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Progress on the three-particle quantization condition

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We report progress on extending the relativistic model-independent quantization condition for three particles, derived previously by two of us, to a broader class of theories, as well as progress on checking the formalism. In particular, we discuss the extension to include the possibility of 2->3 and 3->2 transitions and the calculation of the finite-volume energy shift of an Efimov-like three-particle bound state. The latter agrees with the results obtained previously using non-relativistic quantum mechanics (NRQM).

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1. Introduction

Tremendous progress has been made over the last few years in the calculation of resonance properties from first principles using lattice QCD (LQCD). The present frontier is the determination of the properties of resonances coupling to multiple two-body channels. A recent example is the study of resonances in Ref. [1]. This considers resonances coupling to both the $\pi\eta$ and $K\overline{K}$ channels, albeit with quarks that are heavier than physical. It uses a theoretical formalism—a “two-particle quantization condition" generalized from seminal papers by Lüscher [2, 3]—that relates the spectrum in a finite volume (FV) to the infinite-volume scattering amplitudes.

However, as the quark mass is lowered, an increasing number of resonances couple either dominantly, or in part, to three-particle channels. Examples include $\omega \to 3\pi$, $K^* \to K\pi\pi$ and $N(1440) \to N\pi\pi$ as well as the recently discovered X, Y and Z resonances. If we wish to determine the properties of such resonances from first principles, it is essential to have a generalization of the two-particle quantization condition to one that includes three particles. Such an extension is also needed to use LQCD to study weak decays involving three particles, e.g. $K \to 3\pi$.

In Refs. [4, 5] two of us have provided such a generalization, applicable to three identical, relativistic, spinless particles whose interactions are constrained by a G-parity-like symmetry. We briefly describe this work, referring to Refs. [4, 5] for details. It consists of two parts. The first is a three-particle quantization condition[1]

$$\det(F_3^{-1} + \mathscr{K}_{\mathrm{df},3}) = 0\,. \tag{1.1}$$

where here and below all quantities are infinite-dimensional matrices in the space of on-shell three-particle states in FV.[2] $\mathscr{K}_{\mathrm{df},3}$ is a three-particle generalization of the K-matrix—an infinite-volume quantity that is, however, not physical as it contains an UV cutoff. F_3 is the matrix

$$F_3 = \frac{F_2}{2\omega L^3}\left[\frac{1}{3} - \mathscr{M}_{2,L}F_2 - \mathscr{D}_L^{(u,u)}\frac{F_2}{2\omega L^3}\right], \tag{1.2}$$

where L is the box size (assuming a cubic box), ω the relativistic energy, F_2 is a generalized Lüscher zeta-function (a known volume-dependent matrix), $\mathscr{M}_{2,L}$ is a FV version of the two-particle scattering amplitude, and $\mathscr{D}_L^{(u,u)}$ is the contribution to the FV three-particle scattering amplitude that contains only two-particle interactions. The key point is that F_3 depends only on known, L-dependent kinematic functions and the infinite-volume two-particle scattering amplitude $\mathscr{M}_2$. Thus it can be determined by applying the two-particle quantization condition to the two-particle FV spectrum.

The second part of the three-particle formalism connects $\mathscr{K}_{\mathrm{df},3}$ to the infinite-volume three-particle scattering amplitude $\mathscr{M}_3$ [5]. The latter is obtained using

$$\mathscr{M}_3 = \lim_{L\to\infty}\Big|_{i\epsilon}\mathscr{M}_{3,L}\,, \quad \text{with} \quad \mathscr{M}_{3,L} = \mathscr{S}\left[\mathscr{D}_L^{(u,u)} + \mathscr{L}_L^{(u)}\mathscr{K}_{\mathrm{df},3}\frac{1}{1+F_3\mathscr{K}_{\mathrm{df},3}}\mathscr{R}_L^{(u)}\right]. \tag{1.3}$$

Here the $i\epsilon$ subscript indicates a particular infinite-volume limit, and $\mathscr{M}_{3,L}$ is a FV version of the scattering amplitude. The quantities $\mathscr{L}_L^{(u)}$ and $\mathscr{R}_L^{(u)}$ depend on $\mathscr{M}_2$ and known kinematic functions, like F_3 and $\mathscr{D}_L^{(u,u)}$. Thus if $\mathscr{M}_2$ and $\mathscr{K}_{\mathrm{df},3}$ are obtained, respectively, from the two- and three-particle

[1]This result holds up to exponentially suppressed FV effects, proportional to e^{-mL}, that we ignore throughout.

