Variational approach to N-body interactions in finite volume

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We explore a variational approach to the finite-volume N-body problem. The general formalism for N nonrelativistic spinless particles interacting with periodic pairwise potentials yields N-body secular equations. The solutions depend on the infinite-volume N-body wave functions. Given that the infinite-volume N-body dynamics may be solved by the standard Faddeev approach, the variational N-body formalism can provide a convenient numerical framework for finding discrete energy spectra in periodic lattice structures.

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I. INTRODUCTION

Three-particle channels are important in spectroscopy of excited mesons. For example, G parity forbids a two-pion decay of the $a_1(1260)$ meson so that the width of this axial-vector resonance is determined by its coupling to three pions. The three-pion decay channel is allowed for the exotic π_1 meson with $J^{PC} = 1^{-+}$, while the exotic h_2 with $J^{PC} = 2^{+-}$ could decay to $b_1[\omega\pi]\pi$ and $\rho\pi$. Because of their possible hybrid nature and relation to confinement [1], these mesons are a subject of intense theoretical and experimental investigations [2]. In the baryon sector, the situation is even more complex because two- and three-particle systems often mix. Phenomenologically, it is observed that the $\pi\pi N$ channels have significant influence and cannot be neglected when determining resonance parameters of nucleon excitations. The number of possible quantum numbers $(\pi\Delta^{(*)}, \pi N^*, \sigma N, \rho N, \ldots)$ for a given spin and parity J^P is large so that one has to truncate. Yet, phenomenology can be a guideline to select relevant channels, e.g., by inspecting the involved centrifugal barriers. For example, it is reasonable to assume that the Roper resonance $N(1440)1/2^+$ is dominated by the σN channel (all three particles in the relative S wave) and maybe the $\pi\Delta$ channel, while the ρN channel could be less important at smaller energies where only pions from the low-energy tail of the ρ can be on-shell.

Pioneering calculations in lattice QCD of the spectra of light excited mesons [3] and baryons [4,5] have delivered a semiquantitative picture in which pion masses are large and finite-volume effects are usually neglected. Energy eigenvalues have been calculated for the $a_1(1260)$ [6] using $q\bar{q}$ operators but also a $\rho\pi$ meson-meson operator, though taken at zero momentum, $\pi(\mathbf{0})\rho(\mathbf{0})$. Recently, the Hadron Spectrum Collaboration calculated isospin $I = 2$ $\pi\rho$ scattering although the ρ meson is stable at the pertinent pion mass [7].

Few-body systems above threshold represent the next milestone for the *ab initio* understanding of the strong interaction through lattice QCD calculations. Therefore, the infinite-volume extrapolation of three-body systems has attracted much interest recently [8–34], including an extension to coupled two- to three-body channels [18] and a study of the connection between low-temperature condensation and scattering in lattice ϕ^4 theory [34]. For the three-particle system in finite volume, the energy eigenvalues are expected to change not only quantitatively but also qualitatively above threshold compared to the two-body case. One can easily understand this by considering the noninteracting energies. For two particles of equal mass m in a cube of side length L with periodic boundary conditions, they are given by $E = 2E_{\mathbf{n}}$, where $E_{\mathbf{n}} = \sqrt{m^2 + \mathbf{p_n}^2}$ and $\mathbf{p_n} = (2\pi/L)\mathbf{n}$, $\mathbf{n} \in \mathbb{Z}^3$. In contrast, noninteracting three-body energies are given by $E = E_{\mathbf{n}} + E_{\mathbf{n}'} + E_{\mathbf{n}+\mathbf{n}'}$, where $\mathbf{n}$, $\mathbf{n}' \in \mathbb{Z}^3$. This pattern is entirely different from the two-body case which is expected to be reflected in the interacting spectrum as well. Apart from conceptual challenges, there is also the problem

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of underdetermination, i.e., there is a plethora of possible channels in contrast to scarce data, and, for the selection of relevant channels, similar considerations as in infinite volume will have to be made.

Four-body systems above threshold have so many possible combinations of quantum numbers that one can only hope to address the simplest cases. A prime example is the energy region above the four-pion threshold in $\pi\pi$ scattering. In analyses of experiments, usually the four-pion channel below 1 GeV is neglected given that the experimentally measured partial-wave amplitudes are almost elastic in this energy region (see Refs. [35,36] for a calculation of the inelasticity). Similarly, the existing lattice studies of $\pi\pi$ partial waves exclude the data above the four-pion intermediate states for the infinite-volume extrapolation (see, e.g., Refs. [37–40]).

So far, in the three-body calculations only meson-meson or meson-baryon operators have been used, as opposed to those with three components (such as $\pi\pi\pi$ or $\pi\pi N$). An exception is the N-body threshold calculation of positively charged pions by the NPLQCD Collaboration [41,42]. Energy eigenvalues for the Roper [43] resonance above the $\pi\pi N$ threshold have been calculated recently including nonlocal πN and σN operators. This calculation was performed close to the physical pion mass such that the extracted energy levels lie above the πN but also above the $\pi\pi N$ threshold. An unusual pattern was observed that could originate from the aforementioned three-body dynamics in a coupled $\pi N, \sigma N, \ldots$ channel, where the σ has to be understood as an interacting two-body subsystem and not a stable particle.

In a rough and incomplete classification, there are three major approaches to solving the three-body problem in finite volume in the momentum-space representation: an relativistic, all-orders perturbation theory pursued by Briceño, Hansen, and Sharpe [12–14,18,21], a nonrelativistic dimer formalism by Hammer *et al.* [10,15–17,20], and a method based on three-body unitarity to identify on-shell configurations and, therefore, power-law finite-volume effects by Döring and Mai [8,19,22]. For the latter two approaches, the partial diagonalization of the amplitude according to cubic symmetry was discussed in Ref. [22].

All of these approaches aim at fully mapping out the few-body dynamics, but there are also attempts to obtain essential information from these systems without the need to explicitly take all degrees of freedom into account [28,29]. The first-ever prediction of excited three-body energy eigenvalues of a physical system ($\pi^+\pi^+\pi^+$) from two-body scattering information and lattice threshold eigenvalues [41,42] was achieved recently [8].

A. Variational approach

Most of the approaches to the few-body problem, including the examples discussed above, rely on the momentum representation of the reaction amplitude or correlation function in finite volume. There is, however, an alternative approach based on Faddeev equations and two- and three-body wave functions in configuration space [30–33,44,45]. The finite-volume wave function is related to the infinite-volume wave function by a linear superposition over infinite sets of periodic cubic boxes: the quantization conditions are subsequently obtained from matching conditions [30–33,44,45]. One of the advantages of this approach is that the connection between long-distance correlations over boxes and short-distance interactions within each cubic box is made explicit by constructing the finite-volume wave function.

In the present work, we set up and explore the foundations of a potentially convenient numerical approach to the N-body interaction in finite volume. The formalism presented in this work is based on the variational method [46,47] combined with the Faddeev approach [48–51]. A brief summary of the variational principle and Faddeev approach are presented in Appendices A and B as a short reference for readers that are not familiar with the above-mentioned methods.

Based on the traditional variational principle, the secular equation may be obtained by considering $\delta\Lambda = 0$ with $\Lambda = \langle\Phi|E - \hat{H}^{(L)}|\Phi\rangle$, where both the N-body Hamiltonian $\hat{H}^{(L)} = \hat{T} + \sum_{i<j}\hat{V}^{(L)}_{(ij)}$ and the trial wave function Φ display periodicity in the cubic lattice, $\hat{T}$ is the kinetic energy operator, and $\hat{V}^{(L)}_{(ij)}$ stands for the periodic pairwise interaction between the ith and jth particle. Instead of the traditional approach, in this work we write the total wave function as a sum of multiple terms [48–51]: $\Phi = \sum^{N}_{(i<j)=1}\Phi^{(ij)}$. Each component of the total wave function $\Phi^{(ij)}$ is required to satisfy the equation $(E - \hat{T})|\Phi^{(ij)}\rangle = \hat{V}^{(L)}_{(ij)}|\Phi\rangle$. Therefore, a single Schrödinger equation, $(E - \hat{H}^{(L)})|\Phi\rangle = 0$, is turned into $N(N-1)/2$ coupled equations. The advantage of the Faddeev approach is to allow one to incorporate the dominant subsystem structures in an adequate way and to use two-body scattering amplitudes as input for the N-body dynamical equations. By splitting the complete N-body wave function, ultimately $N(N-1)/2$ secular equations may be obtained by considering

$$\delta[\langle\Phi|(E - \hat{T})|\Phi^{(ij)}\rangle - \langle\Phi|\hat{V}^{(L)}_{(ij)}|\Phi\rangle] = 0. \tag{1}$$

As will be shown in Sec. III, the secular equations obtained from Eq. (1) resemble two-body secular equations.

In solid state and condensed matter physics, the linear combination of atomic orbital (LCAO) method for the calculations of the electronic structure of periodic systems [52] provides an elegant way to construct a wave function that satisfies periodic boundary conditions. The trial wave function that describes electrons traveling in a periodic crystal is constructed by linear superposition of all atomic

orbital solutions of an isolated atom centered at each cell of the crystal. In this way, the periodic boundary conditions of the wave function are automatically guaranteed, and the energy spectra are given by secular equations from the variational principle. Similarly, as also suggested in Refs. [30–32,45], the trial finite-volume N-body wave function may be constructed from the N-body infinite-volume wave function, $\Phi(\{\mathbf{x}\})=\sum_{\{\mathbf{n}_\mathbf{x}\}\in\mathbb{Z}^3}\Psi(\{\mathbf{x}+\mathbf{n}_\mathbf{x}L\})$, where Ψ is the solution of the corresponding infinite-volume Schrödinger equation, $(E-\hat{H})|\Psi\rangle=0$, and the set $\{\mathbf{x}\}$ stands for the complete set of particle positions. Hence, the trial finite-volume N-body wave function satisfies periodic boundary conditions by construction. In principle, the infinite-volume wave function may be solved by standard methods, such as Faddeev's approach [48–51].

The immediate gain of the variational approach for finite-volume systems is evident. 1) The construction of the finite-volume wave function from the infinite-volume wave function presents a clear connection between short-range N-body dynamics within each image of the cubic box and long-range correlations in the entire periodic lattice structure. The N-body dynamics within each cubic box is determined by N-body Faddeev equations. The long-range correlation effect accumulated from all cubic boxes is implemented by the linear superposition of all wave functions centered at each image of cubic boxes. 2) The quantization conditions (secular equations) due to the periodic structure of the lattice are imposed by a variational approach, and eventually yield the discrete energy spectra of the system in finite volume. 3) The variational formalism is mathematically transparent and may be suitable for the numerical evaluation of the N-body finite-volume problem. However, it comes at the price of sacrificing the explicit analytical expressions of quantization conditions as present in the Lüscher formula [53] for the two-body problem and at the high cost of computation of the N-body phase space integration.

As we present here the first attempt to calculate the N-body interaction in finite volume with the proposed methods, and also for the sake of simplification of the discussion, in this work, we only consider a simple model with N nonrelativistic spinless particles interacting through pairwise short-range potentials. Given the infinite-volume wave function, Ψ, that may be solved by the Faddeev approach and is used as input to the finite-volume problem, the quantization conditions for the finite-volume N-body interaction are obtained and presented in Sec. II. In principle, three-body forces and coupled-channel effects may be included in the formalism as well. However, such type of effects are not considered in the present work. In addition, bound states below threshold may be described by the analytic continuation of scattering amplitudes. In the present work, we focus on the N-body problem with pairwise interactions. The discussion of the three-body force, coupled-channel effect, and bound states below threshold will be given in future publications.

An effective two-body formalism may be determined by integrating out the rest of the degrees of freedoms of the N-body system. The resemblance of the N-body quantization condition to the two-body quantization condition will be discussed in Sec. II E. Finally, in Appendix C we also present some main results for a pairwise short-range δ-function potential. The renormalization issue due to the singular nature of the δ-function interaction in three dimensions is also discussed.

The paper is organized as follows. In Sec. II we present the derivation and main results of the variational approach to the N-body interaction in finite volume. The discussion and summary are given in Sec. III.

