($L = 2.5$ fm and $m_\pi \in \{291, 352, 491, 591\}$ MeV); 2) This repulsive $\pi\pi$ channel is a critical test bed for our formalism [20, 26] with respect to its flexibility.

In particular, our program consists of prediction of the full (up to the 4π threshold) finite-volume spectrum using experimentally available data. Subsequently, we will fix the remaining parameter (genuine 3-body coupling) to the ground-state energy level of the $\pi^+\pi^+\pi^+$ system [24, 25], predicting higher levels up to the 5π threshold.

Quantization condition In the following, we will use the 3-body quantization condition [20] derived from the unitary, relativistic 3-body isobar scattering amplitude [26]. After the projection to the irreducible representations (irreps) of the cubic group (see Sec. IV of Ref. [21]), it reads

$$\det \left(B_{uu'}^{\Gamma_{ss'}} + \frac{2E_s L^3}{\vartheta(s)} \tau_s^{-1} \delta_{ss'} \delta_{uu'} \right) = 0, \quad (1)$$

where the determinant is taken with respect to the basis index $u^{(\prime)}$ for a given irrep $\Gamma \in \{A_1, A_2, E, T_1, T_2\}$ and $s^{(\prime)}$ denotes the sets of momenta related by cubic symmetry (“shells”). On a shell s , the number of points is denoted by $\vartheta(s)$ and the energy of pions by $E_s := E_{\mathbf{p}} := \sqrt{m_\pi^2 + \mathbf{p}^2}$, respectively. In the following, we will work in the center of mass system of three pions with the total four-momentum $P = (W_3, \mathbf{0})$, suppressing the dependence of W_3 for brevity.

Condition (1) contains two parts: the driving term $B_{uu'}^{\Gamma_{ss'}}$ of the isobar-spectator interaction and the isobar propagator τ_s . The form of these terms is fixed by 3-body unitarity up to real valued functions C and K . In particular, and before the projection to the irreps [21], they read

$$B_{\mathbf{q}\mathbf{p}} = -\frac{f((P-2\mathbf{q}-\mathbf{p})^2)f((P-\mathbf{q}-2\mathbf{p})^2)}{2E_{\mathbf{q}+\mathbf{p}}(W_3-E_{\mathbf{p}}-E_{\mathbf{q}}-E_{\mathbf{q}+\mathbf{p}})} + C_{\mathbf{q}\mathbf{p}}, \quad (2)$$

$$\tau_{\mathbf{q}}^{-1} = K_{\mathbf{q}}^{-1} - \frac{J_{\mathbf{q}}}{L^3} \sum_{\mathbf{x} \in \frac{2\pi}{q} \mathbb{Z}^3} \sum_{\pm} \frac{\left(f \left((P_{\mathbf{q}}^* \pm 2\mathbf{k}_{\mathbf{x},\mathbf{q}}^*)^2 \right) \right)^2}{4\sqrt{\sigma_{\mathbf{q}}} E_{\mathbf{k}_{\mathbf{x},\mathbf{q}}^*} \left(\sqrt{\sigma_{\mathbf{q}}} \pm 2E_{\mathbf{k}_{\mathbf{x},\mathbf{q}}^*} \right)},$$

where \mathbf{p}/\mathbf{q} are the three-momenta of the in/outgoing spectator pions (being identical for the propagator) and $P_{\mathbf{q}}^* := (\sqrt{\sigma_{\mathbf{q}}}, \mathbf{0})$ is the four-momentum of the isobar (two-pion system) boosted to its reference frame. The invariant mass squared of the latter reads $\sigma_{\mathbf{q}} = W_3^2 + m_\pi^2 - 2W_3 E_{\mathbf{q}}$. The three-momentum of pions \mathbf{x} boosted by \mathbf{q} is denoted by $\mathbf{k}_{\mathbf{x},\mathbf{q}}^*$ with $J_{\mathbf{q}}$ being the corresponding Jacobian. Furthermore, the form-factor $f(Q^2)$ yields a smooth cutoff of an otherwise log-divergent self-energy part of the isobar propagator (second term in τ^{-1} of Eq. (2)). Note, that this cutoff-dependence cancels in the full quantization condition (1) by the functions C and K . Specifically, we have chosen here $f(Q^2) = 1/(1 + e^{-(\Lambda/2-1)^2 + Q^2/4})$.

