Threshold expansion of the three-particle quantization condition

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We recently derived a quantization condition for the energy of three relativistic particles in a cubic box [M. T. Hansen and S. R. Sharpe, Phys. Rev. D **90**, 116003 (2014); M. T. Hansen and S. R. Sharpe, Phys. Rev. D **92**, 114509 (2015)]. Here we use this condition to study the energy level closest to the three-particle threshold when the total three-momentum vanishes. We expand this energy in powers of $1/L$, where L is the linear extent of the finite volume. The expansion begins at $\mathcal{O}(1/L^3)$, and we determine the coefficients of the terms through $\mathcal{O}(1/L^6)$. As is also the case for the two-particle threshold energy, the $1/L^3$, $1/L^4$ and $1/L^5$ coefficients depend only on the two-particle scattering length a. These can be compared to previous results obtained using nonrelativistic quantum mechanics [K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957); S. R. Beane, W. Detmold, and M. J. Savage, Phys. Rev. D **76**, 074507 (2007); S. Tan, Phys. Rev. A **78**, 013636 (2008)], and we find complete agreement. The $1/L^6$ coefficients depend additionally on the two-particle effective range r (just as in the two-particle case) and on a suitably defined threshold three-particle scattering amplitude (a new feature for three particles). A second new feature in the three-particle case is that logarithmic dependence on L appears at $\mathcal{O}(1/L^6)$. Relativistic effects enter at this order, and the only comparison possible with the nonrelativistic result is for the coefficient of the logarithm, where we again find agreement. For a more thorough check of the $1/L^6$ result, and thus of the quantization condition, we also compare to a perturbative calculation of the threshold energy in relativistic $\lambda\phi^4$ theory, which we have recently presented in [M. T. Hansen and S. R. Sharpe, Phys. Rev. D **93**, 014506 (2016)]. Here, all terms can be compared, and we find full agreement.

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I. INTRODUCTION

In two recent papers, we derived a relationship between the spectrum of three relativistic particles in a periodic box and on-shell, infinite-volume two-to-two and three-to-three scattering amplitudes [1,2]. In the first paper, Ref. [1], we related the finite-volume spectrum to an unphysical infinite-volume three-to-three scattering quantity that we denoted $\mathcal{K}_{\mathrm{df},3}$. The formalism was then completed in Ref. [2], where we presented the purely infinite-volume relation between $\mathcal{K}_{\mathrm{df},3}$ and the standard three-to-three scattering amplitude, $\mathcal{M}_3$. As the derivation of these results is lengthy and involved, it is important to check them as thoroughly as possible. Some checks were made in Refs. [1,2], but the purpose of the present paper is to provide a more significant check. We do so by calculating, in our formalism, the energy of the state closest to threshold as a function of the inverse box size $1/L$, and by comparing to results obtained using two other methods: nonrelativistic quantum mechanics (NRQM) (as done in Refs. [3–5]) and a perturbative expansion in relativistic $\lambda\phi^4$ theory (a calculation we have recently completed in Ref. [6]). These two methods provide complementary checks of the results of our general formalism.

The result derived in Refs. [1,2] is for a scalar field ϕ with a Z_2 symmetry, $\phi \to -\phi$, so that only even legged vertices appear. This theory is studied in a cubic box with side length L and periodic boundary conditions in all three spatial directions. The absence of $2 \to 3$ transitions means that a direct comparison can be made to the nonrelativistic approach, since in the latter particle number is conserved.

The analysis of Refs. [1,2] allows for nonzero total three-momentum, $\vec{P}$, in the finite-volume frame. However, since Refs. [3–6] consider only zero total three-momentum, we restrict ourselves here to $\vec{P} = 0$. This means that the threshold occurs when the total energy satisfies $E = 3m$, with m the physical mass of the scalar particle. In the absence of interactions, this is also the energy of the lowest-lying three-particle state in the box, with all particles at rest. Including interactions, the energy of this state will shift by an amount

$$\Delta E_{\mathrm{th}} = E - 3m, \tag{1}$$

which should go to zero as $L \to \infty$. For two particles, it is well known that $\Delta E_{\mathrm{th}} \propto a/L^3 + \mathcal{O}(1/L^4)$, with a the scattering length (see Ref. [7] and references therein).

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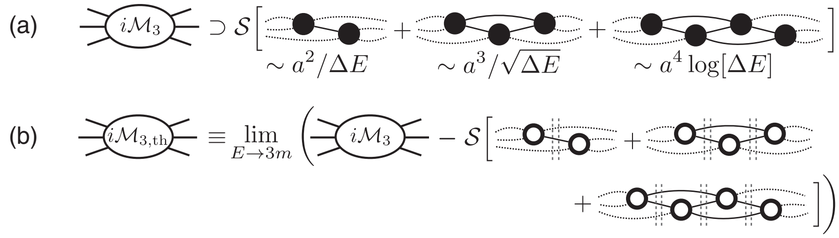

FIG. 1. (a) The three-to-three scattering amplitude contains three types of pairwise scattering diagrams that lead to divergences at threshold. The scaling of the divergence with the shift from threshold, ΔE, and the two-particle scattering length, a, is shown. (b) We define a finite threshold scattering amplitude by subtracting the singular parts of these diagrams before sending the energy to $3m$. The rings, in contrast to filled circles, indicate that only the two-to-two scattering amplitude near threshold appears in the subtraction. The vertical dashed lines indicate that a simple pole is used in place of the fully dressed propagator. Detailed definitions are given in Sec. III D.

The $1/L^3$ factor arises because the two particles, both of which have spatially uniform wave functions, need to be close to each other in order to interact. We expect that $\Delta E_{\rm th}$ for three particles should scale with the same power of $1/L$, since one possible process is a pairwise interaction with the third particle spectating. Similarly, a localized three-particle interaction should lead to a contribution scaling as $1/L^6$, since all three particles must be close. These expectations are indeed borne out of the results of Refs. [4–6].

It should be noted that, in finite volume, there is an infinite tower of states with energies $E_n(L)$ satisfying $\lim_{L\to\infty} E_n(L) = 3m$. We are only interested in the lowest lying level in this infinite set, for which, as noted above, $\Delta E = \mathcal{O}(1/L^3)$. In particular, we are not concerned with excited states that, in the noninteracting limit, contain at least two particles with nonzero momenta. The energy shifts for such states scale as $\Delta E = \mathcal{O}(1/L^2)$ with positive coefficients. Our quantization condition could also be used to develop the $1/L$ expansion of the energy shifts for these excited states, but we do not pursue this in the present article.

In light of these considerations we expand the energy shift as

$$\Delta E_{\rm th} = \sum_{n=3}^{\infty} \frac{a_n(L)}{L^n} \tag{2}$$

and determine the $a_n(L)$ up to $n = 6$. We include a possible L dependence in the coefficients, since Refs. [4–6] find a logarithmic dependence for $a_6(L)$.

As we will show, our results for a_{3-5}, as well as the logarithmic, volume-dependent term in $a_6(L)$, agree with those from Refs. [3–5] (which were also checked in Ref. [6]). We cannot, however, make a useful comparison with the NRQM results for the volume-independent part of $a_6(L)$ for two reasons. First, as we discovered in Ref. [6], there are differences between the nonrelativistic and relativistic results for the two-particle threshold energy shift at $\mathcal{O}(1/L^6)$. Such differences arise from relativistic kinematics, and we expect these to persist also in the three-particle case. Second, this is the order at which a three-particle interaction first appears, and the definition of this quantity is scheme dependent. The schemes used in the two NRQM calculations differ from that used in our formalism (as well as from each other), and the relationship between these schemes is not known at present. It is primarily because of this issue that we carried out the perturbative calculation of Ref. [6], since in that calculation we could use the same scheme for defining the three-particle interaction, and thus provide an unambiguous check for $a_6(L)$.[1]

Since the scheme dependence of the three-particle interaction plays an important role in the following, we briefly recall how this issue arises. The quantity that one naively expects to enter the $1/L^6$ energy shift in a relativistic theory is the infinite-volume three-to-three scattering amplitude at threshold. This cannot be the case, however, since this amplitude diverges as $\Delta E = E - 3m$ vanishes.[2] The divergences are due to the three pairwise scattering diagrams shown in Fig. 1(a), and they scale as $a^2/\Delta E$, $a^3/\sqrt{\Delta E}$ and $a^4 \log(\Delta E)$, respectively, where a is the scattering length. The existence of such singularities is a general field-theoretic result that was established long ago [9–12]. Our formalism accommodates these divergences by finding that $\Delta E_{\rm th}$ depends on a modified quantity, $\mathcal{M}_{3,\rm th}$, given by subtracting the divergent terms from $\mathcal{M}_3$ [see Fig. 1(b) as well as Eq. (114) below]. The choice of subtraction is, however, ambiguous and introduces dependence on a cutoff scale and scheme.

The remainder of this paper is organized as follows. In the following section we summarize the quantization condition of Ref. [1], which takes the form of a determinant of formally infinite-dimensional matrices. The core of this paper is Sec. III, in which we describe the development of the threshold expansion. The central difficulty is that, at

[1] See also Ref. [8] for a recent review of results for three particles in a finite volume.

[2] As discussed later, there are also divergences above threshold. We imagine here choosing the kinematics such that the above-threshold divergences are avoided, and then moving towards threshold, at which point the divergences cannot be avoided.

$\mathcal{O}(1/L^6)$ in the expansion of $\Delta E_{\rm th}$, all entries in the infinite-dimensional matrices contribute. We thus first recast the quantization condition into a more useful form, given in Eq. (33). We then analyze the reduced result by understanding the $1/L$ scaling of its components. The analysis is rather involved and lengthy, and requires the introduction of the threshold amplitude $\mathcal{M}_{3,\rm th}$ discussed above. Brief conclusions are given in Sec. IV. Technical calculations are collected in three appendixes.

II. SUMMARY OF QUANTIZATION CONDITION

In this section we recall the three-particle quantization condition from Ref. [1]. This condition determines the spectral energies E_i to be those values for which

$$\det[1 + F_3 \mathcal{K}_{\rm df,3}] = 0. \tag{3}$$

Here, F_3 and $\mathcal{K}_{\rm df,3}$ are matrices, to be defined below, that depend on E (and, in the case of F_3, also on L). Particle interactions enter through two infinite-volume scattering quantities: the three-particle quantity $\mathcal{K}_{\rm df,3}$, shown explicitly, and the two-particle K matrix $\mathcal{K}_2$, contained in F_3.

$\mathcal{K}_{\rm df,3}$ is a three-particle divergence-free K matrix. It depends on the same (on-shell) kinematic variables as $\mathcal{M}_3$, and is invariant under the interchange of the external particle momenta. It differs from the standard three-to-three scattering amplitude in two important ways [1,2]. First, physical divergences, which are known to occur in the three-particle scattering amplitude $\mathcal{M}_3$, are absent in $\mathcal{K}_{\rm df,3}$. These divergences are due to pairwise scatterings separated by arbitrarily long-lived intermediate states [see Fig. 1(a)]. Second, loop integrals defining $\mathcal{K}_{\rm df,3}$ are evaluated with a pole prescription differing from the standard $i\epsilon$ prescription. This feature is needed to properly accommodate finite-volume effects from the two-particle unitary cusp. The issue of two-particle cusps plays a minor role in the threshold expansion so we do not describe it here. We direct the interested reader to Refs. [1,2,8] for a thorough discussion.

The precise relation between $\mathcal{K}_{\rm df,3}$ and $\mathcal{M}_3$ is given in Ref. [2]. First, one uses an integral equation to convert $\mathcal{K}_{\rm df,3}$ to $\mathcal{M}_{\rm df,3}$. The latter is an intermediate quantity that, like $\mathcal{K}_{\rm df,3}$, has no singularities due to long-lived intermediate states. Unlike $\mathcal{K}_{\rm df,3}$, however, $\mathcal{M}_{\rm df,3}$ is defined with the standard $i\epsilon$-pole prescription and is therefore more closely related to the standard scattering amplitude. $\mathcal{M}_{\rm df,3}$ is defined in Eq. (93) below. Second, one adds back in the singular terms. These depend only on kinematic variables as well as the on-shell two-to-two scattering amplitude. As we see below, the threshold expansion of Eq. (3) actually reproduces the integral equation that converts $\mathcal{K}_{\rm df,3}$ to $\mathcal{M}_{\rm df,3}$. In addition, the expansion produces an infinite series of terms that convert $\mathcal{M}_{\rm df,3}$ to the quantity $\mathcal{M}_{3,\rm th}$ introduced above. Of the three quantities, $\mathcal{K}_{\rm df,3}$, $\mathcal{M}_{\rm df,3}$ and $\mathcal{M}_{3,\rm th}$, only the latter appears in our final result for the threshold expansion. This is also the quantity that is most closely related to the standard scattering amplitude.

We now explain the matrix indices of $\mathcal{K}_{\rm df,3}$ and F_3. These specify the incoming and outgoing configuration of three on-shell particles with $\vec{P} = 0$ and given total energy E. We arbitrarily pick one of the three incoming particles and label its momentum $\vec{k}$, and similarly label one of the outgoing momenta $\vec{k}'$. We sometimes refer to these two particles as "spectators," for reasons that will become clear below. In infinite volume $\vec{k}$ and $\vec{k}'$ are continuous, but the quantization condition, Eq. (3), depends only on $\mathcal{K}_{\rm df,3}$ for finite-volume momenta satisfying $\vec{k}, \vec{k}' \in (2\pi/L)\mathbb{Z}^3$. With $\vec{k}$, $\vec{k}'$ specified, the total momentum and energy of the remaining two particles are also determined, separately for the in- and out-states. Thus, the only remaining degrees of freedom are the incoming and outgoing two-particle orbital angular momenta in their respective center-of-mass (CM) frames. We specify these using spherical harmonic indices: ℓ, m for the in-state and ℓ', m' for the out-state. Altogether, for fixed E (and $\vec{P} = 0$), $\mathcal{K}_{\rm df,3}$ depends on $\vec{k}', \ell', m'$ and $\vec{k}, \ell, m$. Since these quantities take discrete values, it is convenient to view $\mathcal{K}_{\rm df,3}$ as a matrix, i.e. $\mathcal{K}_{\rm df,3} = \mathcal{K}_{{\rm df},3;k',\ell',m';k,\ell,m}$. Equivalently, $\mathcal{K}_{\rm df,3}$ is a linear operator acting on a space with orthonormal basis vectors $|\vec{k}, \ell, m\rangle$, such that

$$\langle \vec{k}', \ell', m' | \mathcal{K}_{\rm df,3} | \vec{k}, \ell, m\rangle = \mathcal{K}_{{\rm df},3;k',\ell',m';k,\ell,m}. \tag{4}$$

The other factor in Eq. (3), F_3, is a matrix acting on the same space. It is given by

$$F_3 = \frac{1}{L^3}\frac{1}{2\omega}\left[\frac{F}{3} - F\frac{1}{\mathcal{K}_2{}^{-1} + F + G}F\right], \tag{5}$$

where we have used the form of the result given (up to trivial rearrangements) in Appendix C of Ref. [1]. Four new matrices enter Eq. (5): $1/(2\omega)$, F, G, and $\mathcal{K}_2$. The first three are kinematical quantities and will be described below. We first discuss $\mathcal{K}_2$, which is given by

$$\mathcal{K}_{2;k',\ell',m';k,\ell,m} = \delta_{k'k}\delta_{\ell'\ell}\delta_{m'm}\frac{16\pi E^*_{2,k}}{q^*_k}\tan\delta_\ell(q^*_k). \tag{6}$$

The physical interpretation of this infinite-volume quantity is that it describes a process in which the spectator particles do not interact (so that $\vec{k} = \vec{k}'$), while the other two particles scatter (so that the two-particle CM angular momentum is conserved). In the two-particle CM frame, the momentum of each particle is denoted q^*_k, while their combined energy is $E^*_{2,k}$. These are given, respectively, by

$$q_k^{*2} = E_{2,k}^{*2}/4 - m^2 \quad \text{and} \quad E_{2,k}^{*2} = (E-\omega_k)^2 - \vec{k}^2, \tag{7}$$

where $\omega_k = \sqrt{\vec{k}^2 + m^2}$. Stripping away the Kronecker deltas from Eq. (6), what remains is the two-particle K matrix, given in terms of the physical, infinite-volume scattering phase shift $\delta_\ell(q_k^*)$.

As written, Eq. (6) is only valid above threshold, i.e. for $(q_k^*)^2 > 0$. However, our formalism also requires $\mathcal{K}_2$ below threshold. This is because, as $\vec{k}^2$ increases, $E_{2,k}^*$ drops below $2m$ and thus $(q_k^*)^2$ becomes negative. The subthreshold result is defined in Ref. [1] and is obtained from the above threshold result, Eq. (6), by two changes. First, one analytically continues the scattering phase shifts below threshold in the standard way using threshold expansions. For example, for $\ell = 0$, one uses

$$q^{-1}[\tan\delta_0(q)] = -a\left[1 + \frac{1}{2}raq^2 + \mathcal{O}[(aq)^4]\right], \tag{8}$$

which is valid for both positive and negative q^2. Here, a is the scattering length in the nuclear physics convention,[3] and r is the effective range. Similar expansions exist for the higher partial waves, but we will only need the result

$$q^{-1}[\tan\delta_\ell(q)] = \mathcal{O}(q^{2\ell}). \tag{9}$$

In addition to the analytic continuation of the phase shift, the subthreshold definition of $\mathcal{K}_2$ includes a term related to the two-particle unitary cusp (and involving the cutoff function H introduced below). However, this term does not contribute to any power of $1/L$ when doing an expansion about the threshold energy. We thus do not describe it in this work.

We now define the remaining matrices contained in F_3. The first is a simple diagonal kinematical matrix,

$$\left[\frac{1}{2\omega}\right]_{k',\ell',m';k,\ell,m} \equiv \delta_{k'k}\delta_{\ell'\ell}\delta_{m'm}\frac{1}{2\omega_k}. \tag{10}$$

The second, G, resembles the three-particle nonrelativistic propagator, decorated by angular dependence. It has both diagonal and off-diagonal entries:

$$G_{p,\ell',m';k,\ell,m} \equiv \left(\frac{k^*}{q_p^*}\right)^{\ell'} \frac{4\pi Y_{\ell',m'}(\hat{k}^*)H(\vec{p})H(\vec{k})Y^*_{\ell,m}(\hat{p}^*)}{2\omega_{kp}(E-\omega_k-\omega_p-\omega_{kp})} \times \left(\frac{p^*}{q_k^*}\right)^{\ell}\frac{1}{2\omega_k L^3}. \tag{11}$$

[3]The convention is such that $a > 0$ for repulsive two-body interactions and $a < 0$ for attractive ones. Thus, we expect the proportionality factor in $\Delta E_{\rm th} \propto a/L^3 + \mathcal{O}(1/L^4)$ to be positive. [See the text after Eq. (1) above.]

Here, q_p^* is defined as for q_k^* in Eq. (7) except with $k \to p$; $\vec{k}^*$ is the result of boosting the vector $\vec{k}$ with velocity $\vec{\beta}_p = \vec{p}/(E-\omega_p)$, and $\vec{p}^*$ is defined by a similar boost with $\vec{k} \leftrightarrow \vec{p}$. In addition, $\omega_{kp} = \sqrt{(\vec{k}+\vec{p})^2 + m^2}$ is the on-shell energy of the particle with the "third" momentum coordinate, $-\vec{k}-\vec{p}$. Finally, H is a cutoff function, defined by[4]

$$H(\vec{k}) = J([E_{2,k}^*/(2m)]^2),$$
$$J(x) \equiv \begin{cases} 0 & x \le 0 \\ \exp\left(-\frac{1}{x}\exp\left[-\frac{1}{1-x}\right]\right) & 0 < x \le 1 \\ 1 & 1 < x. \end{cases} \tag{12}$$

It ensures that the boosts needed to obtain $\vec{p}^*$ and $\vec{k}^*$ are well defined. A key property of $J(x)$ is that it is smooth. In particular, since $J(x) = 1$ for $x \ge 1$, all its derivatives vanish as $x \to 1^-$. Thus, the function remains unity to all orders in a Taylor expansion about $x = 1$. For further discussion of J and H see Ref. [1].

