Rummukainen-Gottlieb formula on a two-particle system with different masses

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A proposal by Lüscher enables us to extract the elastic scattering phases from two-particle energy spectrum in a cubic box using lattice simulations. Rummukainen and Gottlieb further extend it to the moving frame, which is devoted to the system of two identical particles. In this work, we generalize Rummukainen-Gottlieb's formula to the generic two-particle states where two particles are explicitly distinguishable, namely, the masses of the two particles are different. Their relations with the elastic scattering phases of two-particle energy spectrum in the continuum are obtained for both C_{4v} and C_{2v} symmetries. Our analytical results will be very helpful for the study of some resonances, such as kappa, vector kaon, and so on.

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I. INTRODUCTION

Many low-energy hadrons, such as kappa, sigma, can observed as resonances in scattering experiments. The energy eigenvalues of two-particle states with definite symmetry can be obtained by measuring appropriate correlation functions through lattice simulations. Therefore, it is highly desirable to relate these calculated energy eigenvalues to the scattering phases measured by a scattering experiment. This was accomplished through the methods proposed by Lüscher [1–5] for a cubic box. In these references, Lüscher established a nonperturbative relation of the energy of a two-particle state in a cubic box with the corresponding elastic scattering phases in the continuum. The finite size formula presented by Rummukainen and Gottlieb further extended Lüscher's formula to the moving frame (MF) [6]. The studies of two-particle scattering states provided by Feng *et al.* generalized Lüscher's formula in an asymmetric box [7]. These formula have been extensively utilized in different applications [8–19].

For some cases, we have to use the generic two-particle system to extract the resonance parameters in the moving frame. However, all of these aforementioned formulae in the moving frame can apply only to two identical particle systems. For example, to examine the behavior of the κ resonance, it is highly desired for us to investigate the πK scattering with nonzero total momentum modes in the moving frame. In a generic two-particle system, the original Rummukainen-Gottlieb formulae, which only give the relation between the energy eigenvalues of two identical particle states in the finite box and the continuum elastic scattering phase shifts with the nonzero total momentum, must be modified accordingly. To this purpose, we strictly derive the equivalents of the famous Rummukainen-Gottlieb formulae for a generic two-particle system in the moving frame not only from theoretical aspects, but also from practical considerations. This scenario is quite useful in practice since it provides an important feasible method in the study of the κ decay, vector kaon K^* decay, and so on.

The modifications which we must be implemented, as compared with Ref. [6], are mainly concerned with the different symmetries of the two-particle system in a cubic box. The representations of the rotational group are decomposed into irreducible representations of the D_{4h} and D_{2h} cubic groups for the system of two identical particles with the nonzero total momentum in a cubic box [6]. In a generic two-particle state, the symmetry of the system is further reduced. In the case of $\mathbf{d} = (0, 0, 1)$, the basic group becomes C_{4v} instead of D_{4h}; As for $\mathbf{d} = (0, 1, 1)$, the symmetry is further reduced to C_{2v}. Hence, the final expression connecting the energy eigenvalues of the system and the scattering phases is certainly new.

This paper is organized as follows. In Sec. II, we discuss the general properties of the generic two-particle states in a cubic box for free and then interacting cases. In Secs. III and IV, we investigate the theoretical aspects of our alteration: in Sec. III, we extend Rummukainen-Gottlieb formalism to the generic case and derive the fundamental relationship for the phase shift in Eq. (17), and in Sec. IV we present the symmetry considerations. Our brief conclusions are given in Sec. V. Some details of the numerical calculation are provided in the Appendices for reference.

II. GENERIC TWO-PARTICLE STATES ON A CUBIC BOX

In this section we derive the formalisms required for calculating the scattering phase shifts in a periodic cubic box. Here we just consider the continuous space-time. In practice we should apply these results to the discrete periodic lattices, and address for the lattice artifacts [20]. The formulae presented here are enough for analyzing the lattice data. We follow the essential formalisms and notations introduced by Rummukainen and Gottlieb [6], spreading them to the generic two-particle states.