In conclusion, we emphasize that the above expressions are equivalent to the originally derived ones [20] when multiplying the matrix expression in Eq. (1) from left and right with the regular function $\lambda_{\mathbf{q}}$ – the disso-

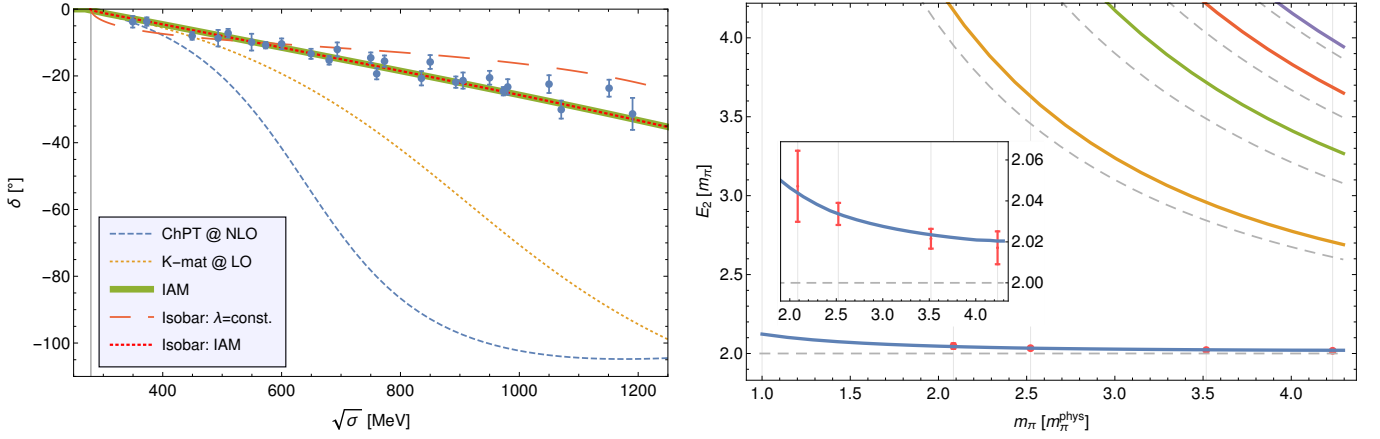


FIG. 1. Left: Comparison of available phase-shift data [27–29] with the prediction of the considered models. Right: Prediction of 2-body energy levels (full) as a function of m_π with dashed lines denoting non-interacting levels. The inset shows a zoom-in on the ground level, where the red points denote the result of the lattice calculation [24, 25].

ciation vertex of the isobar (two-pion system) with the four-momentum $P-q$. In particular, $K_q = \lambda_q^2/(\sigma_q - M_0^2)$ for parameter M_0 as used in the original quantization condition [20]. In general, the quantization condition (1) is a coupled-channel equation with respective “copies” of Eq. (2) and parameters therein. Dealing here with a 3-pion system of maximal isospin in S-wave, only one isobar ($\pi^+\pi^+$ sub-system) is of interest, while the irrep will be fixed throughout this work to $\Gamma = A_1^+$.

Two-body subsystem The 3-body scattering amplitude [26] corresponding to the quantization condition (1) fulfills 2- (in every sub-channel) and 3-body unitarity by construction. The corresponding normalized 2-body scattering amplitude, projected to the S-wave, reads

$$T_2(\sigma) = -(\lambda(\sigma)f(4m_\pi^2 - \sigma))^2 \frac{\hat{\tau}(\sigma)}{32\pi} \quad \text{for} \quad (3)$$

$$\frac{1}{\hat{\tau}(\sigma)} = K^{-1}(\sigma) - \sum_{\pm} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{(f((\sqrt{\sigma} \pm 2E_k)^2 - 4k^2))^2}{4E_k \sqrt{\sigma}(\sqrt{\sigma} \pm 2E_k)},$$

where $\hat{\tau}$ is the infinite-volume counterpart of the isobar propagator τ and σ is the invariant mass squared of the 2-body system. The yet unknown parameters (λ and M_0) will be constrained using the available experimental phase-shifts [27–29] in the following.