The last matrix, F, is a generalization of the zeta functions introduced in Ref. [7]:

$$F_{k',\ell',m';k,\ell,m} \equiv \delta_{k'k}F_{\ell',m';\ell,m}(\vec{k}), \tag{13}$$

$$F_{\ell',m';\ell,m}(\vec{k}) = F^{i\epsilon}_{\ell',m';\ell,m}(\vec{k}) + \rho_{\ell',m';\ell,m}(\vec{k}), \tag{14}$$

$$F^{i\epsilon}_{\ell',m';\ell,m}(\vec{k}) = \frac{1}{2}\left[\frac{1}{L^3}\sum_{\vec{a}} - \int_{\vec{a}}\right]\frac{4\pi Y_{\ell',m'}(\hat{a}^*)Y^*_{\ell,m}(\hat{a}^*)H(\vec{k})H(\vec{a})H(\vec{b}_{ka})}{2\omega_a 2\omega_{ka}(E-\omega_k-\omega_a-\omega_{ka}+i\epsilon)} \times \left(\frac{a^*}{q_k^*}\right)^{\ell+\ell'}. \tag{15}$$

Here, $\int_{\vec{a}} \equiv \int d^3a/(2\pi)^3$, while the sum over $\vec{a}$ runs over all finite-volume momenta, and $\vec{a}^*$ is the vector obtained by boosting $\vec{a}$ to the two-particle CM frame, treating $\vec{k}$ as the spectator momentum, i.e. boosting with velocity $\vec{\beta}_k = \vec{k}/(E-\omega_k)$. Finally, ρ is a phase space factor defined by

$$\rho_{\ell',m';\ell,m}(\vec{k}) \equiv \delta_{\ell'\ell}\delta_{m'm}H(\vec{k})\tilde{\rho}(E_{2,k}^*), \tag{16}$$

$$\tilde{\rho}(E_{2,k}^*) \equiv \frac{1}{16\pi E_{2,k}^*} \times \begin{cases} -iq_k^* & (2m)^2 < E_{2,k}^{*2} \\ |q_k^*| & 0 < E_{2,k}^{*2} \le (2m)^2, \end{cases} \tag{17}$$

The addition of the ρ term to $F^{i\epsilon}$ in Eq. (14) changes the pole prescription from $i\epsilon$ to the "$\widetilde{\rm PV}$" prescription defined in Ref. [1].

[4]Other choices of the function J are possible, as discussed in Ref. [1], but this is the form we use for numerical evaluations.

We close this section by rearranging the matrices appearing in the quantization condition in two minor ways. The first takes care of the powers of $1/q_p^*$ or $1/q_k^*$ (which we collectively refer to as $1/q^*$) contained in G and F. Since we will find that $q^* \sim 1/L$, these terms apparently lead to positive powers of L, complicating the development of the threshold expansion. These powers of $1/q^*$ are, however, misleading, since they are canceled by corresponding positive powers contained within $\mathcal{K}_2$ and $\mathcal{K}_{\mathrm{df},3}$. This is shown for $\mathcal{K}_2$ by the result (9), and for $\mathcal{K}_{\mathrm{df},3}$ by a general result shown in Appendix A of Ref. [1]. It is thus preferable to make this cancellation explicit by introducing factors of the matrix

$$Q_{k',\ell',m';k,\ell,m} \equiv \delta_{k'k}\delta_{\ell'\ell}\delta_{m'm}(q_k^*)^{\ell}. \tag{18}$$

The second change is to insert factors of the matrix $1/(2\omega)$ and its inverse (2ω) such that the symmetric matrix $(2\omega)^{-1}G$ appears.

Specifically, we introduce

$$\tilde{F}_3 = QF_3Q, \qquad \tilde{\mathcal{K}}_{\mathrm{df},3} = Q^{-1}\mathcal{K}_{\mathrm{df},3}Q^{-1},$$
$$\tilde{\mathcal{K}}_2 = (2\omega)Q^{-1}\mathcal{K}_2Q^{-1}, \qquad \tilde{F} = (2\omega)^{-1}QFQ, \quad \text{and}$$
$$\tilde{G} = (2\omega)^{-1}QGQ, \tag{19}$$

in terms of which the quantization condition becomes

$$\det[1 + \tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}] = 0, \tag{20}$$

where

$$\tilde{F}_3 = \frac{1}{L^3}\left[\frac{\tilde{F}}{3} - \tilde{F}\frac{1}{\mathcal{H}}\tilde{F}\right], \tag{21}$$

with

$$\mathcal{H} \equiv \tilde{\mathcal{K}}_2^{-1} + \tilde{F} + \tilde{G}. \tag{22}$$

We stress that both $\tilde{\mathcal{K}}_{\mathrm{df},3}$ and $\tilde{\mathcal{K}}_2$ have a well-defined limit as $q^* \to 0$, and indeed are functions of $(q^*)^2$ that can be analytically continued to negative values. We also note that $\tilde{G}$, $\tilde{F}$ and $\tilde{\mathcal{K}}_2$, and thus also $\mathcal{H}$, are Hermitian.

III. THRESHOLD EXPANSION

To develop the $1/L$ expansion we need to know how the various quantities entering the quantization condition, Eq. (3), scale with $1/L$ when $E \approx 3m$. Specifically, recalling that $\vec{k} = 2\pi\vec{n}/L$ is one of the matrix indices on the quantities in (3), we can work out the scaling assuming that $n = |\vec{n}| = \mathcal{O}(L^0)$ so that $k = \mathcal{O}(1/L) \ll m$. This is the same as assuming that important contributions to the sums over matrix indices occur when all three particles are nonrelativistic. This assumption is naive, since the sums actually range up to values of $\vec{k}$ where $H(\vec{k}) = 0$, for which $k \sim m$. It turns out that the naive scaling gives the correct prediction for the first three orders in the $1/L$ expansion of ΔE_{th}. We demonstrate this in Sec. III E, where we also show how to reach the correct result for the $1/L^6$ contribution, for which the naive scaling is insufficient.

As we explain in detail in the first subsection below, the assumption $|\vec{n}| = \mathcal{O}(L^0)$, together with the assumed form (2) for ΔE_{th}, allows one to determine the scaling with $1/L$ of each of the components of the matrices entering into the quantization condition. We find that the elements of $\tilde{\mathcal{K}}_{\mathrm{df},3}$ are of $\mathcal{O}(L^0)$, which is simply the statement that this is an infinite-volume quantity with a nonzero limit at threshold. The dominant contributions to $\tilde{F}$ and $\tilde{G}$ are also of $\mathcal{O}(L^0)$, so that $\tilde{F}_3 \sim 1/L^3$ due to the explicit volume factor in Eq. (21). Naively, one might conclude that $\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3} \sim 1/L^3$ and cannot cancel the contribution from the unit matrix in Eq. (20), as would be necessary to satisfy the quantization condition. There are two ways to avoid this conclusion. First, the determinant involves a product over $\mathcal{O}(L^3)$ matrix indices, and this multiplicity factor can cancel the $1/L^3$ in $\tilde{F}_3$. Second, the matrix $\mathcal{H}$ can, for an appropriately tuned energy, have an eigenvalue of $\mathcal{O}(1/L^3)$, due to cancellations between the terms in Eq. (22) [which are each of $\mathcal{O}(L^0)$]. This leads to $\tilde{F}_3$ scaling as $\mathcal{O}(L^0)$. Both mechanisms turn out to contribute in the solution to the quantization condition, and we describe them in turn.

To illustrate the impact of having $\mathcal{O}(L^3)$ matrix indices, we expand the determinant in terms of cofactors[5]

$$\det[1 + \tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}] = (1 + [\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}]_{000;000})C_{000} + \sum_{\{k\ell m\}\neq 0} [\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}]_{000;k\ell m}C_{k\ell m}. \tag{23}$$

We focus on the second term. From the discussion above, we know that the matrix elements $[\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}]_{000;k\ell m}$ scale as $1/L^3$. Now we use the result that the infinite-volume limit of $(1/L^3)\sum_{\vec{k}}$ acting on a smooth function equals the integral, $\int d^3k/(2\pi)^3$, of that function. Assuming that C_{klm} scales as L^0, this implies that the second term in (23) in fact scales as L^0 rather than as $1/L^3$. To determine the actual scaling of C_{klm}, one would need to iteratively repeat the cofactor analysis, removing increasingly more rows and columns and evaluating determinants. It is plausible that this could lead to additional L^3 enhancements. In this study, however, we are able to avoid this complicated line of analysis, by recasting the quantization condition in a form that, for studying the threshold energy,

[5] $C_{k\ell m}$ is the determinant of the matrix reached by removing the 000th row and the $k\ell m$th column from $1 + \tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}$, multiplied by an alternating phase.

is simpler to handle. We thus use Eq. (23) only to emphasize that the naive scaling of terms can be invalidated by the presence of sums over the $\mathcal{O}(L^3)$ indices, leading to a potential proliferation of contributions. This observation will play a central role in the subsequent analysis.

To illustrate the second mechanism needed to find the threshold solution of the quantization condition, we adopt the naive scaling worked out in the next subsection. In this scaling, the dominant parts of $\tilde{F}$ and $\tilde{G}$ are, respectively, $\tilde{F}_{00} \equiv \tilde{F}_{000;000}$ and $\tilde{G}_{00} \equiv \tilde{G}_{000;000}$, both of which scale as L^0 (as do all elements of $\tilde{\mathcal{K}}_{\mathrm{df},3}$). Here, we are introducing the abbreviation that the subscript 00 refers to the matrix element with $\vec{k} = \vec{k}' = \vec{0}$ and $\ell = \ell' = m = m' = 0$. The dominant part of $\tilde{F}_3$ is then

$$\tilde{F}_{3;00} \equiv \tilde{F}_{3;000,000} \approx -\frac{1}{L^3}\tilde{F}_{00}[\mathcal{H}^{-1}]_{00}\tilde{F}_{00}, \qquad (24)$$

with all other matrix elements suppressed by additional powers of $1/L$. If this were the entire story, the quantization condition would collapse, as $L \to \infty$, to the algebraic equation

$$1 + \tilde{F}_{3;00}\tilde{\mathcal{K}}_{\mathrm{df},3;00} = 0. \qquad (25)$$

This equation can be solved if ΔE [of the form shown in Eq. (2)] can be tuned such that $\mathcal{H}$ has an eigenvalue that behaves as c/L^3. We call this putative small eigenvalue λ_0. It is also necessary that the corresponding eigenvector, $|\lambda_0\rangle$, have nonzero overlap with $|\vec{0},0,0\rangle$ when $L \to \infty$. In that case $[\mathcal{H}^{-1}]_{00} \sim L^3$, so that $\tilde{F}_{3;00} \sim L^0$ and the quantization condition (25) can be satisfied if ΔE is tuned so that the constant c has the appropriate value. The requisite tuning of the eigenvalue of $\mathcal{H}$ is possible because, as can be seen from Eq. (22), $\mathcal{H}_{00}$ consists of three terms of $\mathcal{O}(L^0)$, two of which ($\tilde{F}$ and $\tilde{G}$) depend on ΔE (as shown in the next subsection).

To obtain the correct expression for the energy of the near-threshold state, one must combine the two mechanisms. The first mechanism alone would require a cancellation between quantities in which all finite-volume sums have been replaced by integrals, so that dependence on L is lost. This cannot lead to the desired volume dependence of Eq. (2). The second mechanism does lead to such a volume dependence—indeed, as we show below, in order that $\lambda_0 \sim 1/L^3$ we must remove L^0, $1/L$ and $1/L^2$ contributions from λ_0, and this fixes the coefficients a_3, a_4 and a_5 in ΔE_{th}. However, to determine the a_6/L^6 term in ΔE_{th}, it turns out that we must control an infinite number of contributions arising because of the first mechanism.

As noted above, we have not found it fruitful to work directly with the expansion given in Eq. (23). Instead, after some trial and error, we have found that an alternative form of the quantization condition allows a simpler analysis. This is

$$\lim_{E\to 3m+\Delta E_{\mathrm{th}}} \langle\lambda_0|\tilde{F}\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}}\tilde{F}|\lambda_0\rangle = \infty, \qquad (26)$$

where $|\lambda_0\rangle$ is the eigenvector of $\mathcal{H}$ introduced above whose eigenvalue λ_0 is tuned to be of $\mathcal{O}(1/L^3)$. We will provide motivation for this form shortly, but first we explain why it is valid. We begin by noting that we expect there to be only one eigenvalue that can be tuned in this way, since only in the element $\mathcal{H}_{00}$ can the requisite cancellation occur. This is consistent with our expectation that there is only a single near-threshold state. Next we note that the matrix element in Eq. (26) can diverge if $\tilde{F}$ diverges or if one of the eigenvalues of $1 + \tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}$ vanishes.[6] The divergence of $\tilde{F}$ only occurs at noninteracting energies and thus does not lead to interesting solutions. We avoid them by requiring ΔE_{th} to have the form indicated in Eq. (2), which differs from all noninteracting energies once L is large enough. With this proviso we see that, whenever Eq. (26) holds, the original quantization condition, Eq. (20), is also satisfied. In fact, Eq. (26) is a stronger condition than (20) because it requires that the eigenvector of $1 + \tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}$ corresponding to the vanishing eigenvalue has nonzero overlap with the vectors $\tilde{F}|\lambda_0\rangle$ and $\tilde{\mathcal{K}}_{\mathrm{df},3}\tilde{F}|\lambda_0\rangle$.

A more physical motivation for the condition (26) is that it corresponds approximately to finding the pole in the correlation function

$$C_{\phi^3}(E) = \int d\tau e^{i(iE)\tau}\langle\tilde{\phi}(\tau,\vec{0})^3\tilde{\phi}(0,\vec{0})^3\rangle, \qquad (27)$$

with $\tilde{\phi}(\tau,\vec{k})$ the spatial Fourier transform, in the finite box, of a scalar field coupling to a single particle. Here, it is understood that the τ integral is performed for real iE. The resulting function can then be analytically continued into the entire complex E plane, with the energy poles then appearing on the real E axis. This correspondence holds because (as shown below) $|\lambda_0\rangle$ differs from the free particle state $|\vec{0},0,0\rangle$ by factors that vanish as $L \to \infty$. In addition, the quantity $\tilde{\mathcal{K}}_{\mathrm{df},3}(1 + \tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3})^{-1}$ expands to a geometric series in which, following the analysis of Ref. [2], we can think of $\tilde{\mathcal{K}}_{\mathrm{df},3}$ as a local three-particle interaction, while the intervening factors of $\tilde{F}_3$ incorporate all possible two-to-two scatterings in finite volume. The form of the correlator $C_{\phi^3}(E)$ is such that, if one were to use it in a numerical lattice calculation, one would pick out the near-threshold state. This is the case because the deviation of the true state from the noninteracting state falls as a power of $1/L$.

[6] Divergences in eigenvalues of $\mathcal{K}_{\mathrm{df},3}$ do not give a solution as they cancel between the numerator and denominator.

In any case, what matters in the following is that Eq. (26) is a valid form for the quantization condition. To see its utility, we define

$$\tilde{F}_3 \equiv \bar{F}_3 + F_3^{\lambda_0}, \tag{28}$$

$$F_3^{\lambda_0} \equiv -\tilde{F}|\lambda_0\rangle \frac{1}{\mathcal{N}_0 L^3 \lambda_0} \langle\lambda_0|\tilde{F}, \tag{29}$$

where $\langle\lambda_0|\lambda_0\rangle = \mathcal{N}_0$.[7] In other words, Eq. (28) splits $\tilde{F}_3$ into a part arising from the small eigenvector of $\mathcal{H}$ and the remainder $\bar{F}_3$, which is not enhanced when ΔE is tuned. Substituting this form into our new quantization condition and performing straightforward manipulations, we find

$$\langle\lambda_0|\tilde{F}\tilde{\mathcal{K}}_{\mathrm{df},3} \frac{1}{1+\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}} \tilde{F}|\lambda_0\rangle$$

$$= \langle\lambda_0|\tilde{F} \frac{1}{[\tilde{\mathcal{K}}_{\mathrm{df},3}]^{-1} + \bar{F}_3 + F_3^{\lambda_0}} \tilde{F}|\lambda_0\rangle, \tag{30}$$

$$= \mathcal{Z} \frac{1}{1 - \mathcal{Z}/(\mathcal{N}_0 L^3 \lambda_0)}, \tag{31}$$

where

$$\mathcal{Z} = \langle\lambda_0|\tilde{F}\tilde{\mathcal{K}}_{\mathrm{df},3} \frac{1}{1+\bar{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}} \tilde{F}|\lambda_0\rangle. \tag{32}$$

We now see the reason for placing factors of $\tilde{F}$ next to the external states in the quantization condition (26). This mirrors the factors that appear in F_3^{00} and leads to a simple final expression (31) involving only the matrix element $\mathcal{Z}$.

Using Eq. (31) we see that the quantization condition can be rewritten as

$$\mathcal{Z} = \mathcal{N}_0 L^3 \lambda_0. \tag{33}$$

We stress that although $\mathcal{Z}$ has a very similar form to the quantity appearing in the quantization condition (26), it does not diverge near threshold. This is because the enhanced contribution to $\tilde{F}_3$ has been removed, and $\bar{F}_3$ is of $\mathcal{O}(1/L^3)$ for all near-threshold energies. In fact, as we show below, $\mathcal{Z}$ is related to the divergence-free three-particle amplitude at threshold, $\mathcal{M}_{\mathrm{df},3}$.

To use Eq. (33) we tune the coefficients a_3, a_4 and a_5 in ΔE_{th} such that $\lambda_0 \sim 1/L^3$. Then we fix a_6 by enforcing (33). Clearly this form of the quantization condition is much simpler than the original version, Eq. (3), since it no longer requires evaluating the formally infinite-dimensional determinant. This simplicity comes, however, at a cost in generality—our new form is only useful for studying the near-threshold state.

In the following subsections we use this reduced quantization condition to determine the $1/L$ expansion of the threshold energy shift. This analysis is organized as follows. We begin in the following subsection by determining the $1/L$ scaling properties of $\tilde{\mathcal{K}}_2$, $\tilde{G}$ and $\tilde{F}$. Next, in Sec. III B, we use these inputs to develop the perturbative expansion of λ_0 and the corresponding state $|\lambda_0\rangle$. Following this, in Sec. III C we prove an important identity relating a matrix element entering the quantization condition and the infinite-volume divergence-free three-particle scattering amplitude. We manipulate this result further in Sec. III D, to reach our final threshold three-particle observable, denoted $\mathcal{M}_{3,\mathrm{th}}$. Finally in Sec. III E we combine results to expand Eq. (33) in powers of $1/L$ and determine the coefficients in ΔE_{th}.

A. Scaling of matrix components with $1/L$

In this subsection we determine how the elements of the matrices $\tilde{\mathcal{K}}_2$, $\tilde{F}$ and $\tilde{G}$ scale with $1/L$ in the regime where the spectator-momentum matrix index satisfies $k \sim 1/L \ll m$. We assume that ΔE scales as $1/L^3$ throughout.

We repeatedly use several simple kinematic results that follow from the definitions in Eq. (7). In the special case $\vec{k} = 0$ we have the exact results

$$\omega_k = \omega_0 = m, \qquad q_0^{*2} = m\Delta E + \frac{\Delta E^2}{4} \equiv q^2, \quad \text{and}$$
$$E_{2,0}^* = 2m + \Delta E = 2\omega_q, \tag{34}$$

where we have introduced the convenient abbreviation q for the three-momentum of each of the nonspectator particles in the case that the spectator has zero momentum. We note that $q^2 \sim \Delta E \sim 1/L^3$. For general $\vec{k} = 2\pi\vec{n}/L \neq \vec{0}$, with $n \sim \mathcal{O}(1)$, we expand in powers of $1/L$, finding

$$\omega_k = m\left(1 + \frac{k^2}{2m^2} + \mathcal{O}[(mL)^{-4}]\right), \tag{35}$$

$$E_{2,k}^* = 2m\left(1 - \frac{3k^2}{8m^2} + \frac{\Delta E}{2m} + \mathcal{O}[(mL)^{-4}]\right), \tag{36}$$

$$q_k^{*2} = -\frac{3k^2}{4} + m\Delta E + m^2\mathcal{O}[(mL)^{-4}]. \tag{37}$$

Note that, unlike for $\vec{k} = 0$, in this case the CM frame of the nonspectator pair is moving relative to the rest frame of the finite volume.