Without loss of generality, we consider two particles with masses m_1 and m_2 for particle 1 and particle 2, respectively. In this work we are specially interested in a system having a nonzero total momentum, namely, the lattice frame or the moving frame [6]. Using a moving frame with total momentum $\mathbf{P} = (2\pi/L)\mathbf{d}$, $\mathbf{d} \in \mathbb{Z}^3$, the energy eigenvalues for our system in the noninteracting case are given by [6]

$$E_{\rm MF} = \sqrt{m_1^2 + p_1^2} + \sqrt{m_2^2 + p_2^2}, \tag{1}$$

where $p_1 = |\mathbf{p}_1|$, $p_2 = |\mathbf{p}_2|$, and $\mathbf{p}_1$, $\mathbf{p}_2$ denote the three-momenta of particle 1 and particle 2, respectively, which satisfy periodic boundary condition,

$$\mathbf{p}_i = \frac{2\pi}{L}\mathbf{n}_i, \qquad \mathbf{n}_i \in \mathbb{Z}^3, \tag{2}$$

and the relation

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{P}. \tag{3}$$

In the center-of-mass (CM) frame, the total center-of-mass momentum disappears, namely,

$$p^* = |\mathbf{p}^*|, \qquad \mathbf{p}^* = \mathbf{p}_1^* = -\mathbf{p}_2^*, \tag{4}$$

where $\mathbf{p}^* = (2\pi/L)\mathbf{n}$, and $\mathbf{n} \in \mathbb{Z}^3$. Here and hereafter we denote the center-of-mass momenta with an asterisk (*). The possible energy eigenvalues of two-particle system are given by

$$E_{\rm CM} = \sqrt{m_1^2 + p^{*2}} + \sqrt{m_2^2 + p^{*2}}. \tag{5}$$

The relativistic four-momentum squared is invariant, and $E_{\rm CM}$ is related to $E_{\rm MF}$ in the moving frame through the Lorentz transformation

$$E_{\rm CM}^2 = E_{\rm MF}^2 - \mathbf{P}^2. \tag{6}$$

In the moving frame, the center-of-mass is moving with a velocity of $\mathbf{v} = \mathbf{P}/E_{\rm MF}$. Using the standard Lorentz transformation with a boost factor $\gamma = 1/\sqrt{1-\mathbf{v}^2}$, the $E_{\rm CM}$ can be obtained through $E_{\rm CM} = \gamma^{-1}E_{\rm MF}$, and momenta $\mathbf{p}_i$ and $\mathbf{p}^*$ are related by the standard Lorentz transformation,

$$\mathbf{p}_1 = \vec{\gamma}(\mathbf{p}^* + \mathbf{v}E_1^*), \qquad \mathbf{p}_2 = -\vec{\gamma}(\mathbf{p}^* - \mathbf{v}E_2^*), \tag{7}$$

where E_1^* and E_2^* are energy eigenvalues of the particle 1 and particle 2 in the center-of-mass frame, respectively,

$$\begin{aligned} E_1^* &= \frac{1}{2E_{\rm CM}}(E_{\rm CM}^2 + m_1^2 - m_2^2), \\ E_2^* &= \frac{1}{2E_{\rm CM}}(E_{\rm CM}^2 + m_2^2 - m_1^2), \end{aligned} \tag{8}$$

and the boost factor acts in the direction of $\mathbf{v}$, here and hereafter we adopt the shorthand notation

$$\vec{\gamma}\mathbf{p} = \gamma\mathbf{p}_\parallel + \mathbf{p}_\perp, \quad \vec{\gamma}^{-1}\mathbf{p} = \gamma^{-1}\mathbf{p}_\parallel + \mathbf{p}_\perp, \tag{9}$$

where $\mathbf{p}_\parallel$ and $\mathbf{p}_\perp$ are components of $\mathbf{p}$ parallel and perpendicular to the center-of-mass velocity, respectively, namely,

$$\mathbf{p}_\parallel = \frac{\mathbf{p}\cdot\mathbf{v}}{|\mathbf{v}|^2}\mathbf{v}, \qquad \mathbf{p}_\perp = \mathbf{p} - \mathbf{p}_\parallel. \tag{10}$$