[2]In any practical application this matrix space must be truncated, as in the two-particle case.

quantization conditions, then $\mathcal{M}_3$ can, in principle, be determined from Eq. (1.3). Working out the details, one finds that this requires solving nested UV-finite integral equations involving on-shell quantities [arising from the implicit matrix indices in Eq. (1.3)] [5].

There are two major limitations of this formalism. First, it assumes a Z_2 symmetry forbidding $1 \to 2$, $2 \to 3$, etc. transitions. Thus it is applicable (to good approximation) to three pions, where G-parity enforces the Z_2 symmetry, but not to most three-particle systems. Second, it requires that the two-particle channel be nonresonant in the kinematic range of interest. For example, in a three-pion system with vanishing total momentum, angular-momentum and $I = 1$, the total energy must satisfy $E < m_\pi + m_R$, where m_R is the position of the pole in the two-particle K-matrix corresponding to the lightest f_0 resonance. This is a very serious limitation on the practical applicability of the formalism.[3]

2. Extensions of the formalism

We are actively working on removing the two limitations just described, and provide a brief update on the status of this work. We have made the most progress on removing the Z_2 symmetry. Based on our analysis so far, we conjecture that the generalized quantization condition is

$$\det\left[\begin{pmatrix} F_2^{-1} & 0 \\ 0 & F_3^{-1} \end{pmatrix} + \begin{pmatrix} \mathcal{K}_2 & \mathcal{K}_{3\to2} \\ \mathcal{K}_{2\to3} & \mathcal{K}_{\mathrm{df},3} \end{pmatrix}\right] = 0\,. \tag{2.1}$$

This rather natural generalization of the three-particle quantization condition (1.1), and the corresponding two-particle result $\det(F_2 + \mathcal{K}_2^{-1}) = 0$, extends the matrix indices to contain both two- and three-particle on-shell FV phase space. This extension arises from the fact that correlators in the Z_2-less theory have cuts containing of any number of on-shell particles. The result (2.1) holds for $m < E < 4m$, where only two and three-particle cuts are allowed. The key point is that physical, on-shell $2 \to 3$ and $3 \to 2$ transitions are allowed, and this leads to the off-diagonal terms in the second matrix in (2.1). These off-diagonal terms contain infinite-volume K-matrices that, like $\mathcal{K}_{\mathrm{df},3}$ (and $\mathcal{K}_2$ below threshold), are unphysical.

One key feature of this conjectured result is that, unlike $\mathcal{K}_{\mathrm{df},3}$, the $2 \to 3$ and $3 \to 2$ K-matrices do not contain divergences arising from long-distance propagation of on-shell particles. $\mathcal{K}_{2\to3}$ and $\mathcal{K}_{3\to2}$ are quasi-local vertices that can be expanded in spherical harmonics.

To establish Eq. (2.1) requires extending the analysis of Ref. [4]. One begins with the skeleton expansion of a FV correlator, locates the position of all possible power-law FV dependence (which are the two- and three-particle cuts), and then replaces FV momentum sums with integrals plus the difference. The skeleton expansion here is more complicated than with a Z_2 symmetry, requiring a large number of additional Bethe-Salpeter kernels. Nevertheless, we have a partial argument leading to (2.1), and hope to complete it soon.

Having done so, the second step will be to relate the four infinite-volume-but-unphysical K-matrices $\{\mathcal{K}_2, \mathcal{K}_{2\to3}, \mathcal{K}_{3\to2}, \mathcal{K}_{\mathrm{df},3}\}$ to the infinite-volume scattering amplitudes $\{\mathcal{M}_2, \mathcal{M}_{2\to3}, \mathcal{M}_{3\to2}, \mathcal{M}_3\}$, i.e. to generalize Eq. (1.3). Our preliminary results indicate that the resulting integral equations are

[3] Other restrictions—to identical, and thus necessarily degenerate, particles and to spinless particles—are expected to be simpler to remove, based on experience with two particles. We do not discuss these here.

coupled, so that all four K-matrices must be known at a given energy in order to determine any of the scattering amplitudes.