We have explored several ansatzes for the functional form of λ , collecting the outcome as depicted in Fig. 1. In the simplest case ($\lambda = \text{const.}$) we fit λ and M_0 to the experimental data obtaining a sufficiently good agreement with data. This, however, cannot be guaranteed at unphysical pion masses, unless one uses input from chiral perturbation theory. The perturbative amplitude of the next-to-leading chiral order [30] and the unitarized amplitude using only the leading chiral order describe the data well only in close proximity to the $\pi\pi$ -threshold. We found that the Inverse Amplitude Method (IAM), see Refs. [31, 32], i.e. $T_{\text{LO}}^2/(T_{\text{LO}} - T_{\text{NLO}})$, shows the

best agreement with the data. Furthermore, it can be expressed in the form of Eq. (3), demanding

$$\lambda^2 = (M_0^2 - \sigma) \left(\frac{d}{4\pi^2} + \frac{T_{\text{LO}} - \bar{T}_{\text{NLO}}}{T_{\text{LO}}^2} \right)^{-1}, \quad (4)$$

where \bar{T}_{NLO} denotes the next-to-leading order chiral amplitude [30] without the s-channel loop, which depends on low-energy constants (LECs) taken from the same reference. The constant d compensates for the fact that dimensional regularization was used in Ref. [30], while in the present ansatz we use form-factors to regulate the divergences. We found that choosing $\Lambda = 42m_\pi$ corresponds to $d = 0.86$ such that the both formulations of the scattering amplitude coincide perfectly, see, e.g., left panel of Fig. 1, which also holds for all pion masses in question. In particular, the scattering lengths read for unphysical pion masses

$$a_{291} = -0.1478_{-0.0550}^{+0.0356}, \quad a_{352} = -0.2016_{-0.1008}^{+0.0663}, \quad (5)$$

$$a_{491} = -0.3622_{-0.1395}^{+0.1914}, \quad a_{591} = -0.5406_{-0.1728}^{+0.3645},$$

and $a_{139.57} = -0.0433(37)$ for the physical one, which compares perfectly with $-0.0444(10)$ from Roy equation analysis [33]. The uncertainties are determined from resampling of the LECs taking uncorrelated error bars from Ref. [30].

Unitarity, correct description of data and proper chiral behavior are the only features required for the realistic prediction of the finite volume spectrum. Therefore, having fixed λ as described before, we predict the $\pi^+\pi^+$ finite-volume spectrum ($L = 2.5$ fm), determining the roots of τ^{-1} from Eq. (2) in the 2-body energy $\sqrt{\sigma}$. Note that this is equivalent to Lüscher’s method [1, 2] up to exponentially suppressed terms.

The result is depicted in the right panel of Fig. (1), while the numerical values for the physical and the pion

m_π [MeV]	139.57	291	352	491	591
E_2^1 [m_π]	$2.1228^{+0.0068}_{-0.0069}$	$2.0437^{+0.0071}_{-0.0086}$	$2.0334^{+0.0076}_{-0.0086}$	$2.0233^{+0.0105}_{-0.0098}$	$2.0204^{+0.0200}_{-0.0106}$
Refs. [24, 25]	—	2.0471(27)(65)	2.0336(22)(22)	2.0215(16)(13)	2.0171(16)(19)
E_2^2 [m_π]	—	—	$3.6245^{+0.0746}_{-0.0299}$	$2.9556^{+0.0728}_{-0.0263}$	$2.7045^{+0.0827}_{-0.0271}$
E_2^3 [m_π]	—	—	—	$3.7114^{+0.1482}_{-0.0737}$	$3.2911^{+0.1241}_{-0.0688}$
E_2^4 [m_π]	—	—	—	—	$3.6802^{+0.0707}_{-0.0902}$
E_2^5 [m_π]	—	—	—	—	$3.9829^{+0.0500}_{-0.0299}$
E_3^1 [m_π]	$3.6564^{+0.1014}_{-0.0847}$	$*3.1444^{+0.0171}_{-0.0192}$	$*3.1058^{+0.0091}_{-0.0147}$	$*3.0655^{+0.0029}_{-0.0095}$	$*3.0537^{+0.0048}_{-0.0119}$
Refs. [24, 25]	—	3.1458(49)(125)	3.1050(27)(27)	3.0665(26)(22)	3.0516(27)(53)
E_3^2 [m_π]	—	—	$4.7301^{+0.1577}_{-0.1027}$	$4.0031^{+0.0196}_{-0.1836}$	$3.7315^{+0.0309}_{-0.0742}$
E_3^3 [m_π]	—	—	—	$4.7043^{+0.0126}_{-0.5923}$	$4.2621^{+0.0001}_{-0.1739}$
E_3^4 [m_π]	—	—	—	$4.7890^{+0.0506}_{-0.1722}$	$4.3155^{+0.0837}_{-0.1341}$
E_3^5 [m_π]	—	—	—	—	$4.5913^{+0.0001}_{-0.1995}$
E_3^6 [m_π]	—	—	—	—	$4.6634^{+0.0001}_{-0.1070}$
E_3^7 [m_π]	—	—	—	—	$4.6995^{+0.0001}_{-0.0661}$