Therefore, by inspecting Eqs. (3), (7), and (8), it can be seen that the $\mathbf{p}^*$ are quantized to the values

$$\mathbf{p}^* = \frac{2\pi}{L}\mathbf{r}, \qquad \mathbf{r} \in P_{\mathbf{d}}, \tag{11}$$

where the set $P_{\mathbf{d}}$ is

$$P_{\mathbf{d}} = \left\{\mathbf{r}|\mathbf{r} = \vec{\gamma}^{-1}\left[\mathbf{n} + \frac{\mathbf{d}}{2}\cdot\left(1 + \frac{m_2^2 - m_1^2}{E_{\rm CM}^2}\right)\right], \mathbf{n} \in \mathbb{Z}^3\right\}. \tag{12}$$

In the interacting case, the $\bar{E}_{\rm CM}$ is given by

$$\bar{E}_{\rm CM} = \sqrt{m_1^2 + k^2} + \sqrt{m_2^2 + k^2}, \qquad k = \frac{2\pi}{L}q, \tag{13}$$

where q is no longer required to be a integer, which is stemmed from a quantized momentum mode. Solving this equation for scattering momentum k we get

$$k = \frac{1}{2\bar{E}_{\rm CM}}\sqrt{[\bar{E}_{\rm CM}^2 - (m_1 - m_2)^2][\bar{E}_{\rm CM}^2 - (m_1 + m_2)^2]}. \tag{14}$$

We can rewrite Eq. (14) to an elegant form as

$$k^2 = \frac{\bar{E}_{\rm CM}^2}{4} + \frac{(m_1^2 - m_2^2)^2}{4\bar{E}_{\rm CM}^2} - \frac{m_1^2 + m_2^2}{2}. \tag{15}$$

It is exactly this energy shift between the noninteracting situation and the interacting case, namely, $\bar{E}_{\rm CM} - E_{\rm CM}$ (or equivalently $|\mathbf{n}|^2 - q^2$), that we can calculate the two-particle scattering phase.

As it is done in Ref. [6], in the current study, we mainly investigate two moving frames. One is $\mathbf{d} = (0, 0, 1)$, where energy eigenstates transform under the tetragonal group C_{4v}, only the irreducible representation A_1 is relevant for two-particle scattering states in infinite volume with angular momentum $l = 0$. Another one is $\mathbf{d} = (0, 1, 1)$, where energy eigenstates transform under the tetragonal group C_{2v}, only the irreducible representation A_1 is relevant for two-particle s-wave scattering states in infinite volume. For the other cases, like $\mathbf{d} = (1, 1, 1)$, etc., we can easily work out from almost the same way without difficulty.

Assuming that the phase shifts δ_l with $l = 1, 2, 3, \ldots$ are negligible in the energy range of interest, the phase shift δ_0 is related to the momentum k by

$$\tan\delta_0(k) = \frac{\gamma\pi^{3/2}q}{\mathcal{Z}_{00}^{\mathbf{d}}(1; q^2)}, \tag{16}$$

where $k = (2\pi/L)q$, and the modified zeta function is formally defined by

$$\mathcal{Z}^{\mathbf{d}}_{00}(s;q^2) = \sum_{\mathbf{r}\in P_d} \frac{1}{(|\mathbf{r}|^2 - q^2)^s}, \tag{17}$$

and the set $P_{\mathbf{d}}$ is

$$P_{\mathbf{d}} = \left\{\mathbf{r}|\mathbf{r} = \hat{\vec{\gamma}}^{-1}\left[\mathbf{n} + \frac{\mathbf{d}}{2}\cdot\left(1 + \frac{m_2^2 - m_1^2}{E_{\mathrm{CM}}^2}\right)\right], \mathbf{n}\in\mathbb{Z}^3\right\}. \tag{18}$$