We consider first the $1/L$ scaling of $\tilde{\mathcal{K}}_2$, which we recall is a diagonal matrix. Since this is an infinite-volume quantity, L dependence enters only through ΔE. The

[7] We use an unnormalized state $|\lambda_0\rangle$ since this proves convenient when studying this state and its eigenvalue using Raleigh-Schrödinger perturbation theory, as we do in Sec. III B.

leading term is of $\mathcal{O}(L^0)$ and is simply given by the value of $\tilde{\mathcal{K}}_2$ at threshold in the appropriate partial wave. As noted above, this is nonvanishing for all ℓ, m because of the factors of Q^{-1} in the definition (19). It turns out that the only explicit expression we need is for the $\vec{k}=0$, $\ell=0, m=0$ element.[8] This can be obtained by inserting the threshold expansion, Eq. (8), into the definitions (6) and (19), and using the kinematic results of Eq. (34):

$$\tilde{\mathcal{K}}_{2;00} = -64\pi m^2 a\left\{1+\frac{\Delta E}{2m}[1+ram^2]+\mathcal{O}\left[\frac{1}{(mL)^6}\right]\right\}. \tag{38}$$

At this stage, we reiterate that we are considering in this subsection only what we have called the "naive" scaling behavior, valid when $k\sim 1/L \ll m$. It turns out that *all* entries of $\tilde{\mathcal{K}}_2$ (i.e. all $\vec{k}$, ℓ and m) actually contribute to ΔE at $\mathcal{O}(1/L^6)$, due to the high-momentum ends of the sums over indices. This is explained in Sec. III B.

The scaling of the elements of $\tilde{G}$ is more complicated. Recall that $\tilde{G}$ is given by Eq. (11) with the factors of q_k^* removed and an overall factor of $1/(2\omega_p)$ included:

$$\tilde{G}_{p,\ell',m';k,\ell,m} \equiv \frac{1}{L^3}\frac{1}{2\omega_p}\frac{4\pi(k^*)^{\ell'}Y_{\ell',m'}(\hat{k}^*)H(\vec{p})H(\vec{k})(p^*)^{\ell}Y^*_{\ell,m}(\hat{p}^*)}{2\omega_{kp}(E-\omega_k-\omega_p-\omega_{kp})}\frac{1}{2\omega_k}. \tag{39}$$

We begin with the generic case in which one or both of $\vec{k}$ and $\vec{p}$ are of $\mathcal{O}(1/L)$, from which it follows that both $\vec{p}^*$ and $\vec{k}^*$ are also of this order. Noting that the energy denominator then behaves as $E-\omega_k-\omega_p-\omega_{kp}\sim 1/L^2$, we see from Eq. (39) that the generic scaling is

$$\tilde{G}_{p,\ell',m';k,\ell,m}\sim\frac{1}{L^{1+\ell+\ell'}} \qquad (\vec{k}\neq 0 \quad \text{and/or} \quad \vec{p}\neq 0). \tag{40}$$

The exceptions to this scaling are the $\vec{k}=\vec{p}=0$ elements. These are special because k^* and p^* now vanish, and the energy denominator scales as $E-3m=\Delta E\sim 1/L^3$ rather than $1/L^2$. These results imply that the $\vec{k}=\vec{p}=0$ elements of $\tilde{G}$ vanish unless $\ell=\ell'=0$, while the 00 element is of $\mathcal{O}(L^0)$, rather than $\mathcal{O}(1/L)$ as the generic scaling would predict.

The upshot is that, in the naive scaling regime, the dominant contributions are from the $\ell=\ell'=0$ entries of $\tilde{G}$. These can be obtained directly from the definition Eq. (39). We quote here only the $\vec{k}=\vec{p}=0$ component

$$\tilde{G}_{00}=\frac{1}{8m^3\Delta E L^3}. \tag{41}$$

As we show in Sec. III B, it turns out that only the $\ell=\ell'=0$ entries of $\tilde{G}$ contribute to $\Delta E_{\rm th}$ through $\mathcal{O}(1/L^5)$. As for $\tilde{\mathcal{K}}_2$, all entries of $\tilde{G}$ contribute to $\Delta E_{\rm th}$ at $\mathcal{O}(1/L^6)$ due to the high-momentum ends of the sums.

Finally, we describe the scaling of the elements of $\tilde{F}$, which we recall is given by Eqs. (13)–(15) multiplied by $(2\omega_k)^{-1}(q_k^*)^{\ell+\ell'}$:

$$\begin{aligned}\tilde{F}_{k',\ell',m';k,\ell,m} &\equiv \delta_{k'k}\frac{1}{2}\left[\frac{1}{L^3}\sum_{\vec{a}}-\int_{\vec{a}}\right] \\ &\quad\times\frac{4\pi(a^*)^{\ell+\ell'}Y_{\ell',m'}(\hat{a}^*)Y^*_{\ell,m}(\hat{a}^*)H(\vec{k})H(\vec{a})H(\vec{b}_{ka})}{2\omega_k 2\omega_a 2\omega_{ka}(E-\omega_k-\omega_a-\omega_{ka}+i\epsilon)} \\ &\quad+\delta_{k'k}\frac{(q_k^*)^{\ell+\ell'}}{2\omega_k}\rho_{\ell',m';\ell,m}(\vec{k}).\end{aligned} \tag{42}$$

Note that $\tilde{F}$ diverges whenever E equals the sum of the energies of three free particles, each having a finite-volume momentum (and with the total momentum vanishing). The value of E we are interested in—the near-threshold energy level in the presence of interactions—avoids these divergences. However, the fact that these poles lie nearby can enhance the scaling of $\tilde{F}$.

To determine the nature of this enhancement, we rewrite $\tilde{F}$ in terms of dimensionless variables, using manipulations mirroring those used in Ref. [13]. Dropping contributions to the summand of the sum-integral difference that are nonsingular (and which thus lead only to exponentially suppressed contributions to $\tilde{F}$), we find

$$\begin{aligned}\tilde{F}_{k',\ell',m';k,\ell,m} = \delta_{k'k}\Bigg\{&\left(\frac{H(\vec{k})}{16\pi^2\omega_k(E-\omega_k)}\right)\left(\frac{2\pi}{L}\right)^{1+\ell+\ell'} \\ &\times\mathcal{Z}_{\ell',m';\ell,m}(x^2,\vec{n}_k)+\frac{(q_k^*)^{\ell+\ell'}}{2\omega_k}\rho_{\ell',m';\ell,m}\Bigg\},\end{aligned} \tag{43}$$

$$\mathcal{Z}_{\ell',m';\ell,m}(x^2,\vec{n}_k)=\left[\sum_{\vec{n}_a}-\int_{\vec{n}_a}\right]\times\frac{r^{\ell'+\ell}Y_{\ell',m'}(\hat{r})Y^*_{\ell,m}(\hat{r})H(\vec{a})H(\vec{b}_{ka})}{x^2-r^2+i\epsilon}, \tag{44}$$

where $x=q_k^*L/(2\pi)$, $\vec{a}=2\pi\vec{n}_a/L$, and $\int_{\vec{n}_a}=\int d^3n_a$. The vector $\vec{r}$ is related to $\vec{n}_a$ by

[8] Higher partial waves are suppressed because, in the matrix products that arise, these are always multiplied by entries of $\tilde{G}$ or $\tilde{F}$ with $\ell\neq 0$.

$$r_\parallel = \frac{1}{\gamma}(n_{a\parallel} - |\vec{n}_k|/2), \qquad r_\perp = n_{a\perp}, \qquad \vec{n}_k = \frac{\vec{k}L}{2\pi},$$
$$\gamma = \frac{E-\omega_k}{E^*_{2,k}}, \tag{45}$$

where parallel and perpendicular are relative to the momentum $-\vec{k}$ of the nonspectator pair. Note that r^2 runs over all positive values and zero as $\vec{n}_a$ is varied.

The function in Eq. (44) is simply related to the zeta functions defined in Ref. [14] (in a way described in Refs. [13,15]) except that here we are using a different UV regularization.[9] The key property of this function for the present discussion is that, for fixed $\vec{n}_k$, as $L \to \infty$, $\mathcal{Z}_{\ell',m';\ell,m}(x^2, \vec{n}_k)$ limits to an L-independent function of x^2 that is finite except for an infinite sequence of poles. There is one pole for each term in the sum over $\vec{n}_a$, occurring when x^2 equals the corresponding value of r^2. These are exactly the poles mentioned above that occur when $E = \omega_k + \omega_a + \omega_{ka}$.

We first consider $\vec{k} = \vec{k}' \neq \vec{0}$, so that, using Eq. (37), $x^2 = -3n_k^2/4 + \mathcal{O}(1/L)$. Since x^2 is negative definite, it does not approach the poles of $\mathcal{Z}$, which are all at $x^2 \geq 0$. Thus, there is no enhancement of the scaling, and $\mathcal{Z}(x^2, \vec{n}_k) = \mathcal{O}(L^0)$. The scaling of the first term in $\tilde{F}$ is therefore given by the explicit factors of $1/L$. The ρ-dependent term has the same scaling, and so we conclude that $\tilde{F} \sim 1/L^{1+\ell+\ell'}$ when $\vec{k} = \vec{k}' \neq \vec{0}$.

We next turn to $\vec{k} = \vec{k}' = \vec{n}_k = 0$, in which case x^2 vanishes in the infinite volume limit: $x^2 = q^2L^2/(2\pi)^2 \sim 1/L$. Thus, if $\mathcal{Z}$ has a pole at $x^2 = 0$, there can be an enhancement in the scaling. For $\vec{n}_k = 0$, Eq. (45) gives $r^2 = n_a^2$, so there is indeed a pole at $x^2 = 0$, from the $\vec{n}_a = 0$ term in the sum. However, this pole is present only when $\ell = \ell' = 0$. For nonvanishing angular momenta, the residue vanishes due to the factor of $r^{\ell'+\ell} = n_a^{\ell+\ell'}$. This implies that, even for $\vec{k} = \vec{k}' = 0$, the scaling derived above for $\vec{k} = \vec{k}' \neq 0$ holds when one or both of ℓ and ℓ' are nonvanishing. The only special case is $\vec{k} = \vec{k}' = \ell = \ell' = 0$. Here, the $\vec{n}_a = 0$ term in the sum gives $\mathcal{Z}(x^2, \vec{0}) \sim 1/x^2 \sim L$, and thus $\tilde{F}_{00} \sim L^0$, i.e. enhanced by one power of L compared to the generic scaling. In the subsequent analysis we will need the first four terms in the $1/L$ expansion of $\tilde{F}_{00}$. These are worked out in Appendix A, with the result

$$\tilde{F}_{00} = \frac{1}{16m\omega_q}\left\{\frac{1}{q^2L^3} - \frac{\mathcal{I}}{4\pi^2L} - \frac{q^2L^3\mathcal{J}}{(4\pi^2L)^2} - \frac{(q^2L^3)^2\mathcal{K}}{(4\pi^2L)^3} + \mathcal{O}\left(\frac{1}{L^4}\right)\right\}. \tag{46}$$

[9] Our functions are regulated by the product of H functions, whereas Ref. [14] uses analytic regularization.

Here $\mathcal{I}$, $\mathcal{J}$ and $\mathcal{K}$ are numerical constants defined in Appendix A.

As with $\tilde{\mathcal{K}}_2$ and $\tilde{G}$, the high-momentum entries of $\tilde{F}$ also contribute to ΔE at $\mathcal{O}(1/L^6)$. This contribution comes only from the ρ-dependent term, the second term in Eqs. (42) and (43).

B. Perturbative expansion of λ_0

In this subsection we develop the perturbative expansion of λ_0, the eigenvalue that appears on the left-hand side of our reduced quantization condition, Eq. (33). We recall that λ_0 is the eigenvalue $\mathcal{H}$ [defined in Eq. (22)] that can be tuned to be of $\mathcal{O}(1/L^3)$ by adjusting ΔE. This tuning is required to satisfy Eq. (33). As already mentioned, $\mathcal{H}$ is generally $\mathcal{O}(L^0)$, so that ΔE must be adjusted to cancel three orders to achieve the desired scaling. Such a cancellation is only possible for the 00 entry of $\mathcal{H}$, because only for this entry do $\tilde{G}$ and $\tilde{F}$ contain $\mathcal{O}(L^0)$ parts that can cancel with $\tilde{\mathcal{K}}_2^{-1}$. It follows that λ_0 can be described as a perturbation of this entry and that the corresponding state, $|\lambda_0\rangle$, is a perturbation of $|\vec{0}, 0, 0\rangle$.

We now seek to determine an expression for λ_0 in terms of ΔE. Since $\mathcal{H}$ is Hermitian we can borrow technology from nonrelativistic quantum mechanics. In particular, we analyze λ_0 using a method related to Raleigh-Schrödinger perturbation theory (RSPT). It proves convenient to first slightly rewrite our "Hamiltonian" in terms of the two-particle scattering amplitude $\mathcal{M}_2$ instead of $\mathcal{K}_2$,

$$\mathcal{H} = \tilde{\mathcal{M}}_2^{-1} + \tilde{F}^{i\epsilon} + \tilde{G}, \tag{47}$$

where

$$\mathcal{M}_2{}^{-1} = \mathcal{K}_2^{-1} + \rho, \tag{48}$$

$$\tilde{\mathcal{M}}_2^{-1} = (2\omega)^{-1}Q\mathcal{M}_2{}^{-1}Q = \tilde{\mathcal{K}}_2^{-1} + (2\omega)^{-1}Q\rho Q, \tag{49}$$

$$\tilde{F}^{i\epsilon} = (2\omega)^{-1}QF^{i\epsilon}Q = \tilde{F} - (2\omega)^{-1}Q\rho Q, \tag{50}$$

and $F^{i\epsilon}$ is defined in Eq. (15). The reason for this choice is that, for fixed $k \sim m$, $F^{i\epsilon}(\vec{k})$ is exponentially suppressed as $L \to \infty$, since the summand of the sum-integral difference in (15) is smooth.[10] We use this result repeatedly in the following analysis. The same is not true of $F(\vec{k})$, due to the $\rho(\vec{k})$ term in Eq. (14).

Next, we split $\mathcal{H}$ into a part $\mathcal{H}_0$ that contains all the terms scaling as L^0 in the $k \sim 1/L$ regime, and the remainder, $\mathcal{H}_R$, which is of $\mathcal{O}(1/L)$. As explained in the previous subsection, all nonzero elements of $\tilde{\mathcal{K}}_2$, as well as the

[10] For $\Delta E \sim 1/L^3$ and the spectator momentum $k \sim m$, the nonspectator pair are far below threshold, the energy denominator is of $\mathcal{O}(m)$, and there are no poles.

components $\tilde{F}_{00}$ and $\tilde{G}_{00}$, are of $\mathcal{O}(L^0)$. The ρ terms are of $\mathcal{O}(1/L)$ and thus do not change the scaling. Thus, we introduce the subtracted quantities

$$\not{F}^{i\epsilon} \equiv \tilde{F}^{i\epsilon} - |\vec{0},0,0\rangle \tilde{F}^{i\epsilon}_{00} \langle \vec{0},0,0|, \tag{51}$$

$$\not{G} \equiv \tilde{G} - |\vec{0},0,0\rangle \tilde{G}_{00} \langle \vec{0},0,0|, \tag{52}$$

in which the $\mathcal{O}(L^0)$ component is excised, and split $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_R, \tag{53}$$

$$\mathcal{H}_0 = \tilde{\mathcal{M}}_2^{-1} + |\vec{0},0,0\rangle (\tilde{F}^{i\epsilon}_{00} + \tilde{G}_{00}) \langle \vec{0},0,0|, \tag{54}$$

$$\mathcal{H}_R = \not{F}^{i\epsilon} + \not{G}. \tag{55}$$

By construction, $\mathcal{H}_0$ is diagonal, with eigenvectors $|\vec{k},l,m\rangle$, and corresponding eigenvalues

$$\lambda_0^{(0)} \equiv \lambda_{000}^{(0)} = \tilde{\mathcal{M}}^{-1}_{2;00} + \tilde{F}^{i\epsilon}_{00} + \tilde{G}_{00} = \tilde{\mathcal{K}}^{-1}_{2;00} + \tilde{F}_{00} + \tilde{G}_{00}, \tag{56}$$

$$\lambda^{(0)}_{klm} = \frac{q_k^*}{16\pi E^*_{2,k}} \cot\delta_\ell(q_k^*) + \tilde{\rho}(E^*_{2,k}), \qquad \{\vec{k},l,m\} \neq \{\vec{0},0,0\}. \tag{57}$$

We see again that only $\lambda_0^{(0)}$ can be tuned to be small, while all other eigenvalues are of $\mathcal{O}(L^0)$. One subtlety in the following is that $\mathcal{H}_0$ is not necessarily Hermitian, since the eigenvalues with $\vec{k}=0$ but $\ell \neq 0$ can be complex. This is because $\tilde{\rho}(E^*_{2,k})$ [defined in Eq. (17)] is imaginary if $\Delta E > 0$, which is possible if $\vec{k}=0$. Nevertheless, the eigenvectors of $\mathcal{H}_0$ form an orthonormal basis, and this is sufficient for the subsequent analysis. We note also that $\mathcal{H}_0$ does become Hermitian when $\Delta E = 0$, i.e. when $L \to \infty$.

Using the results for $\tilde{\mathcal{K}}_2$, $\tilde{F}_{00}$ and $\tilde{G}_{00}$ given in Eqs. (38), (41) and (46), respectively, as well as the kinematic relation (34), we can work out the $1/L$ expansion of $\lambda_0^{(0)}$. We obtain

$$\begin{aligned}\lambda_0^{(0)} = & -\frac{1}{64\pi m^2 a}\left[1 - \frac{x(1+ram^2)}{2m^3L^3}\right] \\ & + \frac{1}{16m}\left[\frac{1}{x} - \frac{\mathcal{I}}{4\pi^2 mL} - \frac{\mathcal{J}x}{(4\pi^2 mL)^2} - \frac{\mathcal{K}x^2}{(4\pi^2 mL)^3} \right. \\ & \left. - \frac{3}{4m^3L^3}\right] + \frac{1}{8mx} + \mathcal{O}\left(\frac{1}{L^4}\right),\end{aligned} \tag{58}$$

where the first square brackets contain the expansion of $\tilde{\mathcal{K}}_{2;00}$, the second the expansion of $\tilde{F}_{00}$, the last term is $\tilde{G}_{00}$, and we have introduced the dimensionless variable

$$x \equiv \Delta E L^3 m^2, \tag{59}$$

which is of $\mathcal{O}(L^0)$. In order to tune λ_0 to scale as $1/L^3$, we find that $\lambda_0^{(0)}$ itself must scale as $1/L^2$. This is because the difference, $\lambda_0 - \lambda_0^{(0)}$, contains a term scaling as $1/L^2$ that must be canceled. We defer details of the tuning to Sec. III E, except for one result. This concerns the cancellation of the $\mathcal{O}(L^0)$ part of $\lambda_0^{(0)}$. Using the result $2\tilde{G}_{00} = \tilde{F}_{00} + \mathcal{O}(1/L)$ [which can be read off from Eq. (58)] this cancellation requires $-3\tilde{\mathcal{K}}_{2;00}\tilde{F}_{00} = 1 + \mathcal{O}(1/L)$. We need this result in the following subsection.