We are at an earlier stage in removing the second limitation of the original formalism, namely the requirement that $\mathscr{K}_2$ have no above-threshold poles. Our approach is to use the factorization of the residues of these poles to simplify the resulting expressions, and to explicitly account for the new FV effects that these poles introduce.

3. A new test of the formalism: FV energy shift for a three-particle bound state

In the remainder of this talk I report on a new test of the original three-particle formalism of Refs. [4, 5]. This is based on work with Hansen that is now written up in Ref. [6]. I present here only an overview of the argument.

We think that it is important to provide checks of the formalism, since it is rather involved and required a very lengthy derivation. We have already completed one such check in Refs. [7, 8], where we have determined the energy of the three-particle state closest to threshold in a series in $1/L$. The $1/L^3$, $1/L^4$ and $1/L^5$ terms agree, as expected, with results from NRQM. The $1/L^6$ term contains relativistic effects, and is also the first term in which the three-particle scattering amplitude enters. We have done an auxiliary calculation of the threshold energy in relativistic $\lambda\phi^4$ theory, working through $\mathscr{O}(\lambda^3)$ in perturbation theory [8]. The results for the $1/L^{3-6}$ terms from our formalism and perturbation theory are in complete agreement.

The new check presented here is based on the work of Ref. [9], hereafter referred to as MRR. These authors use NRQM to determine the leading volume dependence of the energy of a three-particle bound state with total momentum $\vec{P}=0$. Specifically, they assume only two-particle potentials, and that these are near the unitary limit of infinite scattering length. In this limit, first considered by Efimov [10], there is a sequence of three-particle bound states.[4] Focusing on one such bound state, MRR find

$$E_B = 3m - \kappa^2/m + \Delta E_3(L)\,, \tag{3.1}$$

$$\Delta E_3(L) = c\frac{\kappa^2}{m}\frac{1}{(\kappa L)^{3/2}}\exp\left(-2\kappa L/\sqrt{3}\right)\left[1+\mathscr{O}\left(\frac{\kappa}{m},\frac{1}{\kappa L}\right)\right]. \tag{3.2}$$

The first equation defines κ, while the second gives the leading volume dependence of the energy. The constant c is known, and depends on the detailed form of the wavefunction of the (infinte-volume) Efimov state.[5] Our aim here is to fully reproduce Eq. (3.2) using our formalism.

The corresponding equation for a two-particle bound state can be determined from Lüscher's original quantization condition (and from NRQM), and takes the form [11]

$$\Delta E_2(L) = -12\frac{\kappa^2}{m}\frac{1}{\kappa L}e^{-\kappa L}\left[1+\mathscr{O}\left(\frac{\kappa}{m},\frac{1}{\kappa L}\right)\right]. \tag{3.3}$$

Thus we see that the three-particle case has a different exponent, different power of $1/L$, and a more complicated constant.

[4] This is true for both signs of the scattering length. Here we assume a positive scattering length so that there are no two-body bound states.

[5] Here we use a slightly different definition of c than that used by MRR or in Ref. [6].

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The calculation of MRR assumes that only s-wave interactions contribute. Making this approximation in our formalism reduces the size of the matrix space in Eqs. (1.1) and (1.3). The matrix index is now given solely by the momentum of one of the three particles—the "spectator"—while the other two are in a relative s-wave.[6] In all subsequent formulae the spectator momentum is shown explicity, and there are no implicit matrix indices.

The logic of the calculation is straightforward.[7] $\mathscr{M}_3$ has, by assumption, a pole at $E = E_B$:

$$\mathscr{M}_3(\vec{p},\vec{k}) = -\frac{\Gamma(\vec{p})\overline{\Gamma}(\vec{k})}{E^2 - E_B^2} + \text{non-pole}\,, \tag{3.4}$$

where the residues are the amputated, on-shell Bethe-Salpeter amplitudes. We also know that, since $\mathscr{M}_{3,L}$ is a FV correlation function, it has poles at the energies of the FV states, and in particular at the shifted FV energy of the bound state. Given Eq. (1.3), we know that, for large L, $\mathscr{M}_{3,L}$ is close to $\mathscr{M}_3$. The idea is then to quantify this closeness by systematically determining the volume dependence of $\mathscr{M}_{3,L}$ using Eq. (1.3).