TABLE I. Energy levels of the $\pi^+\pi^+$ (E_2) and $\pi^+\pi^+\pi^+$ (E_3) system (level order is denoted by the subscript) with error bars from a re-sampling procedure. The Lattice QCD results [24, 25] are quoted in bold font with statistical and systematic uncertainties in first and second parenthesis, respectively. Those fitted to the lattice data via the constant genuine 3-body coupling c are denoted by an asterisk.

masses used in the lattice calculation [24, 25] are collected in Tab. I. The quoted error bars are determined in a re-sampling procedure varying the LECs from [30]. For the energy levels determination our Monte-Carlo sample is restricted to a smaller set (40) for technical reasons, which makes the uncertainties on higher levels somewhat indicative.

The result for the post-dicted ground state level agrees nicely with the lattice calculation ($\chi_{\text{p.p.}}^2 = 0.35$), and is in agreement with the large-volume expansion formula [34] using the scattering lengths from Eq. (5) as input. Notably and unexpectedly, the IAM-like chiral extrapolation seem to work well up to very high pion masses. The excited energy levels quoted in Tab. I and shown in the right panel of Fig. 1 are predictions. Note that no 4-particle cuts have been discussed, such that the prediction is reliable and quoted, therefore, up to $E_2 = 4m_\pi$.

Three-body energy shift Having made a prediction for the $\pi^+\pi^+$ energy levels, we turn now to the main point of the present paper, the finite-volume spectrum of the $\pi^+\pi^+\pi^+$ system, which depends on the 2-body input. In a 3-particle system, the invariant mass of the two-particle system can be sub-threshold ($\sqrt{\sigma_{\mathbf{q}}} < 2m_\pi$) for a sufficiently large momentum of the spectator \mathbf{q} . Note that only right-hand (physical) 2-body singularities are included in the derivation of the 3-body scattering amplitude [20, 26], leading to the quantization condition (1). This is all what is needed for the infinite-volume extrapolation. Furthermore, in the absence of 2-body bound states, the infinite-volume 2-body ampli-

tude, derived through a dispersion relation [26], has to be real and regular in the sub-threshold region. In the 3-body framework, this 2-body sub-threshold contribution is compensated by the (still) unknown real function $C_{\mathbf{q}\mathbf{p}}$. Furthermore, in finite volume, corrections from this region are exponentially suppressed. In summary, one can simply fix $K_{\mathbf{q}}^{-1}$ in the unphysical region to a (real) constant, smoothly connected to the physical region, where it reproduces the IAM-type of scattering amplitude as described before.