For Eq. (16), we note that the almost same result has already existed in Eq. (1) of Ref. [21], where the formula was just presented without any explanation. We can view our work as further confirming and strictly proving this formula. The modified zeta function converges when $\mathrm{Re}2s > l+3$, and can be analytically continued to whole complex plane. The k is the scattering momentum defined from the invariant mass $\sqrt{s}$ as $\sqrt{s} = \bar{E}_{\mathrm{CM}} = \sqrt{k^2 + m_1^2} + \sqrt{k^2 + m_2^2}$. The calculation method of $\mathcal{Z}^{\mathbf{d}}_{00}(1;q^2)$ is discussed in Appendix A and in Ref. [20]. Using Eq. (16), we can obtain the phase shift from the energy eigenvalue calculated in the lattice simulations. If we now set $m_1 = m_2$, all the results in Ref. [6] are elegantly recovered.

III. DERIVATION OF THE PHASE SHIFT FORMULA

In this section we derive the fundamental phase shift formula in Eq. (16) for the generic two-particle system of spin-0. We utilize the formalisms derived in Ref. [6], and generalize them to the generic two-particle system. To make the derivation simple, we are studying the system by the relativistic quantum mechanics.

Throughout this section, we employ the metric tensor sign convention $g_{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$, write the scalar productions in a compact form $p^2 = p\cdot p = p_\mu p^\mu$, etc., and express the quantities in natural units with $\hbar = c = 1$. Here and hereafter we follow the original notations in Ref. [6].

A. Lorentz transformation of wave function

Let us consider the generic system of two spin-0 particles with mass m_1, and m_2, respectively, in an infinite volume. The state of the system is described by the scalar wave function $\psi(x_1, x_2)$, where $x_i = (x_i^0, \mathbf{x}_i)$, $i = 1, 2$ are the four-dimensional Minkowski space-time coordinates of two particles. The wave function transforms under the Lorentz transformations as

$$\psi(x_1,x_2) = \psi'(x_1', x_2') = \psi'(\Lambda x_1, \Lambda x_2), \tag{19}$$

where $(x')^\mu = \Lambda^\mu_\nu x^\nu$ denotes the standard Lorentz transformation of the four-vector x. The wave function depends on two four-vectors x_1, x_2. Moreover, the space and time coordinates are mixed under the Lorentz transformations.

We can make the problem simpler by using the special properties of the center-of-mass frame of the particles. Let us first consider the two noninteracting particles, and in any inertial frame the wave functions satisfy the Klein-Gordon equations

$$\begin{aligned}(\hat{p}_{1\mu}\hat{p}_1^\mu - m_1^2)\psi(x_1,x_2) = 0,\\ (\hat{p}_{2\mu}\hat{p}_2^\mu - m_2^2)\psi(x_1,x_2) = 0,\end{aligned} \tag{20}$$

where $\hat{p}_{i\mu}$, $i = 1, 2$ is the four-momentum operator. It is well known that the problem simplifies if we separate the variables under the transformations

$$X = \frac{m_1x_1 + m_2x_2}{m_1+m_2}, \tag{21}$$

$$x = x_1 - x_2, \tag{22}$$

where X is the position of the center of mass, and x is the relative coordinate of two particles. Let us restrict ourselves to the solutions which are the eigenstates of the center-of-mass momentum operator. Then Eq. (20) can be transformed into the form

$$\left[\left(\frac{m_1}{M}\right)^2\hat{P}_\mu\hat{P}^\mu + \hat{p}_\mu\hat{p}^\mu - \frac{2m_1}{M}\hat{p}_\mu\cdot\hat{P}^\mu + m_1^2\right]\psi(x,X) = 0, \tag{23}$$