$\mathscr{M}_3$ and $\mathscr{M}_{3,L}$ differ because momentum integrals in the former are replaced by sums (i.e. by matrix products) in the latter. We can systematically replace sums with integrals plus sum-integral differences. Since we are working below threshold, with no on-shell intermediate states, the volume dependence of the sum-integral differences is exponentially suppressed, but with the exponent proportional to κL. This leads to a much weaker suppression than that from the contributions proportional to e^{-mL} that we consistently neglect. We keep the terms with the smallest exponential suppression, which turn out to have exponent $-2\kappa L/\sqrt{3}$, and also drop terms suppressed by additional powers of $1/L$. Using the properties of the residue functions Γ and $\overline{\Gamma}$, which will be discussed below, we find that the dominant FV corrections arise from three-particle cuts lying between the scattering of one pair and a different pair (which we label "switch states"). With this simplification we are able to show that the unsymmetrized versions of $\mathscr{M}_{3,L}$ and $\mathscr{M}_3$ satisfy[8]

$$\mathscr{M}_{3,L}^{(u,u)}(\vec{p},\vec{k}) = \mathscr{M}_{3}^{(u,u)}(\vec{p},\vec{k}) + \left[\frac{1}{L^3}\sum_{\vec{\ell}} - \int \frac{d^3\ell}{(2\pi)^3}\right] \mathscr{M}_{3}^{(u,u)}(\vec{p},\vec{\ell})\frac{1}{2\omega_\ell \mathscr{M}_2(\ell)}\mathscr{M}_{3,L}^{(u,u)}(\vec{\ell},\vec{k})\,. \tag{3.5}$$

The unsymmetrized amplitudes have poles at the same positions as the symmetrized ones, and by substituting the pole forms [e.g. Eq. (3.4)] into this equation we find the energy shift to be

$$\Delta E_3(L) = -\frac{1}{2E_B}\left[\frac{1}{L^3}\sum_{\vec{k}} - \int \frac{d^3k}{(2\pi)^3}\right]\frac{\overline{\Gamma}^{(u)}(k)\Gamma^{(u)}(k)}{2\omega_k \mathscr{M}_2(k)}\,. \tag{3.6}$$

Here $\Gamma^{(u)}$, $\overline{\Gamma}^{(u)}$ are the residues appearing in the pole form for the unsymmetrized amplitude $\mathscr{M}_3^{(u,u)}$. Note that these turn out to depend only on the magnitude of the spectator momentum, as does $\mathscr{M}_2$.

[6] In FV this spectator momentum is quantized. Note that the asymmetry inherent in the choice of spectator is removed by subsequent symmetrization in our formalism.

[7] The following description is an updated version of that given in the talk, based on subsequent improvements in the derivation. In particular, we no longer need to make the approximation $\mathscr{K}_{\text{df},3} = 0$.

[8] Unsymmetrized means that the first two-particle interaction occurring in a skeleton expansion of $\mathscr{M}_3$ and $\mathscr{M}_{3,L}$ occurs between the non-spectator pair. $\mathscr{M}_2(\vec{\ell})$ gives the scattering amplitude for two particles with total four-momentum $P_2 = (E - \omega_\ell, -\vec{\ell})$. In the sum, $\vec{\ell} = 2\pi\vec{n}/L$ with $\vec{n}$ a vector of integers.