II. VARIATIONAL N-BODY INTERACTION FORMALISM IN FINITE VOLUME

A. Secular equations of N-body interaction in finite volume

The dynamics of N nonrelativistic particles interacting via pairwise interactions in finite volume with periodic boundary conditions is determined by the Schrödinger equation,

$$\left[E+\sum_{k=1}^{N}\frac{\nabla_{\mathbf{x}_k}^2}{2m}-\sum_{(i<j)=1}^{N}V_{(ij)}^{(L)}(\mathbf{x}_i-\mathbf{x}_j)\right]\Phi(\{\mathbf{x}\})=0, \tag{2}$$

where we take all masses to be equal to m, $\mathbf{x}_i$ denotes particle position, and $\{\mathbf{x}\}\equiv\{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N\}$. The potential between the ith and jth particles is described by $V_{(ij)}^{(L)}$. In finite volume, $V_{(ij)}^{(L)}$ displays periodicity when the distance of the ith and jth particles is larger than the size of the cubic box. $V_{(ij)}^{(L)}$ may be written as the superposition of all the potentials centered at each image of the periodic cubic box,

$$V_{(ij)}^{(L)}(\mathbf{r})=\sum_{\mathbf{n}\in\mathbb{Z}^3}V_{(ij)}(\mathbf{r}+\mathbf{n}L), \tag{3}$$

where $V_{(ij)}$ is the potential between the ith and the jth particle in the same box, and L is the size of the three-dimensional cube. Because of the periodicity of the finite-volume potential, the finite-volume N-particle wave function $\Phi(\{\mathbf{x}\})$ must also satisfy periodic boundary conditions,

$$\Phi(\{\mathbf{x}+\mathbf{n}_\mathbf{x}L\})=\Phi(\{\mathbf{x}\}), \tag{4}$$

where $\{\mathbf{n}_\mathbf{x}\}=\{\mathbf{n}_{\mathbf{x}_1},\mathbf{n}_{\mathbf{x}_2},\ldots,\mathbf{n}_{\mathbf{x}_N}\}$ and $\mathbf{n}_{\mathbf{x}_i}\in\mathbb{Z}^3$.

Following the Faddeev approach [48–51] (which is briefly summarized in Appendix B), the N-body finite-volume wave function may be expressed as the sum of $N(N-1)/2$ terms,

$$\Phi(\{\mathbf{x}\}) = \sum_{(i<j)=1}^{N} \Phi^{(ij)}(\{\mathbf{x}\}), \tag{5}$$

where wave function $\Phi^{(ij)}$ is required to satisfy the equation

$$(E - \hat{T})\Phi^{(ij)}(\{\mathbf{x}\}) = V_{(ij)}^{(L)}(\mathbf{x}_i - \mathbf{x}_j)\Phi(\{\mathbf{x}\}), \tag{6}$$

where $\hat{T} = -\sum_{k=1}^{N} \frac{\nabla_{\mathbf{x}_k}^2}{2m}$. Hence, the Schrödinger equation (2) is converted to $N(N-1)/2$ coupled equations. The N-body finite-volume wave function is normally expanded in terms of a set of periodic basis functions,

$$\Phi(\{\mathbf{x}\}) = \sum_{[J]} c_{[J]} \Phi_{[J]}(\{\mathbf{x}\}), \tag{7}$$

where $[J]$ refers to a complete set of quantum numbers for the N-particle basis wave functions, and $c_{[J]}$ stands for the expansion coefficients that may be determined by the variational principle. Similar to Eq. (5), the basis function $\Phi_{[J]}$ is also given by the sum of $N(N-1)/2$ terms: $\Phi_{[J]} = \sum_{(i<j)=1}^{N} \Phi_{[J]}^{(ij)}$. We remark that the choice of basis functions may be arbitrary, depending on the symmetry of the specific physical system and the convenience of numerical computation. However, the different choices of basis functions should lead to consistent results. A reasonable choice of basis functions should preserve the symmetry of the physical system (such as periodic boundary conditions in finite volume), and numerical results should be stable and converge.

In the finite volume, to fulfill the periodic boundary conditions, the basis functions $\Phi_{[J]}$ are constructed from infinite-volume solutions of the Schrödinger equation. The complete details are given in Sec. II B. In the following we use the two-body problem as a specific example to explain our choice of basis functions $\Phi_{[J]}$ in finite volume. We denote the infinite-volume wave functions by $\Psi_{[J]}$. In the case of two particles in the center-of-mass frame, the solutions of the Schrödinger equation in infinite volume may be determined by the partial-wave expansion of the free incoming wave, $\Psi_{[J]}^{(0)}(\mathbf{r}) = (4\pi) i^J Y_{[J]}(\mathbf{r}) j_J(qr)$, where $[J] = JM$ are partial-wave quantum numbers, $\mathbf{r}$ stands for the relative position of the two particles, and $q = \sqrt{mE}$ is the relative momentum of the particles. Thus, the asymptotic solution of two-body scattering in infinite volume is given by

$$\Psi_{[J]}(\mathbf{r}) \to (4\pi) i^J Y_{[J]}(\mathbf{r})[j_J(qr) + i t_J(q) h_J^+(qr)], \tag{8}$$

where $t_J(q)$ stands for the two-body scattering amplitude. Hence, $\Psi_{[J]}$ can be used as basis functions in infinite volume to construct the corresponding finite-volume basis functions $\Phi_{[J]}$ in order to fulfill the requirement of periodic boundary conditions,

$$\Phi_{[J]}(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \Psi_{[J]}(\mathbf{r} + \mathbf{n}L). \tag{9}$$

Such finite-volume basis functions reflect the periodic lattice structure. It will be shown in Sec. II D that the two-body basis functions $\Phi_{[J]}$ will be related to Lüscher's zeta function [53]. As a general remark, the basis functions should be constructed respecting the cubic symmetry of the problem; however, we do not explicitly address this topic here. Such basis functions will be given by linear superpositions of infinite-volume basis functions; see, e.g., Ref. [22] in which basis functions for "shells" were derived as linear combinations of cubic harmonics which by themselves are superpositions of spherical harmonics.

With the finite-volume wave function expanded in terms of the basis function (7), the variational principle $\partial\Lambda^{(ij)}/\partial c_{[J']}^* = 0$, with $\Lambda^{(ij)}$ given by

$$\Lambda^{(ij)} = \sum_{[J],[J']} c_{[J']}^* \langle \Phi_{[J']} | [(E - \hat{T})|\Phi_{[J]}^{(ij)}\rangle - \hat{V}_{(ij)}^{(L)}|\Phi_{[J]}\rangle] c_{[J]}, \tag{10}$$

yields a set of coupled secular equations,

$$\sum_{[J]} [\langle \Phi_{[J']}|E - \hat{T}|\Phi_{[J]}^{(ij)}\rangle - \langle \Phi_{[J']}|\hat{V}_{(ij)}^{(L)}|\Phi_{[J]}\rangle] c_{[J]} = 0, \tag{11}$$

and summing the above $N(N-1)/2$ equations leads to a familiar form for the secular equation [see also Eq. (A5)],

$$\sum_{[J]} [\langle \Phi_{[J']}|E - \hat{H}^{(L)}|\Phi_{[J]}\rangle] c_{[J]} = 0, \tag{12}$$

where $\hat{H}^{(L)} = \hat{T} + \sum_{(i<j)=1}^{N} \hat{V}_{(ij)}^{(L)}$. A nontrivial solution of Eq. (11) exists, provided all $N(N-1)/2$ determinant conditions

$$\det [\langle \Phi_{[J']}|E - \hat{T}|\Phi_{[J]}^{(ij)}\rangle - \langle \Phi_{[J']}|\hat{V}_{(ij)}^{(L)}|\Phi_{[J]}\rangle] = 0 \tag{13}$$

are satisfied simultaneously. To summarize, given a set of basis functions $\Phi_{[J]}^{(ij)}$ that satisfy periodic boundary conditions, the variational solution for the spectrum of the N-body finite-volume problem is reduced to a solution of the determinant conditions given by Eq. (13).

B. Construction of the finite-volume wave function and reduction of the secular equations

To proceed, a proper choice of basis functions with periodic symmetry $\Phi_{[J]}^{(ij)}$ has to be made. There are numerous examples of periodic basis functions, e.g., devised for calculations of electronic structure in a periodic lattice and other condensed matter or solid state systems. Specifically, in the LCAO method [52], the periodic

variational basis functions for describing electronic states tunneling in a crystal are constructed as a linear superposition of all atomic orbital solutions for an isolated atom located at each unit cell of the crystal. When applied to hadron scattering, instead of using bound-state solutions (as done previously in Refs. [30–32,45]) the basis functions may be constructed from the linear superposition of infinite-volume scattering wave functions centered at each image of the cubic box,

$$\Phi^{(ij)}_{[J]}(\{\mathbf{x}\}) = \frac{1}{\mathcal{N}} \sum_{\{\mathbf{n}_\mathbf{x}\}\in\mathbb{Z}^3} \Psi^{(ij)}_{[J]}(\{\mathbf{x}+\mathbf{n}_\mathbf{x}L\}), \tag{14}$$

where $\{\mathbf{n}_\mathbf{x}\} = \{\mathbf{n}_{\mathbf{x}_1}, \mathbf{n}_{\mathbf{x}_2}, \ldots, \mathbf{n}_{\mathbf{x}_N}\}$, $\mathcal{N} = \sum_{\mathbf{n}\in\mathbb{Z}^3}$ is a normalization factor, and $\Psi^{(ij)}_{[J]}$ satisfies the Schrödinger equation in infinite volume with potentials $V_{(ij)}$,

$$(E-\hat{T})|\Psi^{(ij)}_{[J]}\rangle = \hat{V}_{(ij)}|\Psi_{[J]}\rangle. \tag{15}$$

The total N-body wave function in infinite volume $\Psi_{[J]}$ is the scattering solution of the Schrödinger equation $(E-\hat{T}-\hat{V})|\Psi_{[J]}\rangle = 0$ and may be expressed as

$$\Psi_{[J]} = \Psi^{(0)}_{[J]} + \sum_{(i<j)=1}^{N} \Psi^{(ij)}_{[J]}, \tag{16}$$

where $\Psi^{(0)}_{[J]}$ stands for the free incoming wave and satisfies the free Schrödinger equation $(E-\hat{T})|\Psi^{(0)}_{[J]}\rangle = 0$. For example, the two-body partial-wave free incoming wave is given by $\Psi^{(0)}_{[J]}(\mathbf{r}) = (4\pi)i^J Y_{[J]}(\mathbf{r}) j_J(qr)$, while the corresponding wave function in the three-body case was given in Ref [30]. The periodic symmetry of the finite-volume wave function Φ is satisfied automatically by the construction in Eq. (14). The infinite-volume N-body wave function Ψ may be solved using the standard Faddeev approach. Locally, at each image of the cubic box, assuming the size of the box is large enough, the short distance N-body dynamics is thus described by the solution of the infinite-volume Schrödinger equation Ψ. The long-distance correlations at scales larger than the range of the potential are taken into account through the linear superposition of the infinite-volume wave functions centered at each image of the periodic cubic box; see Eq. (14).

Using Eqs. (14) and (15) and taking into account the periodicity of the finite-volume potential, the secular equations given by Eq. (11) reduce to

$$\sum_{[J]} \langle\Phi_{[J']}|\hat{V}_{(ij)}[|X^{(ij)}_{[J]}\rangle - |\Phi_{[J]}\rangle]c_{[J]} = 0, \tag{17}$$

where

$$X^{(ij)}_{[J]}(\{\mathbf{x}\}) = \sum_{\overline{\{\mathbf{n}_\mathbf{x}\}}_{(i,j)}\in\mathbb{Z}^3} \Psi_{[J]}(\{\mathbf{x}+\mathbf{n}_\mathbf{x}L\}), \tag{18}$$

and $\overline{\{\mathbf{n}_\mathbf{x}\}}_{(i,j)}$ stands for the set $\{\mathbf{n}_\mathbf{x}\}$ excluding two elements: $\mathbf{n}_{\mathbf{x}_i}$ and $\mathbf{n}_{\mathbf{x}_j}$. Furthermore, the $N(N-1)/2$ determinant conditions given by Eq. (13) become

$$\det\left[\langle\Phi_{[J']}|\hat{V}_{(ij)}(|X^{(ij)}_{[J]}\rangle - |\Phi_{[J]}\rangle)\right] = 0. \tag{19}$$

Given the scattering solution of the N-body problem in infinite volume Ψ as input, the finite-volume wave functions Φ and $X^{(ij)}$ can be constructed by using Eqs. (14) and (18), respectively. We remark that the energy dependence of the infinite-volume wave function $\Psi_{[J]}$ has been suppressed so far in our presentation. For the scattering solutions, $\Psi_{[J]}$ does indeed depend on the incoming momenta of particles, because the finite volume wave functions, $\Phi_{[J]}$ and $X^{(ij)}_{[J]}$, are constructed from $\Psi_{[J]}$, hence momenta dependence remains in finite volume wave functions as well. Therefore, using the infinite-volume scattering solutions $\Psi_{[J]}$ as inputs, the finite-volume quantization conditions (19) yield discrete energy spectra as a consequence of the periodic cubic lattice structure. In other words, the discrete energy spectra in finite volume is the result of the long-distance correlation effects of particles in a periodic lattice structure. Meanwhile, the specific patterns of discrete spectra rely on the short-distance interactions that are described by scattering amplitudes or "amplitude-carrier" wave functions $\Psi_{[J]}$ in infinite volume. Ultimately, the quantization conditions play the role of imposing constraints on energy spectra due to periodic boundary conditions. The scattering information in infinite volume and with periodic boundary conditions is combined using finite-volume wave functions $\Phi_{[J]}$ and $X^{(ij)}_{[J]}$.