$$\left[\left(\frac{m_2}{M}\right)^2\hat{P}_\mu\hat{P}^\mu + \hat{p}_\mu\hat{p}^\mu + \frac{2m_2}{M}\hat{p}_\mu\cdot\hat{P}^\mu + m_2^2\right]\psi(x,X) = 0, \tag{24}$$

where

$$\hat{p} = \frac{m_2\hat{p}_1 - m_1\hat{p}_2}{m_1+m_2}, \tag{25}$$

$$\hat{P} = \hat{p}_1 + \hat{p}_2, \tag{26}$$

$$M = m_1 + m_2, \tag{27}$$

$\hat{p}$ is the relative 4-momentum operator, $\hat{P}$ is the total 4-momentum operator, and M is the total mass of two particles.

Adding $1/m_1\times(23)$ to $1/m_2\times(24)$ and subtracting (23) from (24), respectively, yields

$$\left[\frac{M^2}{m_1m_2}\hat{p}_\mu\hat{p}^\mu - M^2 + \hat{P}_\mu\hat{P}^\mu\right]\psi(x,X) = 0, \tag{28}$$

$$\left[\hat{p}_\mu\hat{P}^\mu - \frac{m_1-m_2}{2M}\hat{P}_\mu\hat{P}^\mu - \frac{m_1^2 - m_2^2}{2}\right]\psi(x,X) = 0. \tag{29}$$

It is well known that, without external potentials, the total momentum of the two-particle system is conserved; then we can restrain ourselves to the eigenfunctions of P, namely,

$$\psi(x,X) = e^{-iP_\mu X^\mu}\phi(x), \tag{30}$$

where P_μ is a constant timelike vector, and P is denoted through $P^2 = P_\mu P^\mu$.

In the present study, we are specially interested in the center-of-mass frame, which is denoted as the frame where the spatial components of the total momentum of the system disappear, namely, $\mathbf{P}^* = 0$. Therefore, we can only take the positive kinetic energy solutions $P_0^* = E_{\rm CM}^* > m_1 + m_2$ into consideration. Therefore, Eqs. (28) and (29) can be rewritten as

$$\left(\hat{p}_\mu^* \hat{p}^{*\mu} + \frac{E_{\rm CM}^2 m_1 m_2}{(m_1+m_2)^2} - m_1 m_2\right)\phi_{\rm CM}(x^*) = 0, \quad (31)$$

$$\left(\hat{p}_0^* - \frac{E_{\rm CM}}{2}\frac{m_1 - m_2}{m_1+m_2} - \frac{m_1^2 - m_2^2}{2E_{\rm CM}}\right)\phi_{\rm CM}(x^*) = 0. \quad (32)$$

Equation (32) indicates that $\hat{p}_0^*\phi_{\rm CM}(x^*) \neq 0$ for $m_1 \neq m_2$. By inspecting Eqs. (31) and (32), we can reasonably assume that the wave function $\phi_{\rm CM}(x^*)$ can be expressed in the form,

$$\phi_{\rm CM}(x^*) \equiv e^{i\beta x^{*0}}\phi_{\rm CM}(\mathbf{x}^*), \quad (33)$$

where $x^{*0} = x_1^{*0} - x_2^{*0}$ is the relative temporal separation of two particles, and β is a constant, namely,

$$\beta = \frac{E_{\rm CM}}{2}\frac{m_2 - m_1}{m_1+m_2} + \frac{m_2^2 - m_1^2}{2E_{\rm CM}}. \quad (34)$$

It is obvious that when $m_1 = m_2$, $\beta \to 0$. Therefore, in the center-of-mass frame the wave function depends explicitly on the time variable $t^* \equiv X^{*0} = (m_1 x_1^{*0} + m_2 x_2^{*0})/(m_1+m_2)$, the relative spatial separation of the particles $\mathbf{x}^* = \mathbf{x}_1^* - \mathbf{x}_2^*$, and the relative temporal separation of the particles x^{*0}, namely,

$$\psi_{\rm CM}(x^*, t^*) = e^{-iE_{\rm CM}t^*} e^{i\beta x^{*0}}\phi_{\