To proceed, we need to know the residue functions, which, as noted above, are the amputated, on-shell versions of the Bethe-Salpeter (BS) amplitudes for the bound state. We know the Schrödinger wavefunction of the bound states (reviewed, for example, in Ref. [12]), so the issue is how to obtain the BS amplitudes from the wavefunction. This question was addressed, long ago, in Ref. [13]. This work assumed only instantaneous two-particle interactions and worked in the nonrelativistic limit. These are the assumptions made also by MRR, so the result of Ref. [13] is sufficient for our purposes. Using this result (which we have checked in detail, as a full derivation is not supplied in Ref. [13], and corrected the normalization factor) we find[9]

$$\Gamma^{(u)} = 4\sqrt{3}m^2 \lim_{\text{on shell}} \left[-\frac{\kappa^2}{m} - \sum_{i=1,3}\frac{\vec{p}_i^{\,2}}{2m}\right]\widetilde{\phi}_3 \,. \tag{3.7}$$

$\tilde{\phi}_3$ is the Fourier transform of the part of the wavefunction that corresponds to the unsymmetrized BS amplitude. It satisfies the Fadeev equation, in which only the potential between two of the particles appears. The key point here is that the explicit form of ϕ_3 is known [12]. The meaning of “on shell" is that the free Schrödinger operator, i.e. the term in square brackets, vanishes. The right-hand side does not vanish, however, because $\widetilde{\phi}_3$ diverges. We find

$$\overline{\Gamma}^{(u)}(k)\Gamma^{(u)}(k) = -c\; 64\; 3^{3/4}\pi^{5/2}\frac{m^2}{\kappa^2}\left[1+\frac{3k^2}{4\kappa^2}\right]^{-1} + \dots \,, \tag{3.8}$$

with c the same constant as in Eq. (3.2). Here we have kept only the leading singularity for small k, since this leads to the dominant FV correction when inserted into Eq. (3.6).

To evaluate the Eq. (3.6), we also need $\mathcal{M}_2$ in the unitary limit:

$$\frac{1}{\mathcal{M}_2(k)} = \frac{\kappa}{32\pi m}\left[1+\frac{3k^2}{4\kappa^2}\right]^{1/2} . \tag{3.9}$$

Inserting this and Eq. (3.8) into (3.6), using the Poisson summation formula, and evaluating the integral, we find

$$\Delta E_3(L) = c\frac{\kappa^2}{m}\frac{2}{3^{1/4}\sqrt{\pi}\kappa L}K_1\left(\frac{2\kappa L}{\sqrt{3}}\right) , \tag{3.10}$$

whose asymptotic form agrees with the MRR result, Eq. (3.2).

4. Extension to a moving three-particle bound state

Within our formalism, it is straightforward to generalize this result to a moving frame. In the two-particle case, the corresponding generalization of the rest-frame result, Eq. (3.3), has been given in Ref. [14]. They found, for total momentum $\vec{P} = 2\pi\vec{n}_P/L$, the simple form

$$\Delta E_{2,\vec{P}}(\vec{L}) = f_2[\vec{n}_P]\Delta E_2(L)\,, \qquad f_2[\vec{n}_P] = \tfrac{1}{6}\sum_{\hat{s}} e^{i2\pi\hat{s}\cdot\vec{n}_P/2}\,, \tag{4.1}$$

where the sum runs over the six integer vectors of unit length. Thus the form of the volume dependence is unchanged, but the overall factor depends on $\vec{P}$. This dependence turns out to be

[9] The same result holds for $\overline{\Gamma}^{(u)}$ aside from complex conjugation. This schematic form does not show the arguments of $\Gamma^{(u)}$ and $\widetilde{\phi}_3$, as we do not have space to explain all the details here. For these see Ref. [6].

rather dramatic, e.g. $f_2[\vec{0}] = 1$ while $f_2[(1,1,1)] = -1$. Furthermore, by combining results from different frames, the leading exponential dependence can be canceled [14].

We find a similar form in the three-particle case, but with a different prefactor:

$$\Delta E_{3,\vec{P}}(\vec{L}) = f_3[\vec{n}_P]\Delta E_3(L)\,, \qquad f_3[\vec{n}_P] = \frac{1}{6}\sum_{\hat{s}} e^{i2\pi\hat{s}\cdot\vec{n}_P/3}\,. \tag{4.2}$$

Again the prefactor various rapidly with momentum. The fact that the volume dependence changes only by an overall factor means that, as in the two-particle case, it is possible to cancel the leading dependence by combining results from different frames. In fact, since $f_3[(1,1,0)] = 0$, the volume dependence for $\vec{n}_P = (1,1,0)$ is subleading.

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