The remaining unknown piece of the quantization condition (1) is the isobar-spectator function $C_{\mathbf{q}\mathbf{p}}$ in Eq. (2), corresponding to the 3-body contact interaction. This function can only be determined from a fit to actual data. Fortunately, lattice data are available for the ground state [24, 25] in the same setup as for the two-pion system. Note that in general, $C_{\mathbf{q}\mathbf{p}}$ is a function of the in/outgoing spectator momenta (\mathbf{q}/\mathbf{p}) for a given set of parameters such as cutoff in the form factor and in pion mass. We found that already the simplest choice $C_{\mathbf{q}\mathbf{p}} = c\delta^{(3)}(\mathbf{p}-\mathbf{q})$ leads to a good fit to the data [24, 25], i.e. $\chi_{\text{dof}}^2 = 0.05$ for $c = 0.2 \pm 1.5 \cdot 10^{-10}$. The statistical and systematic data uncertainty were added for this fit, which explains the low value of χ_{dof}^2 .

The result of the fit to the ground level as well as prediction of higher levels are depicted in Fig. 2 (central values). The corresponding numerical values are collected in Tab. I with the uncertainties from a re-sampling due to variations of LECs as before. As an additional check we have fitted the ground state

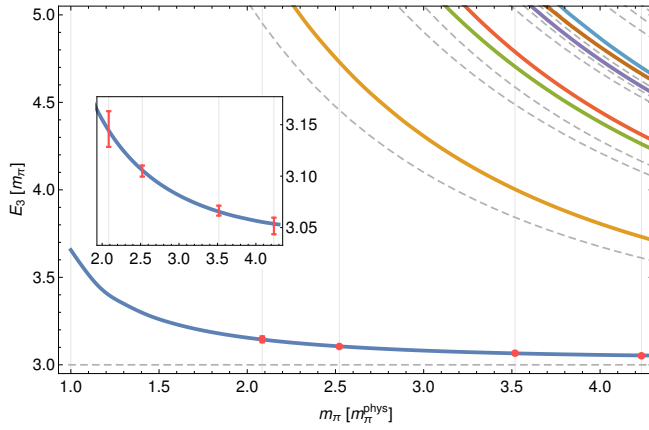


FIG. 2. Prediction of excited energy levels for the $\pi^+\pi^+\pi^+$ -system as a function of pion mass with non-interacting levels represented by dashed lines. The inset shows the zoom-in on the ground level, where the lattice data [24, 25] are shown in red.

levels [24, 25] using the large-volume expansion formula [34] using our scattering lengths (5) and adjusting the unknown 3-body contribution η_3^L (Eqs. (1-5) of [34]). The fit yields $\chi^2_{\text{dof}} = 1.32$ for $\eta_3^L = 1.8 \cdot 10^{-12}$ and $E_3^1 = \{3.1277, 3.1003, 3.0695, 3.0623\} m_\pi$ for $m_\pi = \{291, 352, 491, 591\}$ MeV, respectively. It is interesting to see that not only this confirms our result for the lowest level, but also that the genuine 3-body contribution is similar to c determined before, keeping in mind that the latter was introduced on the level of amplitudes and not a Hamiltonian as η_3^L . Furthermore, it should be noted that in our framework (which is not a Lagrangian framework) c does not directly correspond to a three-body Hamiltonian piece. Besides the emission of a spectator and an isobar it also contains the unstructured emission of three pions from a real-valued three-body term.

On a qualitative level, we observe that the energy levels mimic the pattern of the non-interacting ones shifted to higher energies. This is similar to the 2-body case with the novelty that interacting energy levels not always occur between two non-interacting ones. Furthermore, we have found that all singularities of the argument of the determinant in Eq. (1) are actually simple poles (located at the position of the non-interacting levels), which is a non-trivial fact in 3-body systems.

Conclusion The finite volume spectrum for the $\pi^+\pi^+$ and $\pi^+\pi^+\pi^+$ systems has been analyzed. Using experimental data and a non-perturbative ansatz for the 2-body amplitude we have predicted the $\pi^+\pi^+$ energy levels in finite volume which are in perfect agreement with the lattice data available for the ground state. Finally, using this input and fitting the genuine 3-body contact term to the threshold level determined by the NPLQCD collaboration we have predicted the finite volume spectrum of the $\pi^+\pi^+\pi^+$ system up to $W_3 = 5 m_\pi$.

This is the first prediction of excited levels in a physical three-body system. Possible sources for systematic (choice of parametrization of the 2-body amplitude and its sub-threshold behavior, three-body force, and regularization) and statistical uncertainties have been identified and estimated.

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