The secular equations (17) and corresponding quantization conditions (19) can be further reduced by removing the center-of-mass motion. However, the choice of relative coordinates for the N-body system can normally be made quite arbitrary. In Sec. II C, the specific choice [51] is described by forming the succession of subsystems of N particles in such a way that the subsystems are obtained by successively joining particle 2, particle 3, $\cdots$, particle N to particle 1, i.e., (12), $((12)3)$, $(((12)3)4)$, ….

C. Removal of center-of-mass motion

Since in this work we are mainly interested in scattering solutions, the set of incoming particle momenta is also introduced to label the N-body wave functions $\{\mathbf{p}\} = \{\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N\}$, where $\mathbf{p}_i$ stands for the momentum of the ith incoming particle. The total energy of N particles is given by $E = \sum_{i=1}^{N} p_i^2/2m$. The center-of-mass motion and internal motion of the N-body system can be separated out by changing coordinates. One particular choice

of the relative coordinates and momenta [51] is given, respectively, by

$$\boldsymbol{\rho}_{(12),n} = \sqrt{\frac{2n}{n+1}}\left(\frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_k - \mathbf{x}_{n+1}\right),$$
$$\mathbf{q}_{(12),n} = \sqrt{\frac{n}{2(n+1)}}\left(\frac{1}{n}\sum_{k=1}^{n}\mathbf{p}_k - \mathbf{p}_{n+1}\right), \quad (20)$$

where $n < N$. The quantities $\boldsymbol{\rho}_{(12),n}$ and $\mathbf{q}_{(12),n}$ may be interpreted as the relative coordinates and momentum between the $(n+1)$th particle and the center-of-mass coordinate or momentum of the cluster of particles $(1, 2, \ldots, n)$, respectively. The index (12) is used to label the special choice we made for the relative coordinates and momenta, so that for $n = 1$ the relative coordinates and momenta are defined between particle 1 and particle 2,

$$\boldsymbol{\rho}_{(12),1} = \mathbf{x}_1 - \mathbf{x}_2, \qquad \mathbf{q}_{(12),1} = \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2). \quad (21)$$

The complete sets of relative coordinates and momenta are given by $\{\boldsymbol{\rho}_{(12)}\} = \{\boldsymbol{\rho}_{(12),1}, \boldsymbol{\rho}_{(12),2}, \ldots, \boldsymbol{\rho}_{(12),N-1}\}$ and $\{\mathbf{q}_{(12)}\} = \{\mathbf{q}_{(12),1}, \mathbf{q}_{(12),2}, \cdots, \mathbf{q}_{(12),N-1}\}$, respectively. The center-of-mass coordinate and momentum of the N-body system are

$$\mathbf{R} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i, \mathbf{P} = \sum_{i=1}^{N}\mathbf{p}_i. \quad (22)$$

The total energy of the N-particle system is given by $E = \sum_{n=1}^{N-1}\mathbf{q}_{(12),n}^2/m + \mathbf{P}^2/2mN$, and the kinetic energy operator of the N-body system is

$$\hat{T} = -\sum_{n=1}^{N-1}\frac{\nabla^2_{\boldsymbol{\rho}_{(12),n}}}{m} - \frac{1}{N}\frac{\nabla^2_{\mathbf{R}}}{2m}. \quad (23)$$

In terms of the set $\{\boldsymbol{\rho}_{(12)}\}$, the infinite-volume N-body wave function is given by $\Psi(\{\mathbf{x}\}, \{\mathbf{p}\}) = e^{i\mathbf{P}\cdot\mathbf{R}}\psi(\{\boldsymbol{\rho}_{(12)}\}, \{\mathbf{q}_{(12)}\})$, where the center-of-mass motion is represented by a plane wave $e^{i\mathbf{P}\cdot\mathbf{R}}$ and the wave function ψ describes the internal motions of the N-body system. The same applies to the finite-volume wave function. The N-body wave function representing the relative motion in finite volume is thus given by

$$\phi(\{\boldsymbol{\rho}_{(12)}\}, \{\mathbf{q}_{(12)}\}) = \frac{1}{\mathcal{N}}\sum_{\{\mathbf{n}_\mathbf{x}\}\in\mathbb{Z}^3} e^{i\frac{\mathbf{P}}{N}\sum_{i=1}^{N}\mathbf{n}_{\mathbf{x}_i}}\psi(\{\ddot{\boldsymbol{\rho}}_{(12)}\}, \{\mathbf{q}_{(12)}\}), \quad (24)$$

where the nth element of the set $\{\ddot{\boldsymbol{\rho}}_{(12)}\}$ is

$$\ddot{\boldsymbol{\rho}}_{(12),n} = \boldsymbol{\rho}_{(12),n} + \sqrt{\frac{2n}{n+1}}\left(\frac{1}{n}\sum_{k=1}^{n}\mathbf{n}_{\mathbf{x}_k} - \mathbf{n}_{\mathbf{x}_{n+1}}\right)L. \quad (25)$$

In order to remove one redundant element of the set $\{\mathbf{n}_\mathbf{x}\}$, a subset $\{\mathbf{n}_{(12)}\}$ is introduced,

$$\{\mathbf{n}_{(12)}\} = \{\mathbf{n}_{(12),1}, \mathbf{n}_{(12),2}, \ldots, \mathbf{n}_{(12),N-1}\} \in \mathbb{Z}^3, \quad (26)$$

where the kth element is given by $\mathbf{n}_{(12),k} = \mathbf{n}_{\mathbf{x}_k} - \mathbf{n}_{\mathbf{x}_{k+1}}$. Having introduced the set $\{\mathbf{n}_{(12)}\}$ in this particular way, all of the elements of set $\{\mathbf{n}_{(12)}\}$ still belong in $\mathbb{Z}^3$. We also find

$$\ddot{\boldsymbol{\rho}}_{(12),n} = \boldsymbol{\rho}_{(12),n} + \sqrt{\frac{2}{n(n+1)}}\sum_{k=1}^{n}k\mathbf{n}_{(12),k}L, \quad (27)$$

and

$$\sum_{i=1}^{N}\mathbf{n}_{\mathbf{x}_i} = \sum_{k=1}^{N-1}k\mathbf{n}_{(12),k}L + N\mathbf{n}_{\mathbf{x}_N}. \quad (28)$$

Hence, after removing the center-of-mass motion, the finite-volume relative wave function ϕ is related to ψ by

$$\phi(\{\boldsymbol{\rho}_{(12)}\}, \{\mathbf{q}_{(12)}\}) = \sum_{\{\mathbf{n}_{(12)}\}\in\mathbb{Z}^3} e^{i\frac{\mathbf{P}}{N}\left(\sum_{k=1}^{N-1}k\mathbf{n}_{(12),k}\right)L}\psi(\{\ddot{\boldsymbol{\rho}}_{(12)}\}, \{\mathbf{q}_{(12)}\}) \quad (29)$$

and ϕ satisfies periodic boundary conditions,

$$\phi(\{\ddot{\boldsymbol{\rho}}_{(12)}\}, \{\mathbf{q}_{(12)}\}) = e^{-i\frac{\mathbf{P}}{N}\left(\sum_{k=1}^{N-1}k\mathbf{n}_{(12),k}\right)L}\phi(\{\boldsymbol{\rho}_{(12)}\}, \{\mathbf{q}_{(12)}\}). \quad (30)$$

Clearly, the set $\{\boldsymbol{\rho}_{(12)}\}$ cannot be the only choice of independent relative coordinates. By exchanging the labels of each particle, such as $1 \leftrightarrow i$ and $2 \leftrightarrow j$ in set $\{\boldsymbol{\rho}_{(12)}\}$, another independent coordinate set $\{\boldsymbol{\rho}_{(ij)}\}$ may be obtained. For example, by relabeling $2 \leftrightarrow 3$ in $\{\boldsymbol{\rho}_{(12)}\}$, the elements of set $\{\boldsymbol{\rho}_{(13)}\}$ are given by

$$\boldsymbol{\rho}_{(13),1} = \mathbf{x}_1 - \mathbf{x}_3 = \frac{\boldsymbol{\rho}_{(12),1} + \sqrt{3}\boldsymbol{\rho}_{(12),2}}{2},$$
$$\boldsymbol{\rho}_{(13),2} = \frac{2}{\sqrt{3}}\left(\frac{\mathbf{x}_1 + \mathbf{x}_3}{2} - \mathbf{x}_2\right) = \frac{\sqrt{3}\boldsymbol{\rho}_{(12),1} - \boldsymbol{\rho}_{(12),2}}{2},$$
$$\boldsymbol{\rho}_{(13),n} = \boldsymbol{\rho}_{(12),n}, \qquad n > 2. \quad (31)$$

The different sets $\{\boldsymbol{\rho}_{(ij)}\}$ and $\{\boldsymbol{\rho}_{(i'j')}\}$ are linked by a linear transformation,

$$\{\boldsymbol{\rho}_{(ij)}\} = \Gamma^{(ij),(i'j')}\{\boldsymbol{\rho}_{(i'j')}\}; \quad (32)$$

for example,

$$\Gamma^{(13),(12)} = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & \mathbb{I} \end{bmatrix}. \quad (33)$$

Because it is constructed in this way, the transfer matrix Γ between two different sets is an orthogonal matrix, $\Gamma^T\Gamma = \mathbb{I}$. Hence, both the sum $\sum_{n=1}^{N-1}\boldsymbol{\rho}_{(ij),n}^2$ and the N-body volume element $\int\prod_{n=1}^{N-1} d\boldsymbol{\rho}_{(ij),n}$ are invariant under this transformation of sets. Similarly, both the total energy and kinetic energy operator are also invariant under a transformation between sets of relative coordinates and momenta.

With the introduction of these sets of relative coordinates, the finite-volume N-body wave function $\phi_{[J]}$ may be written as

$$\phi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) = \sum_{(i<j)=1}^{N}\phi_{[J]}^{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\}), \quad (34)$$

where $\phi_{[J]}^{(ij)}$ satisfies

$$\begin{aligned}&(\sigma^2-\hat{T}_{\rho})\phi_{[J]}^{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\})\\&\quad= mV_{(ij)}^{(L)}(\boldsymbol{\rho}_{(ij),1})\phi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}),\end{aligned} \quad (35)$$

and we introduced rescaled total energy and kinetic energy operators, $\sigma^2 = mE - \mathbf{P}^2/2N$ and $\hat{T}_{\boldsymbol{\rho}} = -\sum_{n=1}^{N-1}\nabla^2_{\boldsymbol{\rho}_{(ij),n}}$. The construction of $\phi_{[J]}^{(ij)}$ is given by

$$\begin{aligned}\phi_{[J]}^{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\}) = &\sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3} e^{i\frac{\mathbf{P}}{N}\cdot(\sum_{n=1}^{N-1}n\mathbf{n}_{(ij),n})L}\\&\times\psi_{[J]}^{(ij)}(\{\ddot{\boldsymbol{\rho}}_{(ij)}\},\{q_{(12)}\}),\end{aligned} \quad (36)$$

where $\{\mathbf{n}_{(ij)}\} = \{\mathbf{n}_{(ij),1},\mathbf{n}_{(ij),2},\ldots,\mathbf{n}_{(ij),N-1}\}$, and the set $\{\mathbf{n}_{(ij)}\}$ may be related to $\{\mathbf{n}_{(12)}\}$ by relabeling $1\leftrightarrow i$ and $2\leftrightarrow j$. The set $\{\ddot{\boldsymbol{\rho}}_{(ij)}\}$ is defined by

$$\ddot{\boldsymbol{\rho}}_{(ij),n} = \boldsymbol{\rho}_{(ij),n} + \sqrt{\frac{2}{n(n+1)}}\sum_{k=1}^{n}k\mathbf{n}_{(ij),k}L, \quad (\mathbf{n}_{(ij),k}\in\mathbb{Z}^3). \quad (37)$$

The wave functions $\psi_{[J]}^{(ij)}$ are the solutions of infinite-volume Schrödinger equations,

$$\begin{aligned}&(\sigma^2-\hat{T}_{\rho})\psi_{[J]}^{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\})\\&\quad= mV_{(ij)}(\boldsymbol{\rho}_{(ij),1})\psi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}),\end{aligned} \quad (38)$$

and the total infinite-volume N-body wave function is given by $\psi_{[J]} = \psi_{[J]}^{(0)} + \sum_{(i<j)=1}^{N}\psi_{[J]}^{(ij)}$, where $\psi_{[J]}^{(0)}$ refers to the incoming free wave.