We now work out the perturbative expansion for λ_0 and the corresponding eigenvector $|\lambda_0\rangle$ in powers of $\mathcal{H}_R$. A standard starting point for developing RSPT is

$$|\lambda_0\rangle = |\lambda_0^{(0)}\rangle + \mathcal{R}_0(\mathcal{H}_R - \lambda_0 + \lambda_0^{(0)})|\lambda_0\rangle, \tag{60}$$

$$\mathcal{R}_0 \equiv \frac{1 - |\lambda_0^{(0)}\rangle\langle\lambda_0^{(0)}|}{\lambda_0^{(0)} - \mathcal{H}_0}, \tag{61}$$

where $|\lambda_0^{(0)}\rangle = |\vec{0},0,0\rangle$ is the unperturbed state. Note that, in this formulation, $|\lambda_0\rangle$ satisfies $\langle\lambda_0^{(0)}|\lambda_0\rangle = 1$, implying that $|\lambda^0\rangle$ as defined in Eq. (60) is not normalized to unity, $\mathcal{N}_0 = \langle\lambda_0|\lambda_0\rangle \neq 1$. Iterating Eq. (60) yields

$$|\lambda_0\rangle = \sum_{n=0}^{\infty} |\lambda_0^{(n)}\rangle, \tag{62}$$

with

$$|\lambda_0^{(n)}\rangle \equiv [\mathcal{R}_0(\mathcal{H}_R - \lambda_0 + \lambda_0^{(0)})]^n |\lambda_0^{(0)}\rangle. \tag{63}$$

Contracting with $\langle\lambda_0^{(0)}|\mathcal{H}$ leads to the perturbative expansion for the eigenvalue

$$\lambda_0 = \lambda_0^{(0)} + \sum_{n=0}^{\infty} \lambda_0^{(n+1)}, \tag{64}$$

$$\lambda_0^{(n+1)} \equiv [\mathcal{H}_R[\mathcal{R}_0(\mathcal{H}_R - \lambda_0 + \lambda_0^{(0)})]^n]_{00}. \tag{65}$$

To obtain standard RSPT one inserts the expansion for λ_0 and reexpands in powers of $\mathcal{H}_R$. We will not take this step but rather work with the forms above, containing λ_0. This is possible because we will find that, at the order in $1/L$ that we work, we can set $\lambda_0^{(0)} - \lambda_0$ to zero on the right-hand sides of Eqs. (63) and (65).

We first analyze the perturbative shift to the eigenvalue. Naively, since $\mathcal{H}_R \sim 1/L$, we might expect that a third-order calculation is sufficient to obtain the desired accuracy, $\lambda_0 \sim 1/L^3$. However, as described in the introduction to this section, this scaling breaks down for $k \sim m$, and for such large momenta it turns out that an all-orders summation is needed.

The first-order shift $\lambda_0^{(1)}$ vanishes, since $\not{G}$ and $\not{F}^{i\epsilon}$ are both defined with a vanishing 00th component. Thus, the first nonvanishing correction appears at second order:

$$\lambda_0^{(2)} = [(\not{F}^{i\epsilon} + \not{G})\mathcal{R}_0(\not{F}^{i\epsilon} + \not{G})]_{00}. \tag{66}$$

To obtain this form we have used the result

$$[(\not{F}^{i\epsilon} + \not{G})\mathcal{R}_0(-\lambda_0 + \lambda_0^{(0)})]_{00} = 0, \tag{67}$$

which follows from the fact that $\mathcal{R}_0$ has all zeroes in its first column. We can further reduce $\lambda_0^{(2)}$ by using the fact that $\lambda_0^{(0)}$ will be tuned to be of $\mathcal{O}(1/L^2)$. This implies

$$\mathcal{R}_0 = -\tilde{\mathcal{M}}_2 + \mathcal{O}(1/L^2), \tag{68}$$

and substituting into Eq. (66) gives

$$\lambda_0^{(2)} = \sum_{\vec{k},\ell,m} \not{G}_{000;k\ell m}[-\tilde{\mathcal{M}}_2 + \mathcal{O}(1/L^2)]_{k\ell m;k\ell m}\not{G}_{k\ell m;000} + \sum_{\ell m} \not{F}^{i\epsilon}_{000;0\ell m}[-\tilde{\mathcal{M}}_2 + \mathcal{O}(1/L^2)]_{0\ell m;0\ell m}\not{F}^{i\epsilon}_{0\ell m;000}, \tag{69}$$

where we have written out all sums explicitly. In writing this form we have used the facts that $\not{F}^{i\epsilon}$ is diagonal in $\vec{k}$, that the slashed quantities have no 00 element, and that $\not{G}_{000;0lm}$ vanishes whenever $\ell \neq 0$.

We want to pick out contributions falling no faster than $1/L^3$ from Eq. (69). We do so by keeping terms that have the desired scaling either in the low-momentum ($k \sim 1/L$) regime or in the high-momentum ($k \sim m$) regime, or both. For low momenta, the dominant contribution comes from the first term with $\ell = 0$, for then $\not{G} = \mathcal{O}(1/L)$. Thus, the first term scales as $1/L^2$ (and the dominant contribution arises when intermediate angular momentum vanishes). In the second term, only $\ell \neq 0$ contributes, with the leading term coming from $\ell = 4$. Since $\not{F}^{i\epsilon}_{000;040} = \mathcal{O}(1/L^5)$, the second term scales as $1/L^{10}$ and can be dropped in the low-momentum regime.[11] In fact, for this term this is the only relevant regime, since there is no sum over $\vec{k}$.

What remains is to analyze the first term in Eq. (69) in the high-momentum regime, $k \sim m$. Then the only explicit L dependence arises from the overall factor of $1/L^3$ in $\not{G}$. At first sight this leads to a $1/L^6$ scaling since there are two factors of $\not{G}$. However, the total number of terms in the high-momentum part of the sum scales as L^3, canceling one of the factors of $1/L^3$. This is just an application of the result that, for a smooth function[12] $f(\vec{k})$,

$$\frac{1}{L^3}\sum_{\vec{k}} f(\vec{k}) = \int \frac{d^3k}{(2\pi)^3} f(\vec{k}) + \mathcal{O}(e^{-mL}). \tag{70}$$

The resulting integral is independent of L, and we are dropping exponentially suppressed corrections. The conclusion is that the high-momentum contribution to $\not{G}[-\tilde{\mathcal{M}}_2]\not{G}$ scales as $1/L^3$. While subleading to the low-momentum $1/L^2$ scaling, it is still of an order that we must keep. We also note that, in contrast to the low-momentum result, higher angular-momentum contributions are not suppressed when $k \sim m$.

The net result is that

$$\lambda_0^{(2)} = [\not{G}[-\tilde{\mathcal{M}}_2]\not{G}]_{00} + \mathcal{O}\left(\frac{1}{L^4}\right), \tag{71}$$

where no constraint is placed on the intermediate matrix indices.

We now turn to the third-order perturbative correction, which takes the form

$$\lambda_0^{(3)} = [(\not{F}^{i\epsilon} + \not{G})\mathcal{R}_0(\not{F}^{i\epsilon} + \not{G} - \lambda_0 + \lambda_0^{(0)})\mathcal{R}_0(\not{F}^{i\epsilon} + \not{G})]_{00}, \tag{72}$$

$$= [\not{G}[-\tilde{\mathcal{M}}_2](\not{F}^{i\epsilon} + \not{G} - \lambda_0 + \lambda_0^{(0)})[-\tilde{\mathcal{M}}_2]\not{G}]_{00} + \mathcal{O}\left(\frac{1}{L^6}\right). \tag{73}$$

There are now two summed momenta, which we refer to as k and p, and to determine the scaling we must examine contributions from all possible momentum regimes. First suppose both are of $\mathcal{O}(1/L)$, so that naive scaling can be applied. Then the dominant contribution, scaling as $1/L^3$, comes from the s-wave parts of each factor of $\not{G}$ and $\not{F}^{i\epsilon}$. This is the first example where $\not{F}^{i\epsilon}$ enters the result for λ_0. Note further that since, by assumption, $-\lambda_0 + \lambda_0^{(0)} = \mathcal{O}(1/L^2)$, it leads to a suppressed contribution to $\lambda_0^{(3)}$ of $\mathcal{O}(1/L^4)$. This can be dropped.

We next consider the regime in which both momenta are large, of $\mathcal{O}(L^0)$. Here $F^{i\epsilon}$ is exponentially suppressed and can be dropped. The contribution involving three factors of $\not{G}$ comes with three explicit factors of $1/L^3$, but two of these are canceled by the sums over $\vec{k}$ and $\vec{p}$. Thus, as in the

[11] This follows from the observation that $Y_{40}(\hat{k})$ is the lowest spherical harmonic with $\ell \neq 0$ for which $(1/L^3)\sum_{\vec{k}} Y_{40}(\hat{k}) f(|\vec{k}|) \neq 0$, where $f(|\vec{k}|)$ is any radial function for which the sum converges.

[12] $\tilde{\mathcal{M}}_2$ and $\not{G}$ are both smooth functions in the high-momentum regime, since this corresponds (when $\Delta E \sim 1/L^3$) to the far subthreshold region.

small-momentum regime, this term is $\mathcal{O}(1/L^3)$, but in this regime all partial waves must be kept. This leaves the term containing $-\lambda_0 + \lambda_0^{(0)}$ and two factors of $\mathcal{G}$. Since $-\lambda_0 + \lambda_0^{(0)} = \mathcal{O}(1/L^2)$, this contribution has an explicit factor of $1/L^8$, one power larger than the explicit factor on the three-$\mathcal{G}$ term. However, since $-\lambda_0 + \lambda_0^{(0)}$ is diagonal, this contribution is only enhanced by one sum rather than two, leading to an overall $1/L^5$ scaling. Thus this term can also be dropped.

The final region to consider is that in which one momentum is small and the other large. Since $F^{i\epsilon}$ and $-\lambda_0 + \lambda_0^{(0)}$ are diagonal in momentum space, this regime is only possible for the term containing three $\mathcal{G}$s. Since we are keeping this term for all momenta anyway, no special attention to this case is needed.

Based on these considerations, we deduce that

$$\lambda_0^{(3)} = \sum_{\vec{k}} \mathcal{G}_{0k} \tilde{\mathcal{M}}_{2;kk} F^{i\epsilon}_{kk} \tilde{\mathcal{M}}_{2,kk} \mathcal{G}_{k0} + [\mathcal{G}[-\tilde{\mathcal{M}}_2]\mathcal{G}[-\tilde{\mathcal{M}}_2]\mathcal{G}]_{00} + \mathcal{O}\left(\frac{1}{L^4}\right). \quad (74)$$

Here, the notation in the matrices in the first term indicates that only $\ell = 0$ components are kept, e.g. $F^{i\epsilon}_{kk} \equiv F^{i\epsilon}_{k00;k00}$. By contrast, the intermediate indices are summed over all momenta and all partial waves in the second term. We stress again that the first term is dominated by small momenta, while in the second all momenta contribute.

The generalization to higher orders is now clear. For $n > 3$ one has four or more factors drawn from $\mathcal{G}$, $F^{i\epsilon}$ and $-\lambda_0 + \lambda_0^{(0)}$. This means that the low-momentum contribution scales as $1/L^4$ or higher and can be dropped. In the high-momentum regime an $\mathcal{O}(1/L^3)$ contribution does arise, given by

$$\lambda_0^{(n)} = [\mathcal{G}[-\tilde{\mathcal{M}}_2\mathcal{G}]^{n-1}] + \mathcal{O}\left(\frac{1}{L^4}\right), \quad \text{for } n > 3. \quad (75)$$

The $n-1$ momentum sums cancel all but one of the factors of $1/L^3$ contained in the $\mathcal{G}$s, so that the overall scaling is $1/L^3$. All other contributions are suppressed.

Summing our results for λ_0 to all orders, we conclude that

$$\lambda_0 = \lambda_0^{(0)} + \sum_{\vec{k}} \mathcal{G}_{0k} \tilde{\mathcal{M}}_{2,kk} F^{i\epsilon}_{kk} \tilde{\mathcal{M}}_{2,kk} \mathcal{G}_{k0} + \sum_{n=1}^{\infty} [\mathcal{G}[-\tilde{\mathcal{M}}_2\mathcal{G}]^n]_{00} + \mathcal{O}\left(\frac{1}{L^4}\right), \quad (76)$$

where, in the last term, all intermediate momenta and partial waves must be kept.

We turn now to the perturbative analysis of the state $|\lambda_0\rangle$, using Eq. (63). We are specifically interested in the two quantities involving this state that enter into the quantization condition Eq. (33). These are the normalization $\mathcal{N}_0$ and the matrix element $\mathcal{Z}$ [Eq. (32)]. For both of these, we need only the leading L^0 behavior when $L \to \infty$ with ΔE tuned such that $\lambda_0 \sim 1/L^3$.

The task of identifying the leading terms is similar to that for λ_0. After making the simplifications that follow from the properties of $\mathcal{G}$, $F^{i\epsilon}$, and $\mathcal{R}_0$, the first two terms can be written

$$|\lambda_0^{(1)}\rangle = [-\tilde{\mathcal{M}}_2](\mathcal{G} + F^{i\epsilon})|\lambda_0^{(0)}\rangle[1 + \mathcal{O}(1/L^2)], \quad (77)$$

$$|\lambda_0^{(2)}\rangle = [-\tilde{\mathcal{M}}_2](\mathcal{G} + F^{i\epsilon} - \lambda_0 + \lambda_0^{(0)})[-\tilde{\mathcal{M}}_2](\mathcal{G} + F^{i\epsilon})|\lambda_0^{(0)}\rangle \times [1 + \mathcal{O}(1/L^2)]. \quad (78)$$

Using these results, we find that the leading-order correction to $\mathcal{N}_0 = \langle\lambda_0|\lambda_0\rangle$ occurs at second order[13]:

$$\mathcal{N}_0 = 1 + \langle\vec{0},0,0|(\mathcal{G} + F^{i\epsilon})^\dagger \tilde{\mathcal{M}}_2^\dagger \tilde{\mathcal{M}}_2(\mathcal{G} + F^{i\epsilon})|\vec{0},0,0\rangle + 2\mathrm{Re}\langle\vec{0},0,0|\tilde{\mathcal{M}}_2(\mathcal{G} + F^{i\epsilon})\tilde{\mathcal{M}}_2(\mathcal{G} + F^{i\epsilon})|\vec{0},0,0\rangle + \mathcal{O}(1/L^3). \quad (79)$$

Here, we are already using the result that higher-order contributions are of $\mathcal{O}(1/L^3)$, as will become clear shortly. Note also that, at this stage, we have to account for the fact, noted above, that $\tilde{\mathcal{M}}_2$ and $F^{i\epsilon}$ are not Hermitian. In the low-momentum regime, both of the second-order terms scale as $1/L^2$, since the dominant terms in $\mathcal{G}$ and $F^{i\epsilon}$ scale as $1/L$. Similarly, at nth order, the low-momentum terms scale as $1/L^n$. In the high-momentum regime, $F^{i\epsilon}$ can be dropped, and each of the $\mathcal{G}$ factors has an explicit $1/L^3$. There is, however, only a single intermediate sum over $\vec{k}$, so the overall scaling is as $1/L^3$. The same can be easily seen to hold at all higher orders. We thus conclude that

$$\mathcal{N}_0 = 1 + \mathcal{O}(1/L^2). \quad (80)$$

Now we turn to the matrix element $\mathcal{Z}$, which can be expanded as a geometric series

$$\mathcal{Z} = \langle\lambda_0|\tilde{F}\tilde{\mathcal{K}}_{\mathrm{df},3}\tilde{F}|\lambda_0\rangle - \langle\lambda_0|\tilde{F}\tilde{\mathcal{K}}_{\mathrm{df},3}\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}\tilde{F}|\lambda_0\rangle + \cdots. \quad (81)$$

Our aim is to substitute the perturbative expansion of $|\lambda_0\rangle$ and determine the L^0 part of $\mathcal{Z}$. We note immediately that the contribution from the low-momentum regime in the results (77) and (78) is suppressed by powers of $1/L$ and

[13]The first-order term vanishes because $\mathcal{G}_{00} = F^{i\epsilon}_{00} = 0$.

can be dropped. The same is true at higher orders. In the high-momentum regime the dominant contribution comes from terms with multiple $\mathcal{G}$s (since, as in the analysis for λ_0, $F^{i\epsilon}$ is exponentially suppressed and the $-\lambda_0 + \lambda_0^{(0)}$ term lacks a momentum sum to cancel the explicit $1/L^2$). This high-momentum contribution is of $\mathcal{O}(L^0)$ and must be kept. To see this scaling, consider the first term on the right-hand side of Eq. (81) and substitute Eq. (77) for $|\lambda_0\rangle$. The presence of a factor of $\mathcal{K}_{\mathrm{df},3}$ in the "middle" of the matrix element implies that there is one momentum sum for each factor of $\mathcal{G}$, and this cancels the $1/L^3$ factors in $\mathcal{G}$. The same cancellation occurs at all orders in perturbation theory, and also for the higher-order terms in the geometric series in Eq. (81). This implies that, in the evaluation of the leading-order contribution to $\mathcal{Z}$, we can make the following substitution for the nth-order term:

$$|\lambda_0^{(n)}\rangle \to [-\tilde{\mathcal{M}}_2\mathcal{G}]^n|\vec{0},0,0\rangle. \tag{82}$$

These leading terms can then be summed into

$$|\lambda_0\rangle \to \frac{1}{1+\tilde{\mathcal{M}}_2\mathcal{G}}|\vec{0},0,0\rangle. \tag{83}$$

Thus, we find

$$\mathcal{Z} = \langle\vec{0},0,0|\frac{1}{1+\mathcal{G}\tilde{\mathcal{M}}_2}\tilde{F}\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}} \times \tilde{F}\frac{1}{1+\tilde{\mathcal{M}}_2\mathcal{G}}|\vec{0},0,0\rangle + \mathcal{O}(1/L). \tag{84}$$

Here, we have used the result that $\tilde{\mathcal{M}}_2$ is Hermitian at $\mathcal{O}(L^0)$.

C. Relation to the divergence-free three-to-three scattering amplitude

In this subsection we demonstrate the following relation between the matrix element appearing in our modified quantization condition, Eq. (33), and the infinite-volume divergence-free three-to-three scattering amplitude at threshold [defined in Eq. (94) below]:

$$\{9(\tilde{\mathcal{K}}_{2;00})^2\mathcal{Z}\}|_{E=3m+\Delta E_{\mathrm{th}}} = \mathcal{M}_{\mathrm{df},3;00} + \mathcal{O}(1/L). \tag{85}$$

This is a key result as it allows us to connect the output of the finite-volume quantization condition to an infinite-volume scattering quantity. We stress that this result only holds when the quantity on the left-hand side is evaluated at $E = 3m + \Delta E_{\mathrm{th}}$; i.e. the energy must be held at the solution to the quantization condition as $L \to \infty$.

We first review the definition of $\mathcal{M}_{\mathrm{df},3}$, given in Eq. (87) of Ref. [2]. To do so we introduce the set of integrals

$$iI^{(u,u)}_{n;\ell'm';\ell m}(\vec{p},\vec{k}) \equiv \int\frac{d^3k_n}{(2\pi)^3 2\omega_{k_n}}\cdots\int\frac{d^3k_1}{(2\pi)^3 2\omega_{k_1}} \times [i\mathcal{M}_2(\vec{p})iG^\infty(\vec{p},\vec{k}_n)i\mathcal{M}_2(\vec{k}_n) \cdots iG^\infty(\vec{k}_1,\vec{k})i\mathcal{M}_2(\vec{k})]_{\ell'm';\ell m}, \tag{86}$$

where n is a positive integer,

$$G^\infty_{\ell'm';\ell m}(\vec{p},\vec{k}) = \left(\frac{k^*}{q_p^*}\right)^{\ell'}\frac{4\pi Y_{\ell',m'}(\hat{k}^*)H(\vec{p})H(\vec{k})Y^*_{\ell,m}(\hat{p}^*)}{2\omega_{kp}(E-\omega_k-\omega_p-\omega_{kp}+i\epsilon)} \times\left(\frac{p^*}{q_k^*}\right)^{\ell}, \tag{87}$$

and

$$\mathcal{M}_{2;\ell',m';\ell,m}(\vec{k}) \equiv \delta_{\ell'\ell}\delta_{m'm}\left[\frac{q_k^*}{16\pi E^*_{2,k}}\cot\delta_\ell(q_k^*) + \tilde{\rho}(E^*_{2,k})\right]^{-1}, \tag{88}$$

is the standard two-to-two scattering amplitude for two particles carrying energy momentum $(E-\omega_k, -\vec{k})$. This differs from the matrix $\mathcal{M}_2$, introduced in Eq. (48) above, only in that $\mathcal{M}_2(\vec{k})$ is defined for continuous $\vec{k}$. The products in the square brackets of Eq. (86) are understood as matrix products over the spherical-harmonic indices. We also extend the definition to $n = 0$ via

$$iI^{(u,u)}_{0;\ell'm';\ell m}(\vec{p},\vec{k}) \equiv [i\mathcal{M}_2(\vec{p})iG^\infty(\vec{p},\vec{k})i\mathcal{M}_2(\vec{k})]_{\ell'm';\ell m}. \tag{89}$$

These definitions are shown diagrammatically in Fig. 2(a). The basic structure is a sequence of on-shell scattering amplitudes alternating with a pole term that interchanges the scattering pair. The superscript (u,u) on $I_n^{(u,u)}(\vec{k},\vec{p})$ indicates that the quantity is unsymmetrized, in the sense that the momenta $\vec{k}$ and $\vec{p}$ are assigned to the particles that are unscattered by the outermost insertions. The factors of G^∞ (represented by the vertical dashed lines in the figure) have the same singularities as propagators in the standard Feynman rules for the diagrams. Thus, the integrals $I_n^{(u,u)}$ are simplified versions of the corresponding Feynman diagrams, having the same singularities, but depending only on on-shell two-to-two scattering amplitudes.