After removing the center-of-mass motion, the determinant conditions are now given by

$$\det\left[\langle\phi_{[J']}|\hat{V}_{(ij)}(|\chi_{[J]}^{(ij)}\rangle - |\phi_{[J]}\rangle)\right] = 0, \quad (39)$$

where

$$\begin{aligned}\chi_{[J]}^{(ij)}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) = &\sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3} e^{i\frac{\mathbf{P}}{N}\cdot(\sum_{n=2}^{N-1}n\mathbf{n}_{(ij),n})L}\\&\times\psi_{[J]}(\Gamma^{(12),(ij)}\{\overline{\ddot{\boldsymbol{\rho}}_{(ij)}}\},\{q_{(12)}\}).\end{aligned} \quad (40)$$

The set $\overline{\{\mathbf{n}_{(ij)}\}}$ refers to $\{\mathbf{n}_{(ij),2},\mathbf{n}_{(ij),3},\ldots,\mathbf{n}_{(ij),N-1}\}$ which is a subset of $\{\mathbf{n}_{(ij)}\}$ by excluding element $\mathbf{n}_{(ij),1}$. The set $\{\overline{\ddot{\boldsymbol{\rho}}_{(ij)}}\}$ is defined by

$$\overline{\ddot{\boldsymbol{\rho}}_{(ij),n}} = \boldsymbol{\rho}_{(ij),n} + \sqrt{\frac{2}{n(n+1)}}\sum_{k=2}^{n}k\mathbf{n}_{(ij),k}L, \quad (\mathbf{n}_{(ij),k}\in\mathbb{Z}^3). \quad (41)$$

Noting the invariance of set $\{n_{(ij)}\}$, we are able to write $\phi_{[J]}$ in a similar way as Eq. (40),

$$\begin{aligned}\phi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) = &\sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3} e^{i\frac{\mathbf{P}}{N}\cdot(\sum_{n=1}^{N-1}n\mathbf{n}_{(ij),n})L}\\&\times\psi_{[J]}(\Gamma^{(12),(ij)}\{\ddot{\boldsymbol{\rho}}_{(ij)}\},\{q_{(12)}\}),\end{aligned} \quad (42)$$

which is equivalent to Eq. (24). Hence, the relation between $\phi_{[J]}$ and $\chi_{[J]}^{(ij)}$ can be made more clear,

$$\begin{aligned}\phi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) = &\sum_{\mathbf{n}_{(ij),1}\in\mathbb{Z}^3} e^{i\frac{\mathbf{P}}{N}\mathbf{n}_{(ij),1}L}\\&\times\chi_{[J]}^{(ij)}(\Gamma^{(12),(ij)}\{\tilde{\boldsymbol{\rho}}_{(ij)}\},\{q_{(12)}\}),\end{aligned} \quad (43)$$

where the nth element of $\{\tilde{\boldsymbol{\rho}}_{(ij)}\}$ is given by

$$\tilde{\boldsymbol{\rho}}_{(ij),n} = \boldsymbol{\rho}_{(ij),n} + \mathbf{n}_{(ij),1}L, \quad (\mathbf{n}_{(ij),1}\in\mathbb{Z}^3), \quad (44)$$

and $\{\ddot{\boldsymbol{\rho}}_{(ij)}\} = \{\bar{\ddot{\boldsymbol{\rho}}}_{(ij)}\} + \{\tilde{\boldsymbol{\rho}}_{(ij)}\}$.

D. Relation to the two-body Lüscher formula

In the simplest case $N = 2$, there is only one relative coordinate and relative momentum so that the particle index can be dropped, and in what follows they are denoted by $\mathbf{r}$ and $\mathbf{q}$, respectively. Notice that $\chi_{[J]}^{(ij)}$ is now reduced to $\psi_{[J]}$ for the two-body system. Therefore, the determinant condition in Eq. (39) is given by

$$\det\left[\langle\phi_{[J']}|\hat{V}(|\psi_{[J]}\rangle - |\phi_{[J]}\rangle)\right] = 0, \quad (45)$$

where $[J] = JM$ stands for quantum numbers of a specific partial wave, and

$$\phi_{[J]}(\mathbf{r},q)=\sum_{\mathbf{n}\in\mathbb{Z}^3}e^{i\frac{\mathbf{p}}{2}\cdot\mathbf{n}L}\psi_{[J]}(\mathbf{r}+\mathbf{n}L,q). \tag{46}$$

Assuming the potential has a finite range, $V(r)=0$ for $R<r<L$, in the region outside of the potential the infinite-volume wave function has the form

$$\begin{aligned}&\psi_{[J]}(\mathbf{r},q)\overset{r>R}{=}\psi^{(\mathrm{out})}_{[J]}(\mathbf{r},q),\\&\psi^{(\mathrm{out})}_{[J]}(\mathbf{r},q)=(4\pi)i^JY_{[J]}(\mathbf{r})[j_J(qr)+it_J(q)h^{(+)}_J(qr)],\end{aligned} \tag{47}$$

where t_J is the partial-wave two-body scattering amplitude, and t_J is normalized by the unitarity relation, $\mathrm{Im}\,[1/t_J]=-1$. Inside the potential region, the wave function is given by the solution of the Schrödinger equation, and is denoted by $\psi^{(in)}_{[J]}(\mathbf{r},q)$ from now on. The matrix element of the determinant condition (45) is given by

$$\int_{r<R}d\mathbf{r}\phi^*_{[J']}(\mathbf{r},q)V(r)[\psi^{(in)}_{[J]}(\mathbf{r},q)-\phi_{[J]}(\mathbf{r},q)]. \tag{48}$$

Using the fact that

$$\begin{aligned}\phi_{[J]}(\mathbf{r},q)&\overset{r\le R}{=}\psi^{(in)}_{[J]}(\mathbf{r},q)-\psi^{(out)}_{[J]}(\mathbf{r},q)\\&+(4\pi)i^Jit_J(q)\sum_{\mathbf{n}\in\mathbb{Z}^3}e^{i\frac{\mathbf{p}}{2}\cdot\mathbf{n}L}Y_{[J]}(\mathbf{r}+\mathbf{n}L)h^{(+)}_J(q|\mathbf{r}+\mathbf{n}L|)\end{aligned} \tag{49}$$

and the relation

$$\begin{aligned}&\sum_{\mathbf{n}\in\mathbb{Z}^3}e^{i\frac{\mathbf{p}}{2}\cdot\mathbf{n}L}Y_{[J]}(\mathbf{r}+\mathbf{n}L)h^{(+)}_J(q|\mathbf{r}+\mathbf{n}L|)\\&=\sum_{[j]}Y_{[j]}(\mathbf{r})[\delta_{[J],[j]}in_J(qr)-i\mathcal{M}^{(\frac{\mathbf{p}}{2})}_{[J],[j]}(q)j_j(qr)],\end{aligned} \tag{50}$$

[derived in Eqs. (B1) and (B3) in Ref. [44]] for the expansion coefficient function of the finite-volume two-body Green's function $\mathcal{M}^{(\frac{\mathbf{p}}{2})}_{[J],[j]}$, we find

$$\begin{aligned}&\langle\phi_{[J']}|\hat{V}(|\psi_{[J]}\rangle-|\phi_{[J]}\rangle)\\&=\sum_{[j]}\left[\int_{r<R}d\mathbf{r}\phi^*_{[J']}(\mathbf{r},q)V(r)j_j(qr)Y_{[j]}(\mathbf{r})\right]\\&\quad\times(4\pi)i^J[\delta_{[J],[j]}(1+it_J(q))-t_J(q)\mathcal{M}^{(\frac{\mathbf{p}}{2})}_{[J],[j]}(q)].\end{aligned} \tag{51}$$

Therefore, the determinant condition for the two-body problem (45) yields Lüscher's formula,

$$\det\left[\delta_{[J],[j]}\left(\frac{1}{t_J(q)}+i\right)-\mathcal{M}^{(\frac{\mathbf{p}}{2})}_{[J],[j]}(q)\right]=0. \tag{52}$$

Hence, the variational approach to the finite-volume few-body system is consistent with the Lüscher approach.

E. Effective two-body formalism

In this section we would like to show that the N-body quantization conditions may be recast in a similar form as the two-body quantization condition in Eq. (45).

Before proceeding to the N-body interaction, let us first rewrite the two-body quantization condition of Eq. (45) by using the periodicity of the finite-volume wave function. We find

$$\phi^*_{[J']}(\mathbf{r},q)\phi_{[J]}(\mathbf{r},q)=\sum_{\mathbf{n}\in\mathbb{Z}^3}\phi^*_{[J']}(\mathbf{r}+\mathbf{n}L,q)\psi_{[J]}(\mathbf{r}+\mathbf{n}L,q). \tag{53}$$

Therefore, the two-body quantization condition (45) may be expressed as

$$\det\left[\int d\mathbf{r}V(r)\left[\Omega_{[J'],[J]}(\mathbf{r},q)-\sum_{\mathbf{n}\in\mathbb{Z}^3}\Omega_{[J'],[J]}(\mathbf{r}+\mathbf{n}L,q)\right]\right]=0, \tag{54}$$

where $\Omega_{[J'],[J]}(\mathbf{r},q)=\phi^*_{[J']}(\mathbf{r},q)\psi_{[J]}(\mathbf{r},q)$.

Next, for the N-body problem we revisit the determinant condition in the (ij) channel in a explicit format,

$$\begin{aligned}&\det\Bigg[\int\prod_{n=1}^{N-1}d\boldsymbol{\rho}_{(ij),n}\phi^*_{[J']}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})mV_{(ij)}(\boldsymbol{\rho}_{(ij),1})\\&\quad\times[\chi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})-\phi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})]\Bigg]=0,\end{aligned} \tag{55}$$

where $\chi^{(ij)}_{[J]}$ and $\phi_{[J]}$ are given by Eqs. (40) and (43), respectively. Because of the relation between $\chi^{(ij)}_{[J]}$ and $\phi_{[J]}$ given in Eq. (43), similarly to Eq. (54), it is advantageous to introduce the quantity $\Omega^{(ij)}(\boldsymbol{\rho}_{(ij),1})$ again by integrating out all of the relative coordinates except for $\boldsymbol{\rho}_{(ij),1}$,

$$\begin{aligned}&\Omega^{(ij)}_{[J'],[J]}(\boldsymbol{\rho}_{(ij),1},\{q_{(12)}\})\\&=\int\prod_{n=2}^{N-1}d\boldsymbol{\rho}_{(ij),n}\phi^*_{[J']}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})\chi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}).\end{aligned} \tag{56}$$

Using the periodicity of the wave function ϕ, the quantization conditions (55) now have a form that resembles the two-body quantization condition given in Eq. (54),

$$\begin{aligned}&\det\Bigg\{\int d\boldsymbol{\rho}_{(ij),1}V_{(ij)}(\boldsymbol{\rho}_{(ij),1})\Bigg[\Omega^{(ij)}_{[J'],[J]}(\boldsymbol{\rho}_{(ij),1},\{q_{(12)}\})\\&\quad-\sum_{\mathbf{n}\in\mathbb{Z}^3}\Omega^{(ij)}_{[J'],[J]}(\boldsymbol{\rho}_{(ij),1}+\mathbf{n}L,\{q_{(12)}\})\Bigg]\Bigg\}=0.\end{aligned} \tag{57}$$

When all of the interactions $V_{(i'j')}$ except the interaction between the ith and jth particle are turned off, clearly the quantization condition in the (ij) channel in Eq. (57) is thus reduced to the two-body quantization condition given in Eq. (54).

III. DISCUSSION AND CONCLUSION

A. Resemblance to the isobar model

In the past, isobar models [54–67] have been a useful tool to describe few-body interactions, in which the few-body interaction is treated by taking into account all possible recombinations of two-body subsystems. The two-body subsystems are considered as the dominant contribution compared to the three-body force, and the few-body interaction correction to the two-body subsystem is generated by rescattering between all possible pairs. In order to show the similarity of this approach to the isobar formulation [54–67], we consider a special case, i.e., a three-body system with two light spinless particles and one infinitely heavy spinless particle stationed at the origin. The heavy particle is labeled as the third particle. The system may be described by

$$\left[E+\frac{1}{2m}\sum_{i=1}^{2}\nabla_{\mathbf{r}_i}^2-\sum_{i=1}^{2}V^{(L)}(r_i)+U^{(L)}(\mathbf{r}_1-\mathbf{r}_2)\right]\times\phi(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2)=0, \tag{58}$$

where $V^{(L)}$ represents the interactions between the heavy particle and one of the light particles, and $U^{(L)}$ stands for the interaction between the two light particles. Again, we use the superscript (L) to identify the periodic potential in finite volume. We also assume that $U^{(L)}$ is a weak interaction, so that the interaction between the two light particles is treated as a perturbation, which serves the purpose of this work. Therefore, the corresponding infinite-volume wave function must have the form

$$\psi(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2)=\psi(\mathbf{r}_1;\mathbf{q}_1)\psi(\mathbf{r}_2;\mathbf{q}_2)+\delta\psi(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2), \tag{59}$$

where the first term is the solution of the system with zero interaction between two lights particles. The second term, $\delta\psi$, can be considered as a perturbative contribution when the weak U potential is turned on. The two-body infinite-volume wave function $\psi(\mathbf{r}_i;\mathbf{q}_i)$ is given by the solution of

$$\left[\frac{q_i^2+\nabla_{\mathbf{r}_i}^2}{2m}-V(r_i)\right]\psi(\mathbf{r}_i;\mathbf{q}_i)=0, \tag{60}$$

with $E=q_1^2/2m+q_2^2/2m$. Following the argument provided in previous sections, the finite-volume wave function is constructed from the infinite-volume wave function. The two ingredients ϕ and $\chi^{(1/2)}$ of the secular equations thus also have the forms

$$\phi(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2)=\phi(\mathbf{r}_1;\mathbf{q}_1)\phi(\mathbf{r}_2;\mathbf{q}_2)+\delta\phi(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2) \tag{61}$$

and

$$\begin{aligned}&\chi^{(1)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2)\\&\quad=\psi(\mathbf{r}_1;\mathbf{q}_1)\phi(\mathbf{r}_2;\mathbf{q}_2)+\delta\chi^{(1)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2),\\&\chi^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2)\\&\quad=\phi(\mathbf{r}_1;\mathbf{q}_1)\psi(\mathbf{r}_2;\mathbf{q}_2)+\delta\chi^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{q}_1,\mathbf{q}_2),\end{aligned} \tag{62}$$

where $\phi(\mathbf{r}_i;\mathbf{q}_i)=\sum_{\mathbf{n}_i\in\mathbb{Z}^3}\psi(\mathbf{r}_i+\mathbf{n}_iL;\mathbf{q}_i)$. The construction of $\delta\phi$ and $\delta\chi^{(i)}$ can also be performed based on $\delta\psi$, but the specific expressions are not crucial for our brief discussion. The two secular equations may also be treated as a perturbation; for example, for the channel (13) we obtain

$$\sum_{[J]}\left[\int d\mathbf{r}_1\left(\int d\mathbf{r}_2\phi^*_{[J']}(\mathbf{r}_1,\mathbf{r}_2;q_1,q_2)\phi_{[L_2]}(\mathbf{r}_2;q_2)\right)V(r_1)\times[\psi_{[L_1]}(\mathbf{r}_1;q_1)-\phi_{[L_1]}(\mathbf{r}_1;q_1)]+\delta U_{[J'],[J]}\right]c_{[J]}=0, \tag{63}$$

where δU stands for the perturbative contribution to the secular equation from the weak U potential. The three-body quantum number set $[J]$ is constructed from two-body quantum numbers $[L_i]$ by $[J]=[L_1]\otimes[L_2]$. In the limit of $\delta U\to 0$, two secular equations yield two independent two-body quantization conditions,

$$\det\left[\delta_{[L_i],[l_i]}\left(\frac{1}{t_{L_i}(q_i)}+i\right)-\mathcal{M}^{(\mathbf{0})}_{[L_i],[l_i]}(q_i)\right]=0,\quad i=1,2, \tag{64}$$

and both q_i's are quantized independently according to the corresponding Lüscher formula. The three-body correction with a weak U potential may be obtained by perturbation. In the current approach, the physical picture is presented in a way that is similar to the three-body rescattering effect corrected isobar model [54–66]. That is to say that the three-body system considered in this subsection can be treated as two two-body isobar subsystems [(13) and (23)], which yield two independent two-body quantization conditions for $q_{1,2}$. The three-body rescattering correction to isobar subsystems produces an energy shift on quantized two-body energies: $q_1^2/2m+q_2^2/2m+\delta E$.

B. Summary

In this work, we proposed a variational approach to the finite-volume N-body problem. In order to fulfill the periodic boundary conditions, the trial wave functions were constructed by linear superposition of all of the solutions of the infinite-volume wave functions centered at each image of the periodic cubic boxes, given that the infinite-volume wave functions may be obtained by standard methods. In this approach, the short-range N-body dynamics is local to each box and long-range correlations correspond to particles traveling through the entire periodic structure of the lattice. In other words, the short-range dynamics are determined by infinite-volume wave functions, and finite-volume wave functions control the long-range correlations that eventually yield the discrete energy spectra because of the periodic structure of the lattice. No explicit analytic expressions between discrete lattice eigenvalues and the scattering amplitude (such as those present in the two-body Lüscher formula) can be given by the variational approach for $N > 2$. Instead, the discrete energy spectra and N-body scattering amplitudes are linked in a rather complicated way. Nevertheless, the method has potential advantages for systems with $N \gg 2$. By combining the variational approach with the Faddeev approach, the $N(N-1)/2$ quantization conditions were ultimately obtained. In the end, these quantization conditions can be expressed in a way that resembles rescattering in the isobar approach. The overall rescattering corrections can also be written as a collective effect by integrating out the of degrees of freedom other then as selected two-body subsystem.

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APPENDIX A: VARIATIONAL PRINCIPLE

For a complex system, most calculations are based on approximate methods: the variational principle is one of the most commonly used approaches. In this section, we briefly outline the main idea of the variational principle as the approximate solution to a general quantum system [46,47], which satisfies the Schrödinger equation,

$$\hat{H}\Psi\rangle = E|\Psi\rangle. \tag{A1}$$

The trial wave function Ψ may be expanded in terms of a set of basis functions that satisfy certain boundary conditions or symmetries of the system,

$$|\Psi\rangle = \sum_n c_n |n\rangle. \tag{A2}$$

The solution of the Schrödinger equation is thus given by the variational principle:

$$\frac{\partial \Lambda}{\partial c_n^*} = 0, \tag{A3}$$

where

$$\Lambda = \sum_{n,n'} c_n^* \langle n|E - \hat{H}|n'\rangle c_{n'}. \tag{A4}$$

Thus, the variational principle yields secular equations,

$$\sum_{n'} [E\langle n|n'\rangle - \langle n|\hat{H}|n'\rangle] c_{n'} = 0, \tag{A5}$$

and the nontrivial solutions exist only if

$$\det\,[E\langle n|n'\rangle - \langle n|\hat{H}|n'\rangle] = 0. \tag{A6}$$

APPENDIX B: N-BODY FADDEEV EQUATIONS IN INFINITE VOLUME

In this Appendix, for completeness we give a brief summary of the Faddeev equations for the general interaction of N particles. The nonrelativistic N-body dynamics is described by the Schrödinger equation,

$$(E - \hat{T} - \hat{V})|\Psi\rangle = 0. \tag{B1}$$

Assuming only pairwise interactions among particles, $\hat{V} = \sum_{(i<j)=1}^{N} \hat{V}_{(ij)}$, the scattering solution of an N-body wave function is normally written as the sum of multiple terms [48–51],

$$|\Psi\rangle = |\Psi^{(0)}\rangle + \sum_{(i<j)=1}^{N} |\Psi^{(ij)}\rangle, \tag{B2}$$

where $\Psi^{(0)}$ stands for the free initial incoming wave of the N-particle state, $(E - \hat{T})|\Psi^{(0)}\rangle = 0$, and $\Psi^{(ij)}$ satisfies the equation

$$(E - \hat{T})|\Psi^{(ij)}\rangle = \hat{V}_{(ij)}|\Psi\rangle. \tag{B3}$$

In this way, the N-body Schrödinger equation is turned into $N(N-1)/2$ coupled equations,

$$|\Psi^{(ij)}\rangle = \hat{G}_{(ij)}\hat{V}_{(ij)}\left[|\Psi^{(0)}\rangle + \sum_{(i'<j')=1}^{N;(i'j'\neq ij)} |\Psi^{(i'j')}\rangle\right], \quad \text{(B4)}$$

where the Green's function operator $\hat{G}_{(ij)}$ is given by

$$\hat{G}_{(ij)} = (E - \hat{T} - \hat{V}_{(ij)} + i\epsilon)^{-1}. \quad \text{(B5)}$$

$\hat{G}_{(ij)}$ is related to the two-body scattering amplitude $\hat{t}_{ij}$ by

$$\hat{G}_{(ij)} = \hat{G}_{(0)}(1 - \hat{t}_{(ij)}\hat{G}_{(0)}), \quad \text{(B6)}$$

where $\hat{G}_{(0)} = (E - \hat{T} + i\epsilon)^{-1}$ stands for the free two-body Green's function.

The total N-body scattering amplitude $\hat{T}$ is

$$\hat{T}|\Psi^{(0)}\rangle = \sum_{(i<j)=1}^{N} \hat{T}_{(ij)}|\Psi^{(0)}\rangle = -\hat{V}|\Psi\rangle, \quad \text{(B7)}$$

where $\hat{T}_{(ij)}|\Psi^{(0)}\rangle = -\hat{V}_{(ij)}|\Psi\rangle$. Using the relation $\hat{V}_{(ij)}\hat{G}_{(ij)} = -\hat{t}_{(ij)}\hat{G}_{(0)}$ and Eq. (B4), we find that $\hat{T}_{(ij)}$ satisfy the coupled equations

$$\hat{T}_{(ij)} = \hat{t}_{(ij)} - \hat{t}_{(ij)}\hat{G}_{(0)} \sum_{(i'<j')=1}^{N;(i'j'\neq ij)} \hat{T}_{(i'j')}. \quad \text{(B8)}$$

$\hat{T}_{(ij)}$ and $|\Psi^{(ij)}\rangle$ are related by

$$|\Psi^{(ij)}\rangle = -\hat{G}_{(0)}\hat{T}_{(ij)}|\Psi^{(0)}\rangle. \quad \text{(B9)}$$

One of the advantages of the Faddeev approach is that it demonstrates the general relations between the subsystem amplitude and the N-body amplitude in a natural way [see Eq. (B8)], and the two-body amplitude is used as input for the N-body dynamics. In addition, the unitarity relation of the N-body scattering amplitude is also automatically guaranteed by the Faddeev equations.

APPENDIX C: SOLUTIONS OF THE N-BODY PROBLEM WITH δ-FUNCTION POTENTIALS

To give readers a concrete example of our proposed approach to the N-body finite-volume problem, in this Appendix we also include a specific example of short-range interactions between two particles with a δ-function potential.