We next define symmetrized versions of these integrals:

$$iI_n(\vec{p},\hat{a}'^*;\vec{k},\hat{a}^*) \equiv \mathcal{S}[iI^{(u,u)}_{n;\ell'm';\ell m}(\vec{p},\vec{k})] \equiv \sum_{\{\vec{x}',\vec{y}'\}\in\mathcal{P}_{\mathrm{out}}}\sum_{\{\vec{x},\vec{y}\}\in\mathcal{P}_{\mathrm{in}}} \times 4\pi Y^*_{\ell'm'}(\hat{y}'^*)iI^{(u,u)}_{n;\ell'm';\ell m}(\vec{x}',\vec{x})Y_{\ell m}(\hat{y}^*), \tag{90}$$

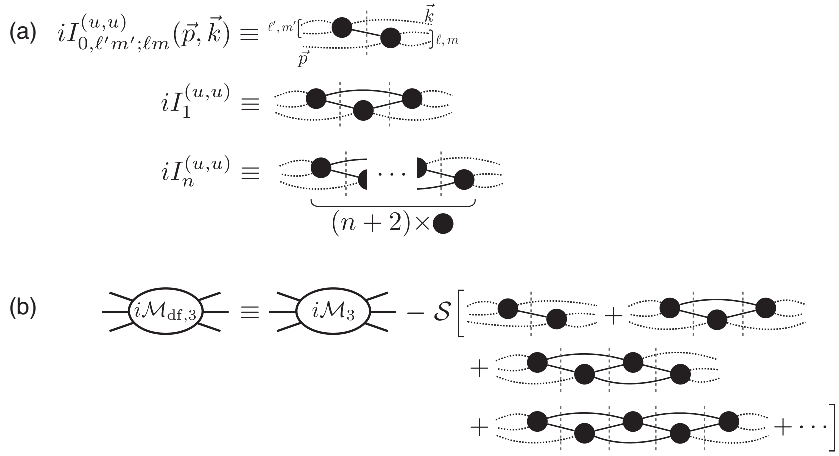

FIG. 2. Diagrammatic definitions of quantities defined in the text. (a) The unsymmetrized subtraction functions, $I_n^{(u,u)}$. Here the black disks represent on-shell projections of $\mathcal{M}_2$, and the vertical dashed lines represent simple poles, used in place of the propagators. For I_0 we have indicated the coordinate dependence, which applies for all of the functions. (b) The divergence-free three-to-three amplitude, $\mathcal{M}_{\mathrm{df},3}$. This quantity is given by subtracting an infinite series of pairwise scattering diagrams, $\sum_{n=0}^{\infty} I_n$, from the standard three-to-three scattering amplitude, $\mathcal{M}_3$. Here, $\mathcal{S}$ indicates that the symmetrized versions of I_n are to be used in the subtraction.

where we sum over possible external momentum assignments

$$\mathcal{P}_{\mathrm{out}} \equiv \{\{\vec{p}, \vec{a}'\}, \{\vec{a}', -\vec{a}' - \vec{p}\}, \{-\vec{a}' - \vec{p}, \vec{p}\}\}, \tag{91}$$

$$\mathcal{P}_{\mathrm{in}} \equiv \{\{\vec{k}, \vec{a}\}, \{\vec{a}, -\vec{a} - \vec{k}\}, \{-\vec{a} - \vec{k}, \vec{k}\}\}. \tag{92}$$

Here, $\vec{k}$, $\vec{a}$ and $-\vec{a}-\vec{k}$ are the momenta of the initial particles, while $\vec{p}$, $\vec{a}'$ and $-\vec{a}'-\vec{p}$ are those of the final particles. The direction $\hat{a}^*$ is that of $\vec{a}$ after boosting to the CM frame of the scattered pair, with $\hat{a}'^*$ defined analogously for the final state. Similarly, when the momentum pair is $\vec{x}, \vec{y}$, $\hat{y}^*$ is defined by boosting $(\omega_y, \vec{y})$ with velocity $\vec{\beta} = \vec{x}/(E-\omega_x)$. Note also that, prior to symmetrization, we have to insert the spherical harmonics and sum over their indices in order to obtain functions of the external momenta.

As we explain in detail in Refs. [1,2], the sum over all symmetrized integrals I_n has the same singularities as the full three-to-three scattering amplitude $\mathcal{M}_3$. Thus, the difference between these quantities, which we denote $\mathcal{M}_{\mathrm{df},3}$, is free of divergences. Explicitly, this is defined as

$$i\mathcal{M}_{\mathrm{df},3}(\vec{p}, \hat{a}'^*; \vec{k}, \hat{a}^*) \equiv i\mathcal{M}_3(\vec{p}, \hat{a}'^*; \vec{k}, \hat{a}^*) - \sum_{n=0}^{\infty} iI_n(\vec{p}, \hat{a}'^*; \vec{k}, \hat{a}^*), \tag{93}$$

and is shown diagrammatically in Fig. 2(b). What is required for Eq. (85) is the value of this amplitude at threshold:

$$\mathcal{M}_{\mathrm{df},3;00} \equiv \mathcal{M}_{\mathrm{df},3}(\vec{0}, \hat{a}'^*; \vec{0}, \hat{a}^*)|_{E=3m}. \tag{94}$$

Note that the right-hand side is, in fact, independent of the direction vectors $\hat{a}'^*$ and $\hat{a}^*$, since $\vec{a}'^* = \vec{a}^* = 0$ when $\vec{p} = \vec{k} = 0$ and $E = 3m$. Thus, we have included no such dependence in $\mathcal{M}_{\mathrm{df},3;00}$. An equivalent definition is given by decomposing $\mathcal{M}_{\mathrm{df},3}(\vec{p}, \hat{a}'^*; \vec{k}, \hat{a}^*)$ in spherical harmonics, keeping only the s-wave term, and evaluating this at threshold. Thus, the index label on $\mathcal{M}_{\mathrm{df},3;00}$ is consistent with that for $\tilde{\mathcal{K}}_2$, $\tilde{G}$ and $\tilde{F}$ used above.

Having explained the definition of the right-hand side of Eq. (85), we now turn to proving the claim. To do so we write out the two sides in more detail. Using the result for $\mathcal{Z}$ worked out in the previous subsection, Eq. (84), we can express the left-hand side of (85) as

$$\{9(\tilde{\mathcal{K}}_{2;00})^2\mathcal{Z}\}|_{E=3m+\Delta E} = \bar{L}\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\bar{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}}\bar{R}|_{E=3m+\Delta E} + \mathcal{O}(1/L). \tag{95}$$

Here, we have introduced the row and column vectors

$$\bar{L}_{k\ell m} = -3\tilde{\mathcal{K}}_{2;00}\left[\frac{1}{1+\mathcal{G}\tilde{\mathcal{M}}_2}\tilde{F}\right]_{000,klm}, \tag{96}$$

$$\bar{R}_{k\ell m} = -3\left[\tilde{F}\frac{1}{1+\tilde{\mathcal{M}}_2\mathcal{G}}\right]_{klm,000}\tilde{\mathcal{K}}_{2;00}. \tag{97}$$

As for the right-hand side, we can rewrite this using the general relation between finite-volume and infinite-volume three-particle scattering amplitudes given in Eq. (80) of Ref. [2]. For the threshold amplitude this relation is

$$\mathcal{M}_{\mathrm{df},3;00} = \lim_{L\to\infty}|_{i\epsilon}\mathcal{S}\left[\left(\frac{1}{3} - \frac{1}{1+\mathcal{M}_{2,L}G}\mathcal{M}_{2,L}F\right)\right. \\ \times \mathcal{K}_{\mathrm{df},3}\frac{1}{1+F_3\mathcal{K}_{\mathrm{df},3}}\left(\frac{1}{3} - \frac{F}{2\omega}\frac{1}{1+G\mathcal{M}_{2,L}} \right. \\ \left.\left.\times \mathcal{M}_{2,L}(2\omega)\right)\right]_{000;000}, \tag{98}$$

where $E = 3m$, and the new matrix is $\mathcal{M}_{2,L}^{-1} \equiv \mathcal{K}_2{}^{-1} + F$. Note that here we are apparently taking a step backwards by expressing the infinite-volume quantity $\mathcal{M}_{\mathrm{df},3;00}$ in terms of the $L \to \infty$ limit of a finite-volume matrix element. The reason for doing so is that the connection to the left-hand side of the desired relation (85) is then much clearer. One new feature in (98) is that the infinite-volume limit is taken using an $i\epsilon$ prescription. As explained in Ref. [2], a prescription is needed to avoid singularities in F and G. The prescription that is required for (98) to hold is that singularities in summands are shifted by $i\epsilon$, after which the infinite-volume limit is well defined.

The symmetrization operator $\mathcal{S}$ in Eq. (98) is essentially the same as that defined in Eq. (90), although there are some subtleties when applied to the finite-volume matrices [2]. These do not concern us here, however, because symmetrization is trivial for the threshold amplitude—it leads simply to an overall factor of 9.

We proceed by rewriting the result (98) in a form that is similar to Eq. (95). After some reorganization (including insertions of appropriate factors of QQ^{-1} and using $Q_{00} = 1$) we find

$$\mathcal{M}_{\mathrm{df},3;00} = \lim_{L\to\infty}|_{i\epsilon}\tilde{L}\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}}\tilde{R}, \tag{99}$$

where $E = 3m$ and the new row and column vectors are

$$\tilde{L}_{k\ell m} = [1 - 3\mathcal{H}^{-1}\tilde{F}]_{000,k\ell m}, \tag{100}$$

$$\tilde{R}_{k\ell m} = [1 - 3\tilde{F}\mathcal{H}^{-1}]_{k\ell m,000}. \tag{101}$$

The result we are aiming to demonstrate can now be rewritten as

$$\lim_{L\to\infty}\bar{L}\,\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\bar{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}}\bar{R}|_{E=3m+\Delta E_{\mathrm{th}}} \\ = \lim_{L\to\infty}|_{i\epsilon}\tilde{L}\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}}\tilde{R}|_{E=3m}. \tag{102}$$

We have chosen the notation in such a way that the results look similar, but we still have significant work to do to demonstrate equality. We stress that the nature of the infinite-volume limits differs between the two sides: on the left-hand side ΔE is tuned to satisfy the quantization condition, while on the right-hand side $\Delta E = 0$.

We first focus on the matrices between the "L" and "R" vectors, and show that

$$\lim_{L\to\infty}\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\bar{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}}|_{E=3m+\Delta E_{\mathrm{th}}} \\ = \lim_{L\to\infty}|_{i\epsilon}\tilde{\mathcal{K}}_{\mathrm{df},3}\frac{1}{1+\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}}|_{E=3m}. \tag{103}$$

We first give a qualitative explanation of this equality. The limit on the right-hand side has been investigated in Ref. [2] and is given by an infinite-volume function $\mathcal{T}_{\ell',m';\ell,m}(\vec{p},\vec{k})$ (where $\vec{p}$ and $\vec{k}$ are the external spectator momenta, both held fixed in the limit). The contribution that survives in the limit comes from large intermediate momenta—contributions from low momenta are suppressed by powers of $1/L$. We note also that, once the limit is taken, we can send $\epsilon \to 0^+$, since the poles are at threshold, and do not need regulation once sums have been converted to integrals. The quantity on the left-hand side differs in two ways: (i) $\tilde{F}_3$ is replaced by $\bar{F}_3 = \tilde{F}_3 - F_3^{\lambda_0}$, and (ii) the infinite-volume limit is approached with the tuned $\Delta E_{\mathrm{th}} = \mathcal{O}(1/L^3)$ rather than $\Delta E = 0$. Note that this limit avoids the poles in F and G that occur at $\Delta E = 0$, so that one does not need to use the $i\epsilon$ prescription at an intermediate stage. Thus, as far as the contributions from large intermediate momenta are concerned, one approaches exactly the same kinematic point as on the right-hand side and should attain the same limit. For large momenta the subtracted part $F_3^{\lambda_0}$ is suppressed by powers of $1/L$. The only complication is that, when approaching the limit with tuned ΔE, there is an enhanced low-momentum contribution to $\tilde{F}_3$, namely, that from $F_3^{\lambda_0}$. This, however, is removed by the subtraction in $\bar{F}_3$, so the left-hand side also receives no low-momentum contributions as $L \to \infty$.

To demonstrate the result in detail we expand both sides of (103) in a geometric series and argue that the results agree order by order. The leading-order terms are identical, so the first nontrivial result to show is

$$\lim_{L\to\infty}\tilde{\mathcal{K}}_{\mathrm{df},3}(\tilde{F}_3 - F_3^{\lambda_0})\tilde{\mathcal{K}}_{\mathrm{df},3}|_{E=3m+\Delta E_{\mathrm{th}}} \\ = \lim_{L\to\infty}|_{i\epsilon}\tilde{\mathcal{K}}_{\mathrm{df},3}\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}|_{E=3m}. \tag{104}$$

Our first step is to replace the $i\epsilon$ regulated limit on the right-hand side with one in which $E - 3m = c/L^3$, with c any constant differing from the tuned value a_3 to be determined below. This avoids the poles in F and G [which are at $E = 3m$ and $E = 3m + \mathcal{O}(1/L^2)$] so that the limit is well defined. In other words we have

$$\lim_{L\to\infty}|_{i\epsilon}\tilde{\mathcal{K}}_{\mathrm{df},3}\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}|_{E=3m} = \lim_{L\to\infty}\tilde{\mathcal{K}}_{\mathrm{df},3}\tilde{F}_3\tilde{\mathcal{K}}_{\mathrm{df},3}|_{E=3m+c/L^3}. \tag{105}$$

Next we argue that on the left-hand side of (104) we can replace $E = 3m + \Delta E_{\rm th}$ with $E = 3m + c/L^3$, with any choice of c:

$$\lim_{L\to\infty} \tilde{\mathcal{K}}_{{\rm df},3}(\tilde F_3 - F_3^{\lambda_0})\tilde{\mathcal{K}}_{{\rm df},3}|_{E=3m+\Delta E_{\rm th}} = \lim_{L\to\infty} \tilde{\mathcal{K}}_{{\rm df},3}(\tilde F_3 - F_3^{\lambda_0})\tilde{\mathcal{K}}_{{\rm df},3}|_{E=3m+c/L^3}. \tag{106}$$

Note here that $F_3^{\lambda_0} = -\tilde F|\lambda_0\rangle\langle\lambda_0|\tilde F/(\mathcal{N}_0 L^3\lambda_0)$ depends on how E is chosen to approach $3m$, since both λ_0 and $|\lambda_0\rangle$ depend on E. To understand this equality consider first the $\tilde F_3$ terms. We recall from our earlier discussion that $\tilde F_3$ has an explicit factor of $1/L^3$, whereas $\tilde{\mathcal{K}}_{{\rm df},3} \sim \mathcal{O}(L^0)$. The $1/L^3$ can only be canceled by a sum over large intermediate momenta (leading to the infinite volume function $\mathcal{T}$ described above) or by the presence of an eigenvalue of $\mathcal{H}$ scaling as $1/L^3$. The latter corresponds to a low-momentum intermediate state since $|\lambda_0\rangle = |\vec 0, 0, 0\rangle + \mathcal{O}(1/L)$. The subtraction on the left-hand side removes this potential $\mathcal{O}(L^0)$ contribution, however, so the difference $\bar F_3$ cannot give rise to an $\mathcal{O}(L^0)$ low-momentum contribution. Thus, it makes no difference precisely how the large volume limit is taken as long as the same asymptote is approached. This is the case for the two sides of (106) for any choice of c.

Finally, we note that the $F_3^{\lambda_0}$ term can be dropped from the right-hand side of Eq. (106),

$$\lim_{L\to\infty} \tilde{\mathcal{K}}_{{\rm df},3}(\tilde F_3 - F_3^{\lambda_0})\tilde{\mathcal{K}}_{{\rm df},3}|_{E=3m+c/L^3} = \lim_{L\to\infty} \tilde{\mathcal{K}}_{{\rm df},3}\tilde F_3\tilde{\mathcal{K}}_{{\rm df},3}|_{E=3m+c/L^3}, \tag{107}$$

as long as $c \neq a_3$. This is simply because the explicit factor of $1/L^3$ in $F_3^{\lambda_0}$ cannot be canceled for an untuned energy.

Combining these three steps we find that the left- and right-hand sides of (104) are equal. This argument can be extended almost verbatim to the higher-order terms in the expansions of Eq. (103), and we do not repeat the discussion. This establishes the desired equality, Eq. (103).

It remains only to relate the "end caps" that appear in Eqs. (95) and (99). We consider first the barred end caps of Eqs. (96) and (97), which are to be evaluated along the tuned energy trajectory $E = 3m + \Delta E_{\rm th}$ in the limit $L \to \infty$. This means that we can replace $\tilde{\mathcal{K}}_{2;00}$ with $\tilde{\mathcal{M}}_{2;00}$, and that, as noted above, following Eq. (59), the combination $-3\tilde{\mathcal{M}}_{2;00}\tilde F_{00}$ has the limiting value of unity. However, $\mathcal{G}$ does not contain an $\mathcal{O}(L^0)$ term when $\Delta E \to 0$, since the potentially large term has been subtracted. Combining these observations we find

$$\lim_{L\to\infty} \bar L_{k\ell m}|_{E=3m+\Delta E_{\rm th}} = \left[-3\tilde{\mathcal{M}}_2\tilde F + 3\tilde{\mathcal{M}}_2\mathcal{G}\tilde{\mathcal{M}}_2\frac{1}{1+\mathcal{G}\tilde{\mathcal{M}}_2}\tilde F\right]_{000,k\ell m} = \left[1 + 3\tilde{\mathcal{M}}_2\mathcal{G}\tilde{\mathcal{M}}_2\frac{1}{1+\mathcal{G}\tilde{\mathcal{M}}_2}\tilde F\right]_{000,k\ell m}, \tag{108}$$

$$\lim_{L\to\infty} \bar R_{k\ell m}|_{E=3m+\Delta E_{\rm th}} = \left[-3\tilde F\tilde{\mathcal{M}}_2 + 3\tilde F\tilde{\mathcal{M}}_2\mathcal{G}\tilde{\mathcal{M}}_2\frac{1}{1+\mathcal{G}\tilde{\mathcal{M}}_2}\right]_{k\ell m,000} = \left[1 + 3\tilde F\tilde{\mathcal{M}}_2\mathcal{G}\tilde{\mathcal{M}}_2\frac{1}{1+\mathcal{G}\tilde{\mathcal{M}}_2}\right]_{k\ell m,000}, \tag{109}$$

where we have left the infinite-volume limit and the constraint $E = 3m + \Delta E_{\rm th}$ implicit in the middle and final equality.

Turning to the "tilded" end caps of Eqs. (100) and (101), the infinite-volume limit is to be taken with $E = 3m$ using the $i\epsilon$ prescription. This means that the enhanced eigenvalue of $\mathcal{H} = \tilde{\mathcal{M}}_2^{-1} + \tilde F^{i\epsilon} + \tilde G$ plays no role. As explained in Ref. [2], $\tilde F^{i\epsilon}$ vanishes in this limit [since it is a difference between a sum and an integral regulated using an $i\epsilon$ prescription; see Eq. (13)]. However, $\tilde F$ does not vanish in general, due to the contribution of the ρ term [see Eq. (14)], although $\tilde F_{00}$ does vanish at threshold, since ρ vanishes there. We find

$$\lim_{L\to\infty}|_{i\epsilon}\tilde L_{k\ell m} = \lim_{L\to\infty}|_{i\epsilon}\left[1 - 3\tilde{\mathcal{M}}_2\frac{1}{1+\tilde G\tilde{\mathcal{M}}_2}\tilde F\right]_{000,k\ell m} = \lim_{L\to\infty}|_{i\epsilon}\left[1 + 3\tilde{\mathcal{M}}_2\tilde G\tilde{\mathcal{M}}_2\frac{1}{1+\tilde G\tilde{\mathcal{M}}_2}\tilde F\right]_{000,k\ell m}, \tag{110}$$

$$\lim_{L\to\infty}|_{i\epsilon}\tilde R_{k\ell m} = \lim_{L\to\infty}|_{i\epsilon}\left[1 - 3\tilde F\tilde{\mathcal{M}}_2\frac{1}{1+\tilde G\tilde{\mathcal{M}}_2}\right]_{k\ell m,000} = \lim_{L\to\infty}|_{i\epsilon}\left[1 + 3\tilde F\tilde{\mathcal{M}}_2\tilde G\tilde{\mathcal{M}}_2\frac{1}{1+\tilde G\tilde{\mathcal{M}}_2}\right]_{k\ell m,000}. \tag{111}$$

To complete the argument we note that the distinction between $\tilde G$ and $\mathcal{G}$ is subleading in L. We deduce

$$\lim_{L\to\infty} \bar L\,|_{E=3m+\Delta E_{\rm th}} = \lim_{L\to\infty}|_{i\epsilon}\tilde L|_{E=3m}, \qquad \lim_{L\to\infty} \bar R\,|_{E=3m+\Delta E_{\rm th}} = \lim_{L\to\infty}|_{i\epsilon}\tilde R|_{E=3m}. \tag{112}$$

Combining Eqs. (103) and (112) completes the demonstration of the desired result, Eq. (85).

D. Relation to minimally subtracted threshold three-to-three amplitude

Using the results (76) and (85), as well as the equality of $\tilde{\mathcal{K}}_{2;00}$ and $\tilde{\mathcal{M}}_{2;00}$ at threshold, we can rewrite the quantization condition (33) as

$$9L^3\left\{(\tilde{\mathcal{K}}_{2;00})^2\lambda_0^{(0)}+\left[[-\tilde{\mathcal{M}}_2]\mathcal{G}\sum_{n=1}^{\infty}[-\tilde{\mathcal{M}}_2\mathcal{G}]^n[-\tilde{\mathcal{M}}_2]\right]_{00}\right.$$
$$\left.+\sum_{\vec{k}}\tilde{\mathcal{M}}_{2,00}\mathcal{G}_{0k}\tilde{\mathcal{M}}_{2,kk}F^{i\epsilon}_{kk}\tilde{\mathcal{M}}_{2,kk}\mathcal{G}_{k0}\tilde{\mathcal{M}}_{2,00}\right\}\Bigg|_{E=3m+\Delta E_{\rm th}}$$
$$=\mathcal{M}_{{\rm df},3;00}+\mathcal{O}(1/L). \tag{113}$$

We recall that the second term in curly braces contains low-momentum contributions scaling as $1/L^2$ and $1/L^3$, and a high-momentum contribution scaling as $1/L^3$, while the third term contains only a low-momentum contribution scaling as $1/L^3$. At this stage we could pull out these low-momentum contributions, evaluate them explicitly, and replace the high-momentum contributions by appropriate infinite-volume integrals. With these expressions in hand we could then determine the coefficients in the expansion (2) for $\Delta E_{\rm th}$. The coefficient a_6 would then depend on the divergence-free amplitude at threshold, $\mathcal{M}_{{\rm df},3;00}$.

However, there is one feature of such a result that is unsatisfactory. We recall that $\mathcal{M}_{{\rm df},3}$ is defined by subtracting from $\mathcal{M}_3$ a series of integrals I_n that remove the physical divergences [see Fig. 2 and Eq. (93)]. The issue is that these integrals, defined in Eq. (86), involve the two-particle scattering amplitude $\mathcal{M}_2$ evaluated far below threshold [since the spectator momenta range up to $k\sim m$ at which point the CM energy of the nonspectator pair is $(3m-\omega_k)^2-k^2\ll 4m^2$]. While there is nothing wrong, in principle, with this (one can obtain the subthreshold amplitude by analytic continuation) it introduces what seems to be an unnecessary complication. The point of the subtractions, after all, is to remove the physical divergences, which occur at threshold.

It turns out, however, that the formalism, and in particular, Eq. (113), is hinting at a remedy. The high-momentum part of the second term in curly braces turns out, as shown below, to exactly cancel the high-momentum (far subthreshold) parts of the integrals I_n contained in $\mathcal{M}_{{\rm df},3;00}$. Thus, we are led to a different definition of the subtracted threshold amplitude that depends only on physical quantities at or above threshold. This is the threshold amplitude $\mathcal{M}_{3,{\rm th}}$ defined schematically in the Introduction. Here, we give its precise definition and then use it to simplify the quantization condition.

Our specific definition of $\mathcal{M}_{3,{\rm th}}$ makes use of the observation that the infinite series of terms subtracted in Eq. (93) is not needed to reach a divergence-free quantity when working with degenerate particles.[14] From the general considerations of Ref. [9] we know that, above threshold, only I_0 and I_1 need to be subtracted. Infrared (IR) divergences are more severe at threshold, but, as shown in Appendix B, I_n with $n\geq 3$ remain finite, so the only additional subtraction we need at threshold is of I_2. In total, then, our first step towards a definition of $\mathcal{M}_{3,{\rm th}}$ is to drop the subtraction of I_n with $n\geq 3$ from $\mathcal{M}_{{\rm df},3;00}$. The next step is to modify the remaining quantities, I_0, I_1 and I_2, to remove the dependence on subthreshold $\mathcal{M}_2$. In fact, since I_0 does not contain an integral [see Eq. (89)], we need only to modify the latter two.

These considerations lead to the definition

$$\mathcal{M}_{3,{\rm th}}\equiv\lim_{\delta\to 0}\left[\mathcal{M}_{3,\delta}(0,\hat{a}'^*;0,\hat{a}^*)-I_{0;\delta}(0,\hat{a}'^*;0,\hat{a}^*)\right.$$
$$-\int_\delta\frac{d^3k_1}{(2\pi)^3}\Xi_1(\vec{k}_1)-\int_\delta\frac{d^3k_1}{(2\pi)^3}\int_\delta\frac{d^3k_2}{(2\pi)^3}$$
$$\left.\times\,\Xi_2(\vec{k}_1,\vec{k}_2)\right]. \tag{114}$$

Here, δ indicates the presence of an IR regularization, to be defined shortly, while Ξ_1 and Ξ_2 are the modified integrands whose integrals replace I_1 and I_2, respectively. They are given in Eqs. (121) and (122) below and depend only on the scattering length a, i.e. not on the scattering amplitude for subthreshold momenta.

We begin our explanation of the definition of $\mathcal{M}_{3,{\rm th}}$ by describing the δ regularization. This consists of two parts. The first is that all IR divergent integrals are cutoff by a lower limit, $k\geq\delta$ (applied in the frame in which $\vec{P}=0$). This is indicated by the subscript on the integrals in Eq. (114). As discussed below, this allows us to set $E=3m$ for these terms, i.e. to work directly at threshold. However, I_0 diverges at threshold when the spectator momenta $\vec{p}$ and $\vec{k}$ vanish:

$$I_0^{(u,u)}(\vec{0},\vec{0})\propto\frac{1}{E-3m}. \tag{115}$$

Thus, we must introduce a second part in the definition of δ regularization: the energy E must approach threshold as $E-3m\propto\delta^4$ with a nonzero proportionality constant. The subscript δ on I_0 in Eq. (114) indicates that $E-3m$ scales in this way. As we explain shortly, the choice of the fourth power of δ allows us to effectively work at threshold for I_1 and I_2 while

[14] The set of integrals that needs to be subtracted is larger if the particles are not degenerate. See Refs. [1,9] for more discussion.

regulating I_0. In fact, any power of δ greater than cubic suffices.[15]

We next determine the form of the modified integrand Ξ_1. We begin with the unsymmetrized form of I_1, which is

$$iI^{(u,u)}_{1;\ell',m';\ell,m}(\vec p;\vec k) \equiv \int \frac{d^3k_1}{(2\pi)^3 2\omega_{k_1}}[i\mathcal{M}_2(\vec p)iG^\infty(\vec p,\vec k_1) \times i\mathcal{M}_2(\vec k_1)iG^\infty(\vec k_1,\vec k)i\mathcal{M}_2(\vec k)]_{\ell',m';\ell,m}. \quad (116)$$

From this integral, we want to pull out the part that leads to the IR divergence at threshold, for this is the only part that we need to subtract from $\mathcal{M}_3$. As explained in Appendix B, IR divergences at threshold are present only if $\vec p = \vec k = 0$ and if all three of the scattering amplitudes $\mathcal{M}_2$ are in the s-wave. Thus, we focus on

$$I^{(u,u)}_{1;00;00}(\vec 0;\vec 0) = \int \frac{d^3k_1}{(2\pi)^3}\frac{\mathcal{M}_{2,s}(\vec k_1)}{2\omega_{k_1}} \times \left(\frac{\mathcal{M}_{2,s}(\vec 0)H(\vec k_1)}{2\omega_{k_1}(E-m-2\omega_{k_1}+i\epsilon)}\right)^2 + \text{IR finite}, \quad (117)$$

where we are using the abbreviation $\mathcal{M}_{2,s}\equiv\mathcal{M}_{2;00;00}$. The "IR finite" term is IR finite at threshold and comes from higher intermediate partial waves. The integral in (117) has a double pole at $k_1=|\vec k_1|=q$, where q [defined in Eq. (34)] is the three-momentum of each particle in the nonspectator pair. This pole is regulated by the $i\epsilon$ prescription that comes with G^∞. However, unlike the case of a single pole, the integral here diverges when $\epsilon\to 0$, for any $E\ge 3m$. This divergence is necessary to cancel the corresponding physical divergence in $\mathcal{M}_3$. The issue at hand is to find a simpler integral that has the same IR divergence at threshold but does not depend, as I_1 does, on $\mathcal{M}_{2,s}(\vec k_1)$ evaluated far below threshold.

To do so we apply the δ regularization to I_1. Then, in the IR regime where $k_1\sim\delta$, we have that

$$E-m-2\omega_{k_1} = -\frac{k_1^2}{m}+E-3m+\mathcal{O}(k_1^4) = -\frac{k_1^2}{m}[1+\mathcal{O}(\delta^2)], \quad (118)$$

since $E-3m$ scales in the same way as the k_1^4 term. This implies that the pole always lies below the cutoff on k_1, so that the integral is well regulated. Since the overall IR divergence is linear ($\int dk_1/k_1^2$) the $\mathcal{O}(\delta^2)$ terms lead to IR-finite corrections and thus can be dropped from the subtraction to $\mathcal{M}_3$. This is why our δ^4 scaling of $E-3m$ is effectively the same as setting $E=3m$. The same holds for I_2, since this integral has a weaker IR divergence.

We conclude that to obtain the same IR divergence as in $I_1^{(u,u)}$ we need only expand the residue of the double pole about $\vec k_1=0$ and keep the constant and linear terms. Since $E-3m$ scales quartically we can set $E=3m$ in this expansion. Similarly we can set ω_{k_1} to m. The factors of $H(\vec k_1)$ equal unity to all orders in a Taylor expansion about threshold, but we do not expand them as they are needed for UV convergence in some terms. Thus, all we need to expand is $\mathcal{M}_{2,s}(\vec k_1)$, which can be done using the relation between $\tilde{\mathcal{M}}_2$ and $\tilde{\mathcal{K}}_2$ [Eq. (48)], the definition of ρ [Eq. (16)], the near-threshold form of $\mathcal{K}_2$ [Eqs. (6) and (8)], and the expression for q_k^2 [Eq. (37)]. The net result is that the modified integrand is[16]

$$\Xi_1^{(u,u)}(\vec k_1)\equiv -\frac{[32\pi ma]^3}{8m}\left[\frac{H(\vec k_1)^2}{k_1^4}+a\frac{\sqrt3}{2}\frac{H(\vec k_1)^3}{k_1^3}\right], \quad (119)$$

and this satisfies

$$\lim_{\delta\to0}\left[I^{(u,u)}_{1;\delta;00;00}(\vec 0,\vec 0)-\int_\delta\frac{d^3k_1}{(2\pi)^3}\Xi_1^{(u,u)}(\vec k_1)\right]=\text{finite}. \quad (120)$$

At threshold, symmetrization leads only to multiplication by 9, so we can replace the subtraction of I_1 with that of the integral of

$$\Xi_1(\vec k_1)=9\Xi_1^{(u,u)}(\vec k_1). \quad (121)$$

This is the quantity entering Eq. (114).

A similar analysis for I_2 leads to the modified integrand

$$\Xi_2(\vec k_1,\vec k_2)=\frac{9}{16m^2}[32m\pi a]^4\frac{H(\vec k_1)^2H(\vec k_2)^2}{k_1^2[k_1^2+k_2^2+(\vec k_1+\vec k_2)^2]k_2^2}. \quad (122)$$

There is only a single term since the integral is only logarithmically IR divergent.

[15]Note that, whatever power one chooses, the square of the scattering particle momentum in $\mathcal{M}_2$ within I_0 will scale in the same way as the energy difference, $q^2\sim E-3m$. Thus, in the $\delta\to0$ limit, both the scattering length and the effective range contribute to the I_0 subtraction. Indeed, since the r-dependent terms are finite, one could choose not to subtract these. This would change the definition of $\mathcal{M}_{3,\text{th}}$ and would also change the explicit r-dependent term in a_6 [see Eq. (136)] to compensate.

[16]This factor of H^2 is not necessary to make the $1/k_1^4$ term UV convergent, but we keep it for the sake of uniformity, since the UV cutoff is needed for the $1/k_1^3$ term.

This completes the explanation of the quantities entering the definition of $\mathcal{M}_{3,\mathrm{th}}$, Eq. (114). To use this to simplify the quantization condition, we need to relate $\mathcal{M}_{3,\mathrm{th}}$ to our original threshold amplitude, $\mathcal{M}_{\mathrm{df},3;00}$. Combining the definition of $\mathcal{M}_{\mathrm{df},3;00}$, given in Eqs. (93) and (94), with the result (114) we find

$$\mathcal{M}_{3,\mathrm{th}} = \mathcal{M}_{\mathrm{df},3;00} + \lim_{\delta\to 0}\left\{\left(I_{1;\delta} - \int_\delta \frac{d^3k_1}{(2\pi)^3}\Xi_1(\vec{k}_1)\right) + \left(I_{2;\delta} - \int_\delta \frac{d^3k_1}{(2\pi)^3}\int_\delta \frac{d^3k_2}{(2\pi)^3}\Xi_2(\vec{k}_1,\vec{k}_2)\right)\right\} + \sum_{n=3}^{\infty} I_n. \tag{123}$$

Since I_0 does not appear, we can set $E = 3m$ in the expression in curly braces. In other words, IR regularization is achieved here simply by cutting off the IR divergent integrals. We are also adopting the notation that I_n or $I_{n;\delta}$ without arguments implies that both spectator momenta vanish and $E = 3m$, so that these are purely s-wave quantities (as for $\mathcal{M}_{\mathrm{df},3;00}$). The interpretation of the result (123) is that the subtraction of $\sum_{n=3}^{\infty} I_n$ is unnecessary for degenerate particles, and so we undo this by adding the series back in. In addition, we add back part of I_1 and I_2, but with a subtraction defined using Ξ_1 and Ξ_2 that keeps $\mathcal{M}_{3,\mathrm{th}}$ finite.

We conclude this section by rewriting the quantization condition (113) in terms of $\mathcal{M}_{3,\mathrm{th}}$. We need the following results:

$$-9L^3[\tilde{\mathcal{M}}_2\mathcal{G}[-\tilde{\mathcal{M}}_2\mathcal{G}]^n\tilde{\mathcal{M}}_2]_{00}|_{E=3m+\Delta E_{\mathrm{th}}} = I_n + \mathcal{O}(1/L) \quad \text{for } n \geq 3, \tag{124}$$

$$-9L^3[\tilde{\mathcal{M}}_2\mathcal{G}[-\tilde{\mathcal{M}}_2\mathcal{G}]^2\tilde{\mathcal{M}}_2]_{00}|_{E=3m+\Delta E_{\mathrm{th}}} - \frac{1}{L^6}\sum_{\vec{k}_1,\vec{k}_2\neq 0}\Xi_2(\vec{k}_1,\vec{k}_2) = \lim_{\delta\to 0}\left[I_{2;\delta} - \int_\delta \frac{d^3k_1}{(2\pi)^3}\int_\delta \frac{d^3k_2}{(2\pi)^3}\Xi_2(\vec{k}_1,\vec{k}_2)\right] + \mathcal{O}(1/L), \tag{125}$$

$$-9L^3[\tilde{\mathcal{M}}_2\mathcal{G}[-\tilde{\mathcal{M}}_2\mathcal{G}]\tilde{\mathcal{M}}_2]_{00}|_{E=3m+\Delta E_{\mathrm{th}}} - \frac{1}{L^3}\sum_{\vec{k}_1\neq 0}\Xi_1(\vec{k}_1) = \lim_{\delta\to 0}\left[I_{1;\delta} - \int_\delta \frac{d^3k_1}{(2\pi)^3}\Xi_1(\vec{k}_1)\right] + \mathcal{O}(1/L), \tag{126}$$

which are demonstrated below. Using these, and the relation (123), we find that the quantization condition can be written as

$$\left\{9L^3(\tilde{\mathcal{K}}_{2;00})^2\lambda_0^{(0)} + 9L^3\sum_{\vec{k}}\tilde{\mathcal{M}}_{2,00}\mathcal{G}_{0k}\tilde{\mathcal{M}}_{2,kk}\mathcal{F}^{ic}_{kk}\tilde{\mathcal{M}}_{2,kk}\mathcal{G}_{k0}\tilde{\mathcal{M}}_{2,00} - \frac{1}{L^3}\sum_{\vec{k}_1\neq 0}\Xi_1(\vec{k}_1) - \frac{1}{L^6}\sum_{\vec{k}_1,\vec{k}_2\neq 0}\Xi_2(\vec{k}_1,\vec{k}_2)\right\}\Bigg|_{E=3m+\Delta E_{\mathrm{th}}} = \mathcal{M}_{3,\mathrm{th}} + \mathcal{O}(1/L). \tag{127}$$

We use Eq. (127) in the following subsection to derive the threshold expansion.

We now return to the demonstration of Eqs. (124)–(126). We first note that, in all three expressions, we can replace $E = 3m + \Delta E_{\mathrm{th}}$ in the first terms with simply $E = 3m$. This is because there are no contributions to these terms that are enhanced by the tuning of ΔE. Thus, shifting the energy away from threshold by ΔE_{th} leads only to corrections suppressed by $1/L^3$. The net result is that all terms in Eqs. (124)–(126) can be evaluated at threshold. Note that for this, it is important that the left-hand sides contain $\mathcal{G}$ rather than G, since the latter diverges at threshold.