1. Two-body interaction with δ-function potential

We consider two-particle scattering with a pairwise δ-function potential, assuming that all particles are spinless and have equal mass. The bare strength of the δ-function potential between the two particles is described by V_0. With the same convention as in Sec. II D, the infinite-volume wave function is given by the Lippmann-Schwinger equation,

$$\psi_{JM}(\mathbf{r}, q) = (4\pi)i^J j_J(qr)Y_{JM}(\mathbf{r}) + \int d\mathbf{r}' G_{(0)}(\mathbf{r}, \mathbf{r}'; q) m V_0 \delta(\mathbf{r}')\psi_{JM}(\mathbf{r}', q), \quad \text{(C1)}$$

where $G_{(0)}$ stands for the free two-body Green's function,

$$G_{(0)}(\mathbf{r}, \mathbf{r}'; q) = \int \frac{d\mathbf{q}'}{(2\pi)^3} \frac{e^{i\mathbf{q}'\cdot(\mathbf{r}-\mathbf{r}')}}{q^2 - \mathbf{q}'^2 + i\epsilon} = -\frac{q}{4\pi} i h_0^{(+)}(q|\mathbf{r} - \mathbf{r}'|). \quad \text{(C2)}$$

The two-body Lippmann-Schwinger equation (C1) has the solution

$$\psi_{JM}(\mathbf{r}, q) = (4\pi)i^J Y_{JM}(\mathbf{r})[j_J(qr) + \delta_{J,0} i t_0(q) h_0^{(+)}(qr)], \quad \text{(C3)}$$

where only the S wave contributes to the two-body scattering amplitude,

$$t_0(q) = -\frac{q}{\frac{4\pi}{mV_0} + iq h_0^{(+)}(qr)|_{r\to 0}}. \quad \text{(C4)}$$

It has been known that singular potentials, such as the δ-function potential, require regularization and renormalization two or higher dimensions [68]. Adopting the renormalization scheme proposed in Ref. [68], a renormalized strength of the δ-function potential V_R is introduced to absorb the divergent part of $h_0^{(+)}(qr)|_{r\to 0} = 1 - \frac{i}{qr}$, and the renormalized and bare strengths are related by

$$\frac{1}{mV_0} = \frac{1}{mV_R} - \frac{1}{4\pi r}\bigg|_{r\to 0}. \quad \text{(C5)}$$

In terms of the renormalized quantity, the S-wave two-body scattering amplitude now reads

$$t_0(q) = -\frac{q}{\frac{4\pi}{mV_R} + iq}, \quad \text{(C6)}$$

and the unitarity relation of the two-body scattering amplitude is guaranteed by $\mathrm{Im}[t_0^{-1}] = -1$.

In finite volume, based on the discussion given in Sec. II D, we find that

$$\psi_{JM}(\mathbf{r},q)-\phi_{JM}(\mathbf{r},q)=(4\pi)i^{J}\sum_{jm_j}j_j(qr)Y_{jm_j}(\mathbf{r}) \times[\delta_{[J],[j]}(1+\delta_{J,0}it_0(q)) -\delta_{J,0}t_0(q)\mathcal{M}^{(\frac{\mathbf{P}}{2})}_{[0],[j]}(q)]. \tag{C7}$$

The nontrivial solutions of the δ-function potential are given only by the S wave, which are determined by

$$\frac{1}{t_0(q)}+i=\mathcal{M}^{(\frac{\mathbf{P}}{2})}_{[0],[0]}(q). \tag{C8}$$

2. N-body interaction with a δ-function potential

a. The solution of the N-body interaction in infinite volume

We again consider a simple model with a short-range δ-function interaction, $V_{(ij)}(\mathbf{x}_i-\mathbf{x}_j)=V_0\delta(\boldsymbol{\rho}_{(ij),1})$. The solution of the N-body interaction may be obtained using the standard Faddeev approach [48–51]. For the scattering with a free N-particle incoming wave, the wave function may be expressed as the sum of $1+N(N-1)/2$ terms,

$$\psi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})=\psi^{(0)}_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) +\sum_{(i<j)=1}^{N}\psi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\}), \tag{C9}$$

where $\psi^{(0)}_{[J]}$ refers to the incoming free wave, and $\psi^{(ij)}_{[J]}$ is given by the Lippmann-Schwinger equation,

$$\psi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\}) =\int\prod_{n=1}^{N-1}d\boldsymbol{\rho}'_{(ij),n}G_{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{\boldsymbol{\rho}'_{(ij)}\};\sigma)mV_0\delta(\boldsymbol{\rho}'_{(ij),1}) \times\left[\psi^{(0)}_{[J]}(\{\boldsymbol{\rho}'_{(12)}\},\{q_{(12)}\}) +\sum_{(i'<j')=1}^{N;(i'j'\neq ij)}\psi^{(i'j')}_{[J]}(\{\boldsymbol{\rho}'_{(i'j')}\},\{q_{(12)}\})\right]. \tag{C10}$$

The Green's function $G_{(ij)}$ satisfies the equation

$$[\sigma^2-\hat{T}_\rho-mV_0\delta(\boldsymbol{\rho}_{(ij),1})]G_{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{\boldsymbol{\rho}'_{(ij)}\};\sigma) =\prod_{n=1}^{N-1}\delta(\boldsymbol{\rho}_{(ij),n}-\boldsymbol{\rho}'_{(ij),n}), \tag{C11}$$

and the solution of Eq. (C11) has the form

$$G_{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{\boldsymbol{\rho}'_{(ij)}\};\sigma) =\int\prod_{n=1}^{N-1}\frac{d\mathbf{q}'_{(ij),n}}{(2\pi)^3}e^{i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot(\boldsymbol{\rho}_{(ij),k}-\boldsymbol{\rho}'_{(ij),k})} \times\frac{\psi(\boldsymbol{\rho}_{(ij),1},\mathbf{q}'_{(ij),1})\psi^*(\boldsymbol{\rho}'_{(ij),1},\mathbf{q}'_{(ij),1})}{\sigma^2-\sum_{n=1}^{N-1}\mathbf{q}'^2_{(ij),n}+i\epsilon}, \tag{C12}$$

where the two-body wave function $\psi(\boldsymbol{\rho}_{(ij),1},\mathbf{q}'_{(ij),1})$ is given by

$$\psi(\boldsymbol{\rho}_{(ij),1},\mathbf{q}_{(ij),1}) =e^{i\mathbf{q}_{(ij),1}\cdot\boldsymbol{\rho}_{(ij),1}}+it_0(q_{(ij),1})h_0^{(+)}(q_{(ij),1}\rho_{(ij),1}). \tag{C13}$$

Using the expression for the two-body wave function in Eq. (C13), we find

$$G_{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{\boldsymbol{\rho}'_{(ij)}\};\sigma) =\int\prod_{n=2}^{N-1}\frac{d\mathbf{q}'_{(ij),n}}{(2\pi)^3}e^{i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot(\boldsymbol{\rho}_{(ij),k}-\boldsymbol{\rho}'_{(ij),k})} \times\left[-\frac{e^{i\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}|\boldsymbol{\rho}_{(ij),1}-\boldsymbol{\rho}'_{(ij),1}|}}{4\pi|\boldsymbol{\rho}_{(ij),1}-\boldsymbol{\rho}'_{(ij),1}|} -\frac{1}{4\pi}\frac{t_0(\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}})}{\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}} \times\frac{e^{i\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}(\rho_{(ij),1}+\rho'_{(ij),1})}}{\rho_{(ij),1}\rho'_{(ij),1}}\right]. \tag{C14}$$

With the renormalization relation given in Eq. (C5), we also find

$$G_{(ij)}(\{\boldsymbol{\rho}_{(ij)}\},\{\boldsymbol{\rho}'_{(ij)}\};\sigma)mV_0\delta(\boldsymbol{\rho}'_{(ij),1}) =\int\prod_{n=2}^{N-1}\frac{d\mathbf{q}'_{(ij),n}}{(2\pi)^3}e^{i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot(\boldsymbol{\rho}_{(ij),k}-\boldsymbol{\rho}'_{(ij),k})} \times it_0\left(\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}\right) \times h_0^{(+)}\left(\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}\rho_{(ij),1}\right)\delta(\boldsymbol{\rho}'_{(ij),1}). \tag{C15}$$

Therefore, we can rewrite $\psi^{(ij)}_{[J]}$ as

$$\psi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\})$$
$$= \int \prod_{n=2}^{N-1} \frac{d\mathbf{q}'_{(ij),n}}{(2\pi)^3} h_0^{(+)}\left(\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}\rho_{(ij),1}\right)$$
$$\times it_0\left(\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}\right) e^{i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot\boldsymbol{\rho}_{(ij),k}}$$
$$\times \int \prod_{n=1}^{N-1} d\boldsymbol{\rho}'_{(ij),n} e^{-i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot\boldsymbol{\rho}'_{(ij),k}}\delta(\boldsymbol{\rho}'_{(ij),1})$$
$$\times \left[\psi^{(0)}_{[J]}(\{\boldsymbol{\rho}'_{(12)}\},\{q_{(12)}\}) + \sum_{(i'<j')=0}^{N;(i'j'\neq ij)} \psi^{(i'j')}_{[J]}(\{\boldsymbol{\rho}'_{(i'j')}\},\{q_{(12)}\})\right]. \quad \text{(C16)}$$

Next, we introduce the scattering amplitudes $T^{(ij)}_{[J]}$ as

$$T^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\})$$
$$= -\int \prod_{n=1}^{N-1} d\boldsymbol{\rho}'_{(ij),n} e^{-i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot\boldsymbol{\rho}'_{(ij),k}}$$
$$\times mV_0\delta(\boldsymbol{\rho}'_{(ij),1})\psi_{[J]}(\{\boldsymbol{\rho}'_{(ij)}\},\{q_{(12)}\}), \quad \text{(C17)}$$

where $\overline{\{\mathbf{q}'_{(ij)}\}} = \{\mathbf{q}'_{(ij),2},\mathbf{q}'_{(ij),3},\ldots,\mathbf{q}'_{(ij),N-1}\}$. Using Eqs. (C16) and (C5), we find that the wave function $\psi^{(ij)}_{[J]}$ and $T^{(ij)}_{[J]}$ are related by

$$\psi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\})$$
$$= \int \prod_{n=2}^{N-1} \frac{d\mathbf{q}'_{(ij),n}}{(2\pi)^3} e^{i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot\boldsymbol{\rho}_{(ij),k}}$$
$$\times ih_0^{(+)}\left(\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}\rho_{(ij),1}\right)$$
$$\times \frac{\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}}{4\pi} T^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\}). \quad \text{(C18)}$$

The $T^{(ij)}_{[J]}$ amplitudes are given by the solutions of coupled integral equations,

$$T^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\}) - \mathbb{T}^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\})$$
$$= \frac{4\pi i t_0\left(\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}\right)}{\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}}$$
$$\times i\int \prod_{n=1}^{N-1} \frac{d\mathbf{q}''_{(ij),n}}{(2\pi)^3} \frac{\prod_{k=2}^{N-1}(2\pi)^3\delta(\mathbf{q}'_{(ij),k} - \mathbf{q}''_{(ij),k})}{\sigma^2 - \sum_{n=1}^{N-1}\mathbf{q}''^2_{(ij),n} + i\epsilon}$$
$$\times \sum_{(i'<j')=1}^{N;(i'j'\neq ij)} T^{(i'j')}_{[J]}(\overline{\{\mathbf{q}''_{(i'j')}\}},\{q_{(12)}\}), \quad \text{(C19)}$$

where

$$\mathbb{T}^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\})$$
$$= \frac{4\pi t_0\left(\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}\right)}{\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}} \int \prod_{n=1}^{N-1} d\boldsymbol{\rho}_{(ij),n}\delta(\boldsymbol{\rho}_{(ij),1})$$
$$\times e^{-i\sum_{k=2}^{N-1}\mathbf{q}'_{(ij),k}\cdot\boldsymbol{\rho}_{(ij),k}}\psi^{(0)}_{[J]}(\{\boldsymbol{\rho}_{(ij}\},\{q_{(12)}\}). \quad \text{(C20)}$$

The total N-body scattering amplitude is given by $T_{[J]} = \sum_{(i<j)=1}^{N} T^{(ij)}_{[J]}$.

b. Construction of finite-volume N-body wave functions

Given the solutions of the infinite-volume wave function $\psi^{(ij)}$, the finite-volume wave function $\phi^{(ij)}$ is obtained using Eq. (36),

$$\phi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\})$$
$$= \sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3} e^{i\frac{\mathbf{P}}{N}\cdot(\sum_{k=1}^{N-1} k\mathbf{n}_{(ij),k})L} \int \prod_{n=2}^{N-1} \frac{d\mathbf{q}'_{(ij),n}}{(2\pi)^3}$$
$$\times e^{i\sum_{n'=2}^{N-1}\mathbf{q}'_{(ij),n'}\cdot(\boldsymbol{\rho}_{(ij),n'} + \sqrt{\frac{2}{n'(n'+1)}}\sum_{k=1}^{n'} k\mathbf{n}_{(ij),k}L)}$$
$$\times ih_0^{(+)}\left(\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}|\boldsymbol{\rho}_{(ij),1} + \mathbf{n}_{(ij),1}L|\right)$$
$$\times \frac{\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}}{4\pi} T^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\}). \quad \text{(C21)}$$