Consider first Eq. (124). Following the arguments of Sec. III A, the high-momentum part of the sums on the left-hand side leads to a contribution scaling as L^0, in which we expect the sums can be replaced by integrals. If any of the sums are restricted to low momenta, then the scaling arguments of Sec. III A can be used to show that the contribution falls as $L \to \infty$. For example, if all the momenta are small, then, using the result that the dominant terms in $\mathcal{G}$ scale as $1/L$, the overall scaling is as $L^{3-(1+n)} = L^{2-n}$, which is subleading for $n \geq 3$. Since all intermediate momenta must be large, we can restrict the sums to run over only nonzero values without making an error when $L \to \infty$. Doing so allows us to replace $\mathcal{G}$ with $\tilde{G}$ in the sums. We can further replace $\tilde{G}$ with G^∞ and $\tilde{\mathcal{M}}_2$ with $\mathcal{M}_2$, as long as we take into account all the factors of 2ω, Q and L^3. Doing so we find that the left- and right-hand sides of Eq. (124) are simply the sum and integral, respectively, of the same summand/integrand, up to subleading corrections.[17] Thus, we can rewrite (124) as

[17]We also need the result that $I_n = 9I_n^{(u,u)}$ at threshold.

$$\left\{\left[\frac{1}{L^3}\sum_{\vec{k}_1\neq 0}\cdots\frac{1}{L^3}\sum_{\vec{k}_n\neq 0}-\int_{\vec{k}_1}\cdots\int_{\vec{k}_n}\right]9i\mathcal{M}_2(0)iG^\infty(0,\vec{k}_1)\cdots iG^\infty(\vec{k}_n,0)\mathcal{M}_2(0)\right\}\Big|_{E=3m}=\mathcal{O}(1/L). \quad (128)$$

We know from Appendix B that, although the integrand diverges in the IR, the singularity is integrable. We also know that the integrand is nonsingular in the high-momentum region, and is UV convergent. Thus, we can use the general result of Ref. [7] that such sum-integral differences vanish as a power of $1/L$. This completes the demonstration of Eq. (124).

Turning to Eq. (125), the argument proceeds along similar lines. We can again replace $\not{G}$ with G as long as we do not allow either of the intermediate momenta to vanish. Here, this is an identity, which follows because $G_{000;0\ell m}=0$ if $\ell\neq 0$. Then, we can manipulate the equation into the form

$$\lim_{\delta\to 0}\left[\frac{1}{L^6}\sum_{\vec{k}_1,\vec{k}_2\neq 0}-\int_\delta\frac{d^3k_1}{(2\pi)^3}\int_\delta\frac{d^3k_2}{(2\pi)^3}\right]\{9i\mathcal{M}_2(0)iG^\infty(0,\vec{k}_1)i\mathcal{M}_2(\vec{k}_1)iG^\infty(\vec{k}_1,\vec{k}_2)i\mathcal{M}_2(\vec{k}_2)iG^\infty(\vec{k}_2,0)i\mathcal{M}_2(0)$$
$$-i\Xi_2(\vec{k}_1,\vec{k}_2)\}|_{E=3m}=\mathcal{O}(1/L). \quad (129)$$

Here, the first term in curly braces does lead to an IR divergent integral, and, correspondingly, a low-momentum contribution to the sum that is of $\mathcal{O}(L^0)$, but both of these are canceled by the Ξ_2 term. Thus, the expression in curly braces is integrable and nonsingular, so the sum-integral difference vanishes as $L\to\infty$.

The argument for Eq. (126) is essentially the same. Again, we can replace $\not{G}$ with G as long as the intermediate sum avoids $\vec{k}_1=0$. The equation can then be manipulated into

$$\lim_{\delta\to 0}\left[\frac{1}{L^3}\sum_{\vec{k}_1\neq 0}-\int_\delta\frac{d^3k_1}{(2\pi)^3}\right]\{9i\mathcal{M}_2(0)iG^\infty(0,\vec{k}_1)i\mathcal{M}_2(\vec{k}_1)iG^\infty(\vec{k}_1,0)i\mathcal{M}_2(0)-i\Xi_1(\vec{k}_1)\}|_{E=3m}=\mathcal{O}(1/L). \quad (130)$$

Once again, the IR singularities cancel, by construction, in the expression in curly braces, so the sum-integral difference vanishes as $L\to\infty$.

E. Solution to the quantization condition

In this section we determine the coefficients a_n in the threshold expansion of $\Delta E_{\rm th}$, Eq. (2), by enforcing the quantization condition, Eq. (127). As noted above, we must tune ΔE to cancel the $\mathcal{O}(L^3)$, $\mathcal{O}(L^2)$ and $\mathcal{O}(L)$ contributions on the left-hand side of this condition. To do so, we need the result for the $1/L$ expansion of $\lambda_0^{(0)}$, given in Eq. (58). The algebraic manipulations needed are straightforward but tedious, and we quote only the final results.

The $\mathcal{O}(L^3)$ and $\mathcal{O}(L^2)$ contributions to the left-hand side of the quantization condition come only from the $\mathcal{O}(L^0)$ and $\mathcal{O}(1/L)$ parts of $\lambda_0^{(0)}$. Thus, these two parts must vanish. Using Eq. (58) we see that canceling the $\mathcal{O}(L^0)$ part of $\lambda_0^{(0)}$ requires

$$a_3=\frac{12\pi a}{m}. \quad (131)$$

This is 3 times the corresponding coefficient for two particles, which is the expected ratio as there are now three pairs that can interact, and is indeed the result found in Refs. [3–6]. We emphasize that both $\tilde{F}_{00}$ and $\tilde{G}_{00}$ contribute to a_3, showing the necessity of both terms even at leading order.

At next order, the cancellation requires

$$\frac{a_4}{a_3}=-\frac{a\mathcal{I}}{\pi}. \quad (132)$$

This is the same *relative* correction as for the two-particle case and agrees with the results of Refs. [3–6].

To proceed one order higher we must determine the leading $\mathcal{O}(L)$ contribution from the sum over Ξ_1, a quantity whose definition is given in Eq. (121). We find[18]

$$\frac{1}{L^3}\sum_{\vec{k}_1\neq 0}\Xi_1(\vec{k}_1)=-\frac{48^2m^2a^3\mathcal{J}}{\pi}L-9\frac{[32m\pi a]^3}{(2m)^3}m^2\frac{1}{L^3}$$
$$\times\sum_{\vec{k}_1\neq 0}\left[\frac{H(\vec{k}_1)^2-1}{k_1^4}+a\frac{\sqrt{3}}{2}\frac{H(\vec{k}_1)^3}{k_1^3}\right]. \quad (133)$$

As we show below, the second term on the right-hand side is of $\mathcal{O}(L^0)$. Combining the $\mathcal{J}$ term from Ξ_1 with that from Eq. (58) we find that canceling the $\mathcal{O}(L)$ terms in Eq. (127) requires

[18]Here, we are using the definition $\mathcal{J}=\sum_{\vec{n}\neq 0}1/(\vec{n}^2)^2$, with $\vec{n}$ a vector of integers. This is equivalent to the definition given in Appendix A.

$$\frac{a_5}{a_3} = \frac{a^2}{\pi^2}(\mathcal{I}^2 + \mathcal{J}). \tag{134}$$

Again this agrees with Refs. [3–6]. We note that the $\mathcal{J}$ term in this result arises both from $\tilde{F}_{00}$ and from the factors of $\tilde{G}_{0k}$ contained in the sum over Ξ_1. Thus, the agreement provides a more stringent test of our formalism.

To determine the final coefficient a_6, we must work out the $L \to \infty$ limits of all the contributions on the right-hand side of the quantization condition (127). We first consider the combination of the term containing $\lambda_0^{(0)}$ with the $\mathcal{O}(L)$ contribution from Ξ_1. Our tuning of ΔE has made this combination of $\mathcal{O}(L^0)$. Explicitly, if we substitute the first three orders of $\Delta E_{\rm th}$ into the expression for $\lambda_0^{(0)}$ we find

$$\lim_{L\to\infty}\left\{9\tilde{\mathcal{K}}_{2;00}^2 L^3 \lambda_0^{(0)} + \frac{48^2 m^2 a^3 \mathcal{J}}{\pi} L\right\}\bigg|_{E=3m+a_3/L^3+a_4/L^4+a_5/L^5} = \frac{576}{\pi^2}\left[a^4 m^2(-\mathcal{I}^3 + \mathcal{I}\mathcal{J} - 9\mathcal{K}) - \pi^3 m^2 a \frac{a_6(L)}{a_3} + 3\pi^4 a^2 + 6\pi^4 m^2 a^3 r\right]. \tag{135}$$

Combining this result with the remaining terms in Eq. (127), which are worked out in Appendix C, and demanding that the equality hold at $\mathcal{O}(L^0)$ then gives the expression for $a_6(L)$. We find

$$\frac{a_6(L)}{a_3} = \left(\frac{a}{\pi}\right)^3\left[-\mathcal{I}^3 + \mathcal{I}\mathcal{J} - 9\mathcal{K} + \frac{16\pi^3}{3}(3\sqrt{3} - 4\pi)\log\left(\frac{mL}{2\pi}\right) + \mathcal{C}_F + \mathcal{C}_4 + \mathcal{C}_5\right] + \frac{64\pi^2 a^2}{m}\mathcal{C}_3 + \frac{3\pi a}{m^2} + 6\pi r a^2 - \frac{\mathcal{M}_{3,\rm thr}}{48 m^3 a_3}. \tag{136}$$

Numerical values for the new constants $\mathcal{C}_F$, $\mathcal{C}_3$, $\mathcal{C}_4$ and $\mathcal{C}_5$ are given in Appendix C, while those for $\mathcal{I}$, $\mathcal{J}$ and $\mathcal{K}$ are given in Appendix A. This completes our calculation of $\Delta E_{\rm th}$ through $\mathcal{O}(1/L^6)$. Together with results for a_3, a_4 and a_5 given, respectively, in Eqs. (131), (132) and (134), this is the main result of the paper.

In a_6 only the logarithmic dependence on L can be compared to that found by the nonrelativistic calculations of Refs. [4,5], and indeed it agrees. The L-independent constants cannot be compared, both because relativistic effects enter at this order and because the nonrelativistic calculations use different definitions for the three-particle threshold amplitude.[19] It is for this reason that we have carried out an independent calculation of the threshold expansion in relativistic $\lambda\phi^4$ theory, working to cubic order [6]. Since a and $a^2 r$ are both of $\mathcal{O}(\lambda)$ in this theory, while $\mathcal{M}_{3,\rm th} = \mathcal{O}(\lambda^2)$, this allows us to check the last four terms on the right-hand side of Eq. (136). We find complete agreement. This check also shows how our definition of $\mathcal{M}_{3,\rm th}$ works in detail through one-loop order. The remaining terms in a_6, i.e. the constants on the right-hand side containing the factor of a^3, have so far not been checked independently. This would require a fourth-order calculation in the $\lambda\phi^4$ theory.

We close this section by commenting on the cutoff dependence of the various quantities in Eq. (136). The constants $\mathcal{C}_3$, $\mathcal{C}_4$ and $\mathcal{C}_5$ depend on the choice of cutoff function H, as does the argument of the logarithm (though not its coefficient). The energy of a physical finite-volume state should not depend on H, and indeed this "scheme dependence" is canceled by that of $\mathcal{M}_{3,\rm th}$. This can be seen explicitly by going back to the definition of $\mathcal{M}_{3,\rm th}$, Eq. (114), in which the dependence on H enters through the functions Ξ_1 and Ξ_2, in exactly the same way as on the left-hand side of the quantization condition (127).

IV. CONCLUSIONS

In this paper, we have shown how to expand the energy of the state closest to threshold for three interacting particles in powers of $1/L$, starting from the quantization condition derived in Refs. [1,2]. This turns out to be quite involved, but also provides insight into the workings of the formalism. We find that the first three nontrivial terms, a_3, a_4 and a_5, as well as the logarithmic dependence in $a_6(L)$, agree with those found previously in calculations using NRQM [3–5]. For a check of the volume-independent part of $a_6(L)$ (where relativistic corrections and the ambiguity in the definition of the three-particle threshold amplitude enter), we have compared to a perturbative calculation in relativistic $\lambda\phi^4$ field theory [6].

[19] Nevertheless, we note that the $\mathcal{I}^3$ and $\mathcal{I}\mathcal{J}$ terms do agree, though not the $\mathcal{K}$ term. We have, however, found that a simple change in the definition of $\mathcal{M}_{3,\rm th}$ also leads to agreement for the $\mathcal{K}$ terms. We do not present the details, however, since other constant terms do not match, and, as noted in the text, the comparison is fundamentally ambiguous anyway.

The two-particle version of the threshold expansion [7] has been successfully used in many numerical simulations of lattice field theories to determine the scattering length a. Using the formula presented here, this can, in principle, be extended to the determination of the (suitably subtracted) three-particle scattering amplitude at threshold. This will require accurate calculations for several volumes of both the two- and three-particle threshold energy shifts; the former is needed to determine a and the effective range r. This will be challenging in practice, since one must control the volume dependence up to $\mathcal{O}(1/L^6)$.

The development of the threshold expansion for three particles is much more challenging than in the two-particle case.[20] The main reason for this difficultly is that the matrices appearing in the quantization condition cannot be truncated when one works at $\mathcal{O}(1/L^6)$. While this adds to the technical challenge, it also led to the conversion of the unphysical quantity $\mathcal{K}_{\mathrm{df},3}$, which appears in the quantization condition, into the physical subtracted threshold amplitude $\mathcal{M}_{3,\mathrm{th}}$. This was essential for the final result for ΔE_{th} to depend only on physical quantities.

One might be concerned that the complications that we have had to deal with here will carry over to the practical application of the three-particle quantization condition. This is not, however, the case. When one does a $1/L$ expansion one loses one of the key simplifying features of the quantization condition. This feature, stressed in Ref. [2], is that, if one truncates the two-particle angular-momentum space, then the matrices of the determinant condition, Eq. (3), become finite. This is because the remaining matrix index, $\vec{k} = 2\pi\vec{n}_k/L$, is automatically truncated by the smooth cutoff function $H(\vec{k})$. In particular, $H(\vec{k})$ vanishes for $k \gtrsim m$ implying that n_k is constrained to satisfy $2\pi n_k \lesssim mL$. Thus, only a finite number of values of $\vec{n}_k$ need be used when applying this formalism to numerical simulations. By contrast, the threshold expansion must be valid for arbitrarily large L, which implies that all $\vec{n}$ can contribute.

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APPENDIX A: EVALUATION OF $\tilde{F}_{00}$

In this appendix we expand the quantity $\tilde{F}_{00}$ in powers of $1/L$ taking $\Delta E = E - 3m$ to scale as $1/L^3$. We recall that $\tilde{F}_{00} \equiv \tilde{F}_{000;000}$, with the latter defined in Eq. (42). For the analysis in the main text, we need to keep terms in $\tilde{F}_{00}$ up to $\mathcal{O}(1/L^3)$.

[20]The latter is given up to $\mathcal{O}(1/L^5)$ in Ref. [7] and to one higher order in Appendix C of Ref. [6].

We start from the expressions given in Eqs. (43) and (44). As the spectator momentum is $\vec{k} = 0$, the scattered pair are already in their CM frame, so the boost factor γ in Eq. (34) is unity. It follows that $\vec{r} = \vec{n}_a$. Thus, we obtain

$$\tilde{F}_{00} = \frac{1}{16m\omega_q}\left\{\frac{1}{q^2L^3} + \frac{1}{4\pi^2 L}\left[\sum_{\vec{n}_a\neq 0} - \tilde{\mathrm{PV}}\int_{\vec{n}_a}\right]\frac{H(\vec{a})^2}{x^2 - n_a^2}\right\}, \tag{A1}$$

where $x = qL/(2\pi)$ and we have used the fact that $\vec{b}_{ka} = -\vec{a}$, and the evenness of $H(\vec{a})$, to rewrite the regulator function. We have also absorbed the ρ term in Eq. (43) into the integral over $\vec{n}_a$ by reverting to the $\tilde{\mathrm{PV}}$ pole prescription. As explained in Ref. [1], this prescription leads to integrals such as that in Eq. (A1) being real and smooth functions of x^2. In particular, the cusp at $x^2 = 0$ present with the $i\epsilon$ prescription is absent with the $\tilde{\mathrm{PV}}$ prescription.

In Eq. (A1), we have pulled out the $\vec{n}_a = 0$ term from the sum since this scales as L^0 [using Eq. (34)]. The remainder scales as $1/L$, as already discussed in Sec. III A. For the sum in Eq. (A1) we can use the fact that $|x^2| \sim 1/L \ll n_a$ (and the absence of the $\vec{n}_a = 0$ term in the sum) to expand the summand in powers of x^2, leading to

$$\sum_{\vec{n}_a\neq 0}\frac{H(\vec{a})^2}{x^2 - n_a^2} = -\sum_{j=0}^{\infty}\left[\frac{q^2L^3}{4\pi^2 L}\right]^j \sum_{\vec{n}_a\neq 0}\frac{H(\vec{a})^2}{(n_a^2)^{1+j}}. \tag{A2}$$

Although H is needed to regulate the UV only for $j = 0$, we cannot drop it from the other terms, as doing so leads to potential power-law corrections. To see this, we note that [using Eq. (7)]

$$\frac{E_{2,a}^{*2}}{4m^2} = \frac{5}{2} - \frac{3}{2}\sqrt{1 + \frac{a^2}{m^2}} + \mathcal{O}\left(\frac{\Delta E}{m}\right), \tag{A3}$$

implying that the regulator function takes the explicit form

$$H(\vec{a}) = J\left(\frac{5}{2} - \frac{3}{2}\sqrt{1 + \frac{n_a^2}{N_{\mathrm{cut}}^2}}\right) + \mathcal{O}\left(\frac{\Delta E}{m}\right) \tag{A4}$$

with

$$N_{\mathrm{cut}} = \frac{mL}{2\pi}. \tag{A5}$$

Given the definition of the function J, Eq. (12), this implies that the sum over $\vec{n}_a$ is cut off (smoothly) at $n_a \approx N_{\mathrm{cut}}$. Since this cutoff depends on L, it can introduce further L dependence in the individual terms of Eq. (A2). For example, in the sum over $H(\vec{a})^2/n_a^4$, it is easy to see that the cutoff leads to a $1/(mL)$ correction. Since this sum arises in a $1/L^2$ term in $\tilde{F}_{00}$, the correction would enter at $\mathcal{O}(1/L^3)$, which is the highest order that we are controlling. Thus, we cannot remove the cutoff at this stage.[21]

We would like to do a similar expansion in powers of x^2 for the integral in Eq. (A1). We know that this must be possible since the $\tilde{\mathrm{PV}}$ prescription leads to smooth, nonsingular dependence on x^2, including at $x^2 = 0$. Naively expanding, however, leads to integrals that diverge at $\vec{n}_a = 0$. To proceed, we first pull out the $x^2 = 0$ term

$$\tilde{\mathrm{PV}}\int_{\vec{n}_a}\frac{H(\vec{a})^2}{x^2-n_a^2} = -\int_{\vec{n}_a}\frac{H(\vec{a})^2}{n_a^2} + \tilde{\mathrm{PV}}\int_{\vec{n}_a}\frac{x^2H(\vec{a})^2}{n_a^2(x^2-n_a^2)}, \tag{A6}$$

where no pole prescription is needed for the IR and UV convergent integral in the first term on the right-hand side. Next, we use the result

$$\tilde{\mathrm{PV}}\int_{\vec{n}_a}\frac{1}{n_a^2(x^2-n_a^2)} = 0, \tag{A7}$$

which can be shown by explicit computation. Note that this integral is finite both in the UV and IR for $x^2 \neq 0$; thus, no regulation is required, and the $x^2 = 0$ result is obtained by smoothness. Subtracting this vanishing integral from that appearing in the second term on the right-hand side of Eq. (A6), we find

$$\tilde{\mathrm{PV}}\int_{\vec{n}_a}\frac{x^2H(\vec{a})^2}{n_a^2(x^2-n_a^2)} = x^2\tilde{\mathrm{PV}}\int_{\vec{n}_a}\frac{H(\vec{a})^2-1}{n_a^2(x^2-n_a^2)}, \tag{A8}$$

$$= -x^2\sum_{j=0}^{\infty}(x^2)^j\int_{\vec{n}_a}\frac{H(\vec{a})^2-1}{(n_a^2)^{2+j}}. \tag{A9}$$

Here, we do a Taylor expansion because the resulting integrals are convergent both in the IR and UV. The IR convergence is assured by the factor of $H(\vec{a})^2 - 1$, a function of n_a^2, all of whose derivatives vanish at $n_a = 0$. The UV convergence is manifest for all j. Once again, despite the UV convergence, we cannot drop the factors of H since they give rise to power-law corrections. Finally, we note that no pole prescription is needed in the integrals in Eq. (A9).

Collecting these results we obtain the $1/L$ expansion for $\tilde{F}_{00}$:

$$\tilde{F}_{00} = \frac{1}{16m\omega_q}\frac{1}{q^2L^3}\left\{1 - \sum_{j=1}^{\infty}\left[\frac{q^2L^3}{4\pi^2L}\right]^j\mathcal{I}_j\right\}. \tag{A10}$$

[21]We can, however, drop the ΔE term in Eq. (A4), since this is proportional to $1/L^3$, pushing the total power to $1/L^5$, i.e. beyond the order we are working.

Here,

$$\mathcal{I}_j = \begin{cases} \left[\sum_{\vec{n}_a\neq 0} - \int_{\vec{n}_a}\right]\frac{H(\vec{a})^2}{\vec{n}_a^2} & j=1 \\ \sum_{\vec{n}_a\neq 0}\frac{H(\vec{a})^2}{(\vec{n}_a)^{2j}} - \int_{\vec{n}_a}\frac{H(\vec{a})^2-1}{(\vec{n}_a)^{2j}} & j\geq 2. \end{cases} \tag{A11}$$

These quantities retain an implicit dependence on L through the cutoff functions. However, this dependence is expected to be exponentially suppressed [falling as $\exp(-N_{\mathrm{cut}})$], since in the derivation of the formalism in Ref. [1] the dependence on the form of H is exponentially suppressed. Indeed, it is simple to check that the leading power-law dependence on N_{cut} cancels between the sums and integrals for $\mathcal{I}_m$ with $m \geq 2$. Furthermore, numerically evaluating the expressions, we observe that the convergence as N_{cut} increases is rapid and consistent with the exponential. Thus, we can replace these quantities with their values when $N_{\mathrm{cut}} \to \infty$. In the notation of Ref. [4] the first three become

$$\mathcal{I}_1 \xrightarrow[{[N_{\mathrm{cut}}\to\infty]}]{} \mathcal{I}, \qquad \mathcal{I}_2 \xrightarrow[{[N_{\mathrm{cut}}\to\infty]}]{} \mathcal{J}, \qquad \mathcal{I}_3 \xrightarrow[{[N_{\mathrm{cut}}\to\infty]}]{} \mathcal{K}. \tag{A12}$$

We have checked that the numerical values we obtain for $\mathcal{I}$, $\mathcal{J}$ and $\mathcal{K}$ agree with those quoted (to about 12 significant figures) in Ref. [4].[22] Quoting only four decimal places, the values are $\mathcal{I} = -8.914$, $\mathcal{J} = 16.532$ and $\mathcal{K} = 8.402$. Making the replacements of Eq. (A12) we obtain the result (46) quoted in the main text.

APPENDIX B: PROOF THAT $I_{n>3}$ ARE FINITE AT THRESHOLD

In this appendix we prove that, for $n \geq 3$, the integrals $I_n(\vec{p}, \hat{a}'^*; \vec{k}, \hat{a}^*)$, defined in Eqs. (86) and (90), are finite at threshold, $E = 3m$. The potential divergence is only in the infrared, since the functions H contained in G^∞ [defined in Eq. (87)] regulate the ultraviolet. As will become clear in the following, the divergences in any I_n occur only when the external spectator momenta are set to $\vec{p} = \vec{k} = 0$, so we primarily consider this case. Setting $\vec{p} = \vec{k} = 0$ at threshold implies in turn that $\vec{a}'^* = \vec{a}^* = 0$, so the I_n are pure s-wave, with no dependence on $\hat{a}'^*$ and $\hat{a}^*$.

When all momenta (both external and internal) are in the IR regime, $k \ll m$, the energy denominators in each factor of G^∞ take their nonrelativistic form

$$E - \omega_k - \omega_p - \omega_{pk} + i\epsilon \to -[\vec{k}^2 + \vec{p}^2 + (\vec{k}+\vec{p})^2 - i\epsilon]/(2m). \tag{B1}$$

[22]Indeed, for $\mathcal{I}_2$ and $\mathcal{I}_3$, the expressions in Eq. (A11) provide a numerically efficient way of evaluating the sums.

Thus, if we set the external momenta to zero and collect the n three-vectors that are being integrated into a $3n$-dimensional vector $\vec{Q} \equiv (\vec{k}_1, \ldots, \vec{k}_n)$, we have (since I_n contains $n+1$ factors of G^∞ and n integrals)[23]

$$I_n \sim \int dQ \int d\Omega Q^{3n-1} \frac{1}{Q^{2(n+1)} f(\Omega)} \propto \int dQ Q^{n-3}. \tag{B2}$$

Here, Ω stands for the collective angular coordinates. Thus, the integral is IR divergent by power-counting for $n = 1$ and 2, while finite for $n \geq 3$. There is, however, another possible source of divergence, namely, that $f(\Omega)$ can have zeroes. This occurs when some, but not all, of the G^∞ factors diverge. It turns out, however, that these zeroes result in no additional divergences since they are canceled by corresponding zeroes in the numerator. Thus, the naive overall power-counting result is correct.

To explain this, we first replace I_n (with vanishing external momenta) with the simpler integral

$$I_{n,\mathrm{IR}} \equiv \int_{\vec{k}_1,\ldots,\vec{k}_n} \frac{1}{2\vec{k}_1^2} \frac{1}{\vec{k}_1^2 + \vec{k}_2^2 + (\vec{k}_1 + \vec{k}_2)^2} \cdots \frac{1}{\vec{k}_{n-1}^2 + \vec{k}_n^2 + (\vec{k}_{n-1} + \vec{k}_n)^2} \frac{1}{2\vec{k}_n^2}. \tag{B3}$$

This removes extraneous factors while maintaining the IR properties of the integral. We have dropped factors of $i\epsilon$ since they are not needed to regularize these integrals when working at threshold.

Next, we consider the $n = 3$ case in detail.

$$I_{3,\mathrm{IR}} \equiv \int_{\vec{k}_1,\vec{k}_2,\vec{k}_3} \frac{1}{2\vec{k}_1^2} \frac{1}{\vec{k}_1^2 + \vec{k}_2^2 + (\vec{k}_1 + \vec{k}_2)^2} \frac{1}{\vec{k}_2^2 + \vec{k}_3^2 + (\vec{k}_2 + \vec{k}_3)^2} \frac{1}{2\vec{k}_3^2}, \tag{B4}$$

$$= \frac{1}{8(2\pi)^6} \int dk_1 \int dk_2 k_2^2 \int d\cos\theta_{12} \int dk_3 \int d\cos\theta_{23} \frac{1}{k_1^2 + k_2^2 + k_1 k_2 \cos\theta_{12}} \frac{1}{k_2^2 + k_3^2 + k_2 k_3 \cos\theta_{23}}, \tag{B5}$$

$$= \frac{1}{8(2\pi)^6} \int dQ \int_0^{\pi/2} d\phi \int_0^{\pi/2} d\theta \int_0^{\pi} d\theta_{12} \int_0^{\pi} d\theta_{23} \times \frac{\sin\theta_{12} \sin\theta_{23} \sin^3\theta \sin^2\phi}{(\sin^2\theta + \sin^2\theta \sin\phi \cos\phi \cos\theta_{12})(\sin^2\theta \sin^2\phi + \cos^2\theta + \sin\theta \sin\phi \cos\theta \cos\theta_{23})}. \tag{B6}$$

Here, we are using the variables $(k_1, k_2, k_3) = Q(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. The lack of divergence in the overall Q integral agrees with our analysis above. One of the possible divergences in the angular integrals occurs when $\theta \approx 0$ (corresponding to $\vec{k}_1$ and $\vec{k}_2$ vanishing but not $\vec{k}_3$). In this limit, the integrand becomes

$$\frac{\sin\theta_{12} \sin\theta_{23} \sin^2\phi\, \theta^3}{(1 + \sin\phi\cos\phi\cos\theta_{12})\theta^2} + \mathcal{O}(\theta^2), \tag{B7}$$

so the integral over θ is finite. There is a similar possible divergence when $\phi \approx 0$, $\theta \approx \pi/2$ (corresponding to $\vec{k}_2$ and $\vec{k}_3$ vanishing but not $\vec{k}_1$), but it is clear from the symmetry of the original expression (B4) under $\vec{k}_1 \leftrightarrow \vec{k}_3$ that this will also lead to a convergent integral. Finally, the divergences when $\vec{k}_1$ and/or $\vec{k}_3$ both vanish (but not $\vec{k}_2$) are manifestly integrable.

An alternative way of stating this result is that, when any pair of momenta vanish, there are two measure factors of k^2 and two denominators vanishing as k^2, so the IR divergence cancels. In this form, the argument is easily generalized to all I_n with $n \geq 3$. If j coordinates vanish there will be j measure factors of k^2 and, at most, j denominators vanishing as k^2. (To achieve this number of diverging denominators the momenta must be sequential and include either the first or last momenta.) Thus, all subintegrals are IR convergent, and we deduce that I_n itself is finite.

The discussion so far assumes that both external momenta are set to zero. If one (or both) are nonvanishing, then it is straightforward to see that the loss of one (or two) potentially vanishing denominators is sufficient to make I_n IR finite for all $n > 0$, including $n = 1$ and 2. This assumes that E is evaluated at threshold. Similarly, all I_n are IR finite if any of the internal angular momenta are taken to be anything other than s-wave. For example, in I_1, whose overall IR divergence is linear [$\int dQ Q^{-2}$ from Eq. (B2)], choosing the internal $\mathcal{M}_2$ to be in a p-wave leads to an extra Q^2 (one factor of Q from each of the adjacent G^∞) and removes the divergence.

[23]Each factor of G^∞ contains a double sum over angular-momentum indices, but we consider here only s-wave contributions, since these dominate in the IR due to the factor of $(k^*)^{\ell'}(p^*)^{\ell} \sim Q^{\ell'+\ell}$ in G^∞.

APPENDIX C: CALCULATION OF FINITE TERMS

In this appendix we calculate the contributions of $\mathcal{O}(L^0)$ arising from the second, third and fourth terms on the left-hand side of the quantization condition Eq. (127). These are needed in Sec. III E to find the coefficients in the expansion of the threshold energy $\Delta E_{\rm th}$.

We begin with

$$\mathcal{X}_F = \lim_{L\to\infty}\left\{9L^3\sum_{\vec k}\tilde{\mathcal{M}}_{2,00}\not{G}_{0k}\tilde{\mathcal{M}}_{2,kk}\not{F}^{i\epsilon}_{kk}\tilde{\mathcal{M}}_{2,kk}\not{G}_{k0}\tilde{\mathcal{M}}_{2,00}\right\}\Bigg|_{E=3m+\Delta E_{\rm th}} \tag{C1}$$

$$= \lim_{L\to\infty}\left\{9L^3\sum_{\vec k\neq 0}\tilde{\mathcal{M}}_{2,00}\tilde{G}_{0k}\tilde{\mathcal{M}}_{2,kk}\tilde{F}^{i\epsilon}_{kk}\tilde{\mathcal{M}}_{2,kk}\tilde{G}_{k0}\tilde{\mathcal{M}}_{2,00}\right\}\Bigg|_{E=3m}. \tag{C2}$$

We recall that the notation here indicates that only s-wave contributions are kept. In the second form we have made two changes. The first is an identity: we can replace the slashed G and $F^{i\epsilon}$ with the tilded versions as long as we remove $\vec k = 0$ from the sum. The second is to work directly at threshold, which is allowed since the absence of the $\vec k = 0$ term means that $\Delta E_{\rm th} \sim 1/L^3$ always leads to a correction suppressed by $1/L$.

We recall from Sec. III A that the sum is dominated by small momenta, so it is legitimate to use nonrelativistic expansions of the various quantities worked out in that section and keep only the leading terms. Thus, $\tilde{\mathcal{M}}_{2,00}$ and $\tilde{\mathcal{M}}_{2,kk}$ can be replaced by the constant $-64\pi m^2 a$ [using Eq. (38) and the equality of $\tilde{\mathcal{M}}_{2,00}$ and $\tilde{\mathcal{K}}_{2;00}$ at threshold]. Using Eq. (39), the leading term in $\tilde{G}_{0k}$ is given by

$$\tilde{G}_{0k}|_{E=3m} = -\frac{1}{L}\frac{1}{32\pi^2 m^2}\frac{1}{n_k^2} + \mathcal{O}(1/L^2), \tag{C3}$$

where $\vec k = 2\pi\vec n_k/L$. Note that in the small-momentum regime we can set $H(\vec k)$ to unity. Finally, using Eq. (43), and recalling that $\tilde F^{i\epsilon}$ differs from $\tilde F$ by dropping the ρ term, we have

$$\tilde F^{i\epsilon}_{kk}|_{E=3m} = \frac{1}{L}\frac{1}{64\pi^2 m^2}\left[\sum_{\vec n_a} - \int_{\vec n_a}\right]\frac{H(\vec a)H(\vec b_{ka})}{x^2 - r^2} + \mathcal{O}(1/L^2), \tag{C4}$$

where $x^2 = -3n_k^2/4$, and $\vec r$ is defined in Eq. (45), except that we can set $\gamma = 1$ in our kinematic regime. Since $r^2 > 0$ while $x^2 < 0$ there is no singularity in the summand/integrand, and thus the $i\epsilon$ regularization can be dropped.

The sum-integral difference can be evaluated using the Poisson summation formula

$$\left[\sum_{\vec n_a} - \int_{\vec n_a}\right]\frac{H(\vec a)H(\vec b_{ka})}{x^2 - r^2} = -\sum_{\vec s\neq 0} e^{i\pi\vec s\cdot\vec n_k}\int d^3 r\, e^{2\pi i\vec s\cdot\vec r}\frac{H(\vec a)H(\vec b_{ka})}{|x|^2 + r^2} \tag{C5}$$

$$= -\pi\sum_{\vec s\neq 0} e^{i\pi\vec s\cdot\vec n_k}\frac{e^{-2\pi|x|s}}{s} + \mathcal{O}(e^{-mL}), \tag{C6}$$

where $\vec s$ is a vector of integers. To obtain the second line we have used the fact that the Fourier transform in the first line is dominated by values of r satisfying $r \lesssim |x| = \mathcal{O}(1)$, which in turn implies that $\vec a$ and $\vec b_{ka}$ are small, so the cutoff functions H can be replaced by unity up to exponentially small corrections. Doing so we can evaluate the integral and obtain the result on the second line. The result shows that the zeta-function (sum-integral difference) falls exponentially with increasing $|x|$. When evaluating this expression numerically, we find that the sum converges rapidly for $|x| \gtrsim 1$.

Combining these results, we find that

$$\mathcal{X}_F = \frac{576 m^2 a^4}{\pi^2}(-4\pi)\sum_{\vec n_k\neq 0}\frac{1}{n_k^4}\sum_{\vec s\neq 0} e^{i\pi\vec s\cdot\vec n_k}\frac{e^{-2\pi|x|s}}{s} \tag{C7}$$

$$\equiv \frac{576 m^2 a^4}{\pi^2}\mathcal{C}_F, \tag{C8}$$

where numerical evaluation leads to $\mathcal{C}_F = -0.493036$. This accuracy is obtained by summing up to $n_k^2 = 11$ and $s^2 = 12$.

We next evaluate the contributions coming from the sum over Ξ_1, i.e. those from the last term in Eq. (133). These are

$$\mathcal{X}_{1A} = \lim_{L\to\infty}\left\{9\frac{[32 m\pi a]^3}{(2m)^3}m^2\frac{1}{L^3}\sum_{\vec k\neq 0}\frac{H(\vec k)^2 - 1}{k^4}\right\}, \tag{C9}$$

$$\mathcal{X}_{1B} = 9\frac{[32m\pi a]^3}{(2m)^3} m^2 \frac{1}{L^3}\sum_{\vec{k}\neq 0} a\frac{\sqrt{3}}{2}\frac{H(\vec{k})^3}{k^3}, \tag{C10}$$

where we are implicitly working at $E = 3m$ in the cutoff functions H. In the second quantity we cannot send $L\to\infty$ but we implicitly discard all terms which vanish as $L\to\infty$. Recalling that the Taylor expansion of H about $\vec{k}=0$ is unity to all orders, we see that the summand of $\mathcal{X}_{1A}$ is nonsingular, so the sum can be replaced by an integral in the $L\to\infty$ limit. This leads to the result

$$\mathcal{X}_{1A} = 576\pi m a^3 64\pi^2 \mathcal{C}_3, \tag{C11}$$

$$\mathcal{C}_3 \equiv \int \frac{d^3k}{(2\pi)^3}\frac{m[H(\vec{k})^2-1]}{k^4} = -0.05806. \tag{C12}$$

For $\mathcal{X}_{1B}$, the summand has a pole so the sum cannot be replaced by an integral. Furthermore, the sum has a logarithmic divergence in the UV that is cut off by H and leads to a $\log(mL)$ dependence. To determine its form we rewrite the expression as

$$\mathcal{X}_{1B} = \frac{576m^2a^4}{\pi^2}4\pi^2\sqrt{3}\sum_{\vec{n}_k}\frac{H(2\pi\vec{n}_k/L)^3}{n_k^3}. \tag{C13}$$

From the definition of H, Eq. (12), we know it vanishes when $(E^*_{2,k})^2$ drops to zero. From the definition of $(E^*_{2,k})^2$ in Eq. (7), we find (when $E=3m$) that it vanishes when $k/m = 4/3$. Thus, in terms of $\vec{n}_k = (L/2\pi)\vec{k}$, the sum is cut off at $(4/3)N_{\rm cut}$ where $N_{\rm cut} = mL/(2\pi)$. Approximating the UV part of the sum with an integral gives the logarithmic dependence, and by numerical evaluation we can determine the constant underneath:

$$\sum_{\vec{n}_k}\frac{H(2\pi\vec{n}_k/L)^3}{n_k^3} = 4\pi\log N_{\rm cut} + 1.54861 + \mathcal{O}(1/L). \tag{C14}$$

Combining these results we find

$$\mathcal{X}_{1B} = \frac{576m^2a^4}{\pi^2}(16\pi^3\sqrt{3}\log N_{\rm cut} + \mathcal{C}_4) + \mathcal{O}(1/L), \tag{C15}$$

$$\mathcal{C}_4 = 105.892. \tag{C16}$$

The final contribution is that from Ξ_2, which is

$$\mathcal{X}_2 = \frac{1}{L^6}\sum_{\vec{k}_1,\vec{k}_2\neq 0}\Xi_2(\vec{k}_1,\vec{k}_2). \tag{C17}$$

This can be evaluated at $E = 3m$ (which only affects the cutoff functions H contained in Ξ_2). Using the definition of Ξ_2, Eq. (122), we find

$$\mathcal{X}_2 = \frac{576m^2a^4}{\pi^2}16\sum_{\vec{n}_1,\vec{n}_2\neq 0}\frac{H(2\pi\vec{n}_1/L)^2 H(2\pi\vec{n}_2/L)^2}{n_1^2[n_1^2+n_2^2+(\vec{n}_1+\vec{n}_2)^2]n_2^2}. \tag{C18}$$

Again the sum has a logarithmic UV divergence, and, pulling this out, we find by numerical evaluation that

$$\mathcal{X}_2 = \frac{576m^2a^4}{\pi^2}\left(\frac{64\pi^4}{3}\log N_{\rm cut} - \mathcal{C}_5\right) + \mathcal{O}(1/L), \tag{C19}$$

$$\mathcal{C}_5 = 1947. \tag{C20}$$

We note that, while the coefficient $\mathcal{C}_5$ appears large, it is approximately the same size as the coefficient of the logarithm: $64\pi^4/3 \approx 2080$.

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