Using the fact that

$$\sum_{n'=2}^{N-1} \mathbf{q}'_{(ij),n'} \cdot \left(\frac{\sum_{k=2}^{n'} k\mathbf{n}'_{(ij),k}}{\sqrt{n'(n'+1)}}\right)L$$
$$= \sum_{k=2}^{N-1}\left(\sum_{n'=k}^{N-1} \frac{\mathbf{q}'_{(ij),n'}}{\sqrt{n'(n'+1)}}\right)\cdot(k\mathbf{n}_{(ij),k})L \quad \text{(C22)}$$

and the Poisson summation formula, we find

$$\phi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\}) = \sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3}\int\prod_{n=2}^{N-1}\frac{d\mathbf{q}'_{(ij),n}}{L^3}e^{i\sum_{n'=2}^{N-1}\mathbf{q}'_{(ij),n'}\cdot\boldsymbol{\rho}_{(ij),n'}}\sum_{k=2}^{N-1}\delta\left(\frac{k\mathbf{P}}{N}+\sum_{n'=k}^{N-1}k\sqrt{\frac{2}{n'(n'+1)}}\mathbf{q}'_{(ij),n'}-\frac{2\pi}{L}\mathbf{n}_{(ij),k}\right)$$
$$\times\sum_{\mathbf{n}_{(ij),1}\in\mathbb{Z}^3}e^{i(\frac{\mathbf{P}}{N}+\sum_{n'=2}^{N-1}\sqrt{\frac{2}{n'(n'+1)}}\mathbf{q}'_{(ij),n'})\cdot\mathbf{n}_{(ij),1}L}ih_0^{(+)}\left(\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}|\boldsymbol{\rho}_{(ij),1}+\mathbf{n}_{(ij),1}L|\right)$$
$$\times\frac{\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}}{4\pi}T^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\}). \tag{C23}$$

The total finite-volume wave function is given by $\phi_{[J]}=\sum_{(i<j)=1}^{N}\phi^{(ij)}_{[J]}$.

Similarly, using Eqs. (40) and (C18), we also find

$$\chi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) = \chi^{(0),(ij)}_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) + \sum_{(i'<j')=1}^{N}\chi^{(i'j'),(ij)}_{[J]}(\{\boldsymbol{\rho}_{(i'j')}\},\{q_{(12)}\}), \tag{C24}$$

where

$$\chi^{(0),(ij)}_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) = \sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3}e^{i\frac{\mathbf{P}}{N}\cdot(\sum_{k=2}^{N-1}k\mathbf{n}_{(ij),k})L}\psi^{(0)}_{[J]}(\Gamma^{(12),(ij)}\{\overline{\boldsymbol{\rho}_{(ij)}}\},\{q_{(12)}\}), \tag{C25}$$

$$\chi^{(ij),(ij)}_{[J]}(\{\boldsymbol{\rho}_{(ij)}\},\{q_{(12)}\}) = \sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3}\int\prod_{n=2}^{N-1}\frac{d\mathbf{q}'_{(ij),n}}{L^3}e^{i\sum_{n'=2}^{N-1}\mathbf{q}'_{(ij),n'}\cdot\boldsymbol{\rho}_{(ij),n'}}\sum_{k=2}^{N-1}\delta\left(\frac{k\mathbf{P}}{N}+\sum_{n'=k}^{N-1}k\sqrt{\frac{2}{n'(n'+1)}}\mathbf{q}'_{(ij),n'}-\frac{2\pi}{L}\mathbf{n}_{(ij),k}\right)$$
$$\times ih_0^{(+)}\left(\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}\rho_{(ij),1}\right)\frac{\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(ij),n}}}{4\pi}T^{(ij)}_{[J]}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\}), \tag{C26}$$

and

$$\chi^{(i'j'),(ij)}_{[J]}(\{\boldsymbol{\rho}_{(i'j')}\},\{q_{(12)}\})\overset{(i'j')\neq(ij)}{=}\int\prod_{n=2}^{N-1}\frac{d\mathbf{q}'_{(i'j'),n}}{(2\pi)^3}e^{i\sum_{k=2}^{N-1}\mathbf{q}'_{(i'j'),k}\cdot\boldsymbol{\rho}_{(i'j'),k}}$$
$$\times\sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3}e^{i\sum_{k=2}^{N-1}(\frac{\mathbf{P}}{N}+\sum_{n=k}^{N-1}\sqrt{\frac{2}{n(n+1)}}(\sum_{n'=2}^{N-1}\mathbf{q}'_{(i'j'),n'}\Gamma^{(i'j'),(ij)}_{n',n}))\cdot(k\mathbf{n}_{(ij),k})L}$$
$$\times ih_0^{(+)}\left(\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(i'j'),n}}|\boldsymbol{\rho}_{(i'j'),1}+\sum_{n=2}^{N-1}\Gamma^{(i'j'),(ij)}_{1,n}\sqrt{\frac{2}{n(n+1)}}\sum_{k=2}^{n}k\mathbf{n}_{(ij),k}L|\right)$$
$$\times\frac{\sqrt{\sigma^2-\sum_{n=2}^{N-1}\mathbf{q}'^2_{(i'j'),n}}}{4\pi}T^{(i'j')}_{[J]}(\overline{\{\mathbf{q}'_{(i'j')}\}},\{q_{(12)}\}). \tag{C27}$$

c. *N*-body secular equations

Given all of the ingredients of the finite-volume wave functions from Eqs. (C23)–(C27), the discrete energy spectra are thus given by $N(N-1)/2$ secular equations,

$$\det\left[\int\prod_{n=1}^{N-1}d\boldsymbol{\rho}_{(ij),n}\phi^*_{[J']}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})mV_0\delta(\boldsymbol{\rho}_{(ij),1})[\chi^{(ij)}_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})-\phi_{[J]}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\})]\right]=0. \tag{C28}$$

As $\boldsymbol{\rho}_{(ij),1} \to \mathbf{0}$, both $\chi^{(ij),(ij)}_{[J]}$ and $\phi^{(ij)}_{[J]}$ appear to have the same ultraviolet-divergent behavior because of the spherical Hankel function, $h^{(+)}_0(\sqrt{\sigma^2 - \sum_{n=2}^{N-1} \mathbf{q}'^2_{(ij),n}}\rho_{(ij),1}) \sim \frac{1}{\rho_{(ij),1}}$; thus, the subtraction of two terms is completely free from ultraviolet divergence. The ultraviolet divergence appears in $\phi^*_{[J']}$ as well. Since V_0 is a bare parameter, in order to remove the ultraviolet divergence a renormalization of the energy is required. Given the fact that

$$mV_0 i h^{(+)}_0(qr) \xrightarrow{r\to 0} \frac{4\pi}{q} - \frac{mV_0}{t_0(q)}, \tag{C29}$$

after the energy shift $E \to E + \delta E$ the divergent contribution of the secular equation can be completely canceled out by the counterterm δE. Thus the renormalized quantity $\phi^*_{[J']} mV_0$ is given by

$$\phi^*_{[J']}(\{\boldsymbol{\rho}_{(12)}\},\{q_{(12)}\}) mV_0 \xrightarrow{\boldsymbol{\rho}_{(ij),1}\to\mathbf{0}} \sum_{\{\mathbf{n}_{(ij)}\}\in\mathbb{Z}^3} \int \prod_{n=2}^{N-1} \frac{d\mathbf{q}'_{(ij),n}}{L^3} e^{-i\sum_{n'=2}^{N-1} \mathbf{q}'_{(ij),n'}\cdot\boldsymbol{\rho}_{(ij),n'}} \sum_{k=2}^{N-1} \delta\left(\frac{k\mathbf{P}}{N} + \sum_{n'=k}^{N-1} k\sqrt{\frac{2}{n'(n'+1)}}\mathbf{q}'_{(ij),n'} - \frac{2\pi}{L}\mathbf{n}_{(ij),k}\right)$$
$$\times T^{(ij)*}_{[J']}(\overline{\{\mathbf{q}'_{(ij)}\}},\{q_{(12)}\}). \tag{C30}$$

3. Three-body interaction with a δ-function potential

The three-body solutions can be derived from the N-body results given in Appendix C 2 by setting $N = 3$. Since the number of particles in the three-body problem is still manageable, we use the shorthand notation

$$\mathbf{r}_{(ij)} = \boldsymbol{\rho}_{(ij),1}, \qquad \mathbf{r}_k = \boldsymbol{\rho}_{(ij),2}, \qquad \mathbf{q}_{(ij)} = \mathbf{q}_{(ij),1}, \qquad \mathbf{q}_k = \mathbf{q}_{(ij),2}, \qquad i \neq j \neq k. \tag{C31}$$

The different sets are related by linear transformations, such as

$$\mathbf{r}_{(13)} = \frac{\mathbf{r}_{(12)} + \sqrt{3}\mathbf{r}_3}{2}, \qquad \mathbf{r}_2 = \frac{\sqrt{3}\mathbf{r}_{(12)} - \mathbf{r}_3}{2}, \qquad \mathbf{q}_{(13)} = \frac{\mathbf{q}_{(12)} + \sqrt{3}\mathbf{q}_3}{2}, \qquad \mathbf{q}_2 = \frac{\sqrt{3}\mathbf{q}_{(12)} - \mathbf{q}_3}{2}. \tag{C32}$$

According to Eq. (C18), the infinite-volume wave function $\psi^{(ij)}_{[J]}$ is given by

$$\psi^{(ij)}_{[J]}(\mathbf{r}_{(ij)},\mathbf{r}_k;q_{(12)},q_3) = \int \frac{d\mathbf{q}}{(2\pi)^3} i h^{(+)}_0\left(\sqrt{\sigma^2 - \mathbf{q}^2} r_{(ij)}\right) e^{i\mathbf{q}\cdot\mathbf{r}_k} \frac{\sqrt{\sigma^2 - \mathbf{q}^2}}{4\pi} T^{(ij)}_{[J]}(\mathbf{q};q_{(12)},q_3), \tag{C33}$$

where the solutions of the T amplitude are given by

$$T^{(ij)}(\mathbf{q};\mathbf{q}_{(12)},\mathbf{q}_3) - \mathbb{T}^{(ij)}(\mathbf{q};\mathbf{q}_{(12)},\mathbf{q}_3) = \frac{4\pi i t_0\left(\sqrt{\sigma^2 - \mathbf{q}^2}\right)}{\sqrt{\sigma^2 - \mathbf{q}^2}} i \int \frac{d\mathbf{q}'}{(2\pi)^3} \frac{T_{(ik)}(\frac{\sqrt{3}}{2}\mathbf{q}';\mathbf{q}_{(12)},\mathbf{q}_3) + T_{(jk)}(\frac{\sqrt{3}}{2}\mathbf{q}';\mathbf{q}_{(12)},\mathbf{q}_3)}{\sigma^2 - \frac{3}{4}\mathbf{q}'^2 - (\frac{\mathbf{q}'}{2} + \frac{2}{\sqrt{3}}\mathbf{q})^2 + i\epsilon}, \tag{C34}$$

where

$$\mathbb{T}^{(ij)}_{[J]}(\mathbf{q};q_{(12)},q_3) = \frac{4\pi t_0\left(\sqrt{\sigma^2 - \mathbf{q}^2}\right)}{\sqrt{\sigma^2 - \mathbf{q}^2}} \int d\mathbf{r}_k e^{-i\mathbf{q}\cdot\mathbf{r}_k} \psi^{(0)}_{[J]}(\mathbf{0},\mathbf{r}_k;q_{(12)},q_3). \tag{C35}$$

In terms of the T amplitude, the finite-volume three-body wave function is taken from Eq. (C23),

$$\phi^{(ij)}_{[J]}(\mathbf{r}_{(ij)},\mathbf{r}_k;q_{(12)},q_3)=\frac{\left(\frac{\sqrt{3}}{2}\right)^3}{L^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{q}=-\frac{\mathbf{P}}{\sqrt{3}}+\frac{\sqrt{3}2\pi}{2\,L}\mathbf{n}} e^{i\mathbf{q}\cdot\mathbf{r}_k}\sum_{\mathbf{n}_{(ij)}\in\mathbb{Z}^3} e^{i(\frac{\mathbf{P}}{3}+\frac{\mathbf{q}}{\sqrt{3}})\cdot\mathbf{n}_{(ij)}L} ih_0^{(+)}\left(\sqrt{\sigma^2-\mathbf{q}^2}|\mathbf{r}_{(ij)}+\mathbf{n}_{(ij)}L|\right)$$
$$\times\frac{\sqrt{\sigma^2-\mathbf{q}^2}}{4\pi}T^{(ij)}_{[J]}(\mathbf{q};q_{(12)},q_3)). \tag{C36}$$

Similarly, from Eqs. (C24), (C26), and (C27), we also find

$$\chi^{(ij)}_{[J]}(\mathbf{r}_{(12)},\mathbf{r}_3;q_{(12)},q_3)=\sum_{(i'<j')=1}^{N}\chi^{(i'j'),(ij)}_{[J]}(\mathbf{r}_{(i'j')},\mathbf{r}_{k'};q_{(12)},q_3), \tag{C37}$$

where

$$\chi^{(ij),(ij)}_{[J]}(\mathbf{r}_{(ij)},\mathbf{r}_k;q_{(12)},q_3)=\frac{\left(\frac{\sqrt{3}}{2}\right)^3}{L^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{q}=-\frac{\mathbf{P}}{\sqrt{3}}+\frac{\sqrt{3}2\pi}{2\,L}\mathbf{n}} e^{i\mathbf{q}\cdot\mathbf{r}_k} ih_0^{(+)}\left(\sqrt{\sigma^2-\mathbf{q}^2}r_{(ij)}\right)\frac{\sqrt{\sigma^2-\mathbf{q}^2}}{4\pi}T^{(ij)}_{[J]}(\mathbf{q};q_{(12)},q_3), \tag{C38}$$

and

$$\chi^{(i'j'),(ij)}_{[J]}(\mathbf{r}_{(i'j')},\mathbf{r}_{k'};q_{(12)},q_3)\overset{(i'j')\neq(ij)}{=}\int\frac{d\mathbf{q}}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{r}_{k'}}\sum_{\mathbf{n}\in\mathbb{Z}^3}e^{i(\frac{2\mathbf{P}}{3}+\frac{2\Gamma^{(i'j'),(ij)}_{2,2}}{\sqrt{3}}\mathbf{q})\cdot\mathbf{n}L}ih_0^{(+)}\left(\sqrt{\sigma^2-\mathbf{q}^2}\left|\mathbf{r}_{(i'j')}+\frac{2\Gamma^{(i'j'),(ij)}_{1,2}}{\sqrt{3}}\mathbf{n}L\right|\right)$$
$$\times\frac{\sqrt{\sigma^2-\mathbf{q}^2}}{4\pi}T^{(i'j')}_{[J]}(\mathbf{q};q_{(12)},q_3). \tag{C39}$$

For the three-body problem, three secular equations may be obtained according to Eq. (C28), but only two of them are independent. For example, for the channel (12), the quantization condition is given by

$$\det\left[\int d\mathbf{r}_3\phi^*_{[J']}(\mathbf{0},\mathbf{r}_3;q_{(12)},q_3)mV_0\Delta\phi^{(12)}_{[J]}(\mathbf{0},\mathbf{r}_3;q_{(12)},q_3)\right]=0, \tag{C40}$$

where

$$\Delta\phi^{(12)}_{[J]}(\mathbf{0},\mathbf{r}_3;q_{(12)},q_3)=-\frac{\left(\frac{\sqrt{3}}{2}\right)^3}{L^3}\sum_{\mathbf{n}_3\in\mathbb{Z}^3}^{\mathbf{q}=-\frac{\mathbf{P}}{\sqrt{3}}+\frac{\sqrt{3}2\pi}{2\,L}\mathbf{n}_3}\frac{\sqrt{\sigma^2-\mathbf{q}^2}}{4\pi}T^{(12)}_{[J]}(\mathbf{q};q_{(12)},q_3)\left[\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{n}\neq\mathbf{0}}e^{i(\frac{\mathbf{P}}{3}+\frac{\mathbf{q}}{\sqrt{3}})\cdot\mathbf{n}L}ih_0^{(+)}(\sqrt{\sigma^2-\mathbf{q}^2}|\mathbf{n}L|)\right]e^{i\mathbf{q}\cdot\mathbf{r}_3}$$
$$+\left[\int\frac{d\mathbf{q}}{(2\pi)^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}e^{i(\frac{2\mathbf{P}}{3}-\frac{\mathbf{q}}{\sqrt{3}})\cdot\mathbf{n}L}-\frac{\left(\frac{\sqrt{3}}{2}\right)^3}{L^3}\sum_{\mathbf{n}_k\in\mathbb{Z}^3}^{\mathbf{q}=-\frac{\mathbf{P}}{\sqrt{3}}+\frac{\sqrt{3}2\pi}{2\,L}\mathbf{n}_k}\sum_{\mathbf{n}\in\mathbb{Z}^3}e^{i(\frac{\mathbf{P}}{3}+\frac{\mathbf{q}}{\sqrt{3}})\cdot\mathbf{n}L}\right]$$
$$\times ih_0^{(+)}\left(\sqrt{\sigma^2-\mathbf{q}^2}\left|\frac{\sqrt{3}\mathbf{r}_3}{2}+\mathbf{n}L\right|\right)e^{-i\mathbf{q}\cdot\frac{\mathbf{r}_3}{2}}\frac{\sqrt{\sigma^2-\mathbf{q}^2}}{4\pi}\sum_{(ij)=13}^{23}T^{(ij)}_{[J]}(\mathbf{q};q_{(12)},q_3). \tag{C41}$$

The renormalized $\phi^*_{[J']}mV_0$ is given by

$$\phi^*_{[J]}(\mathbf{0},\mathbf{r}_3;q_{(12)},q_3)mV_0\to\frac{\left(\frac{\sqrt{3}}{2}\right)^3}{L^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{q}=-\frac{\mathbf{P}}{\sqrt{3}}+\frac{\sqrt{3}2\pi}{2\,L}\mathbf{n}}e^{-i\mathbf{q}\cdot\mathbf{r}_3}T^{(12)*}_{[J']}(\mathbf{q};q_{(12)},q_3). \tag{C42}$$

Normally, the infinite sum of Bessel functions in the above equation has poor convergence, and for numerical purposes a better expression may be given by Eq. (50) in a partial-wave expanded form. It may also be convenient to use an alternative form in Eq. (D7) without partial-wave expansion,

$$\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\mathbf{Q}\cdot\mathbf{n}L} h_0^{(+)}(q|\mathbf{r}+\mathbf{n}L|) = \mathcal{J}^{(\mathbf{Q})}(\mathbf{r},q) + i n_0(qr),$$

where the expression and derivation of $\mathcal{J}^{(\mathbf{Q})}(\mathbf{r},q)$ is presented in Appendix D. In terms of a partial-wave expanded form, $\mathcal{J}^{(\mathbf{Q})}$ is related to Lüscher's form by

$$i\mathcal{J}^{(\mathbf{Q})}(\mathbf{r},q) = \sqrt{4\pi}\sum_{[j]} \mathcal{M}^{(\mathbf{Q})}_{[0],[j]}(q) j_j(qr) Y_{[j]}(\mathbf{r}). \quad \text{(C43)}$$

APPENDIX D: LATTICE SUM OF THE TWO-BODY GREEN'S FUNCTION

An alternative fast algorithm for performing the lattice sum of the two-body Green's function in Eqs. (C23) and (C36) without partial-wave expansion is provided in this Appendix. First of all, using the identity

$$\frac{q}{4\pi} i h_0^{(+)}(qr) = \frac{1}{2\pi\sqrt{\pi}} \int_0^\infty dt e^{-r^2t^2+\frac{q^2}{4t^2}} \quad \text{(D1)}$$

and splitting the integration by an arbitrary parameter η, we can rewrite the lattice sum of the Green's function in Eq. (50) as

$$\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\mathbf{Q}\cdot\mathbf{n}L} h_0^{(+)}(q|\mathbf{r}+\mathbf{n}L|)$$
$$= -\frac{2i}{\sqrt{\pi}q}\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\mathbf{Q}\cdot\mathbf{n}L}\left[\int_0^\eta + \int_\eta^\infty\right] dt e^{-|\mathbf{r}+\mathbf{n}L|^2t^2+\frac{q^2}{4t^2}}. \quad \text{(D2)}$$

For the first term in Eq. (D2), using the identity

$$\frac{1}{2\pi\sqrt{\pi}} e^{-r^2t^2} = \frac{1}{2t^3}\int \frac{d\mathbf{q}'}{(2\pi)^3} e^{-\frac{\mathbf{q}'^2}{4t^2}} e^{i\mathbf{q}'\cdot\mathbf{r}} \quad \text{(D3)}$$

and also applying Poisson summation, we find

$$-\frac{2i}{\sqrt{\pi}q}\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\mathbf{Q}\cdot\mathbf{n}L}\int_0^\eta dt e^{-|\mathbf{r}+\mathbf{n}L|^2t^2+\frac{q^2}{4t^2}}$$
$$= \frac{4\pi i}{q}\frac{1}{L^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{q}'=\frac{2\pi}{L}\mathbf{n}-\mathbf{Q}} \frac{e^{\frac{q^2-\mathbf{q}'^2}{4\eta^2}}}{q^2-\mathbf{q}'^2+i\epsilon} e^{i\mathbf{q}'\cdot\mathbf{r}}. \quad \text{(D4)}$$

For the second term in Eq. (D2), except for $\mathbf{n}=\mathbf{0}$, the convergence of the integration is well defined for a finite value of η; thus, we would like to isolate the $\mathbf{n}=\mathbf{0}$ piece, with the help of the identity

$$-\frac{2i}{\sqrt{\pi}q}\int_\eta^\infty dt e^{-r^2t^2+\frac{q^2}{4t^2}}$$
$$= i n_0(qr) + i\frac{e^{-iqr}\mathrm{erf}(-\frac{iq}{2\eta}+r\eta) - e^{iqr}\mathrm{erf}(-\frac{iq}{2\eta}-r\eta)}{2qr}. \quad \text{(D5)}$$

Therefore, we find

$$-\frac{2i}{\sqrt{\pi}q}\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\mathbf{Q}\cdot\mathbf{n}L}\int_\eta^\infty dt e^{-|\mathbf{r}+\mathbf{n}L|^2t^2+\frac{q^2}{4t^2}}$$
$$= i n_0(qr) + i\frac{e^{-iqr}\mathrm{erf}(-\frac{iq}{2\eta}+r\eta) - e^{iqr}\mathrm{erf}(-\frac{iq}{2\eta}-r\eta)}{2qr}$$
$$-\frac{2i}{\sqrt{\pi}q}\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{n}\neq\mathbf{0}} e^{i\mathbf{Q}\cdot\mathbf{n}L}\int_\eta^\infty dt e^{-|\mathbf{r}+\mathbf{n}L|^2t^2+\frac{q^2}{4t^2}}. \quad \text{(D6)}$$

Putting everything together, we thus obtain a fast-convergent expression for the lattice sum of the Green's function without partial-wave expansion,

$$\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\mathbf{Q}\cdot\mathbf{n}L} h_0^{(+)}(q|\mathbf{r}+\mathbf{n}L|) = \mathcal{J}^{(\mathbf{Q})}(\mathbf{r},q) + i n_0(qr), \quad \text{(D7)}$$

where

$$\mathcal{J}^{(\mathbf{Q})}(\mathbf{r},q) = \frac{4\pi i}{q}\frac{1}{L^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{q}'=\frac{2\pi}{L}\mathbf{n}-\mathbf{Q}} \frac{e^{\frac{q^2-\mathbf{q}'^2}{4\eta^2}}}{q^2-\mathbf{q}'^2+i\epsilon} e^{i\mathbf{q}'\cdot\mathbf{r}}$$
$$+ i\frac{e^{-iqr}\mathrm{erf}(-\frac{iq}{2\eta}+r\eta) - e^{iqr}\mathrm{erf}(-\frac{iq}{2\eta}-r\eta)}{2qr}$$
$$-\frac{2i}{\sqrt{\pi}q}\sum_{\mathbf{n}\in\mathbb{Z}^3}^{\mathbf{n}\neq\mathbf{0}} e^{i\mathbf{Q}\cdot\mathbf{n}L}\int_\eta^\infty dt e^{-|\mathbf{r}+\mathbf{n}L|^2t^2+\frac{q^2}{4t^2}}. \quad \text{(D8)}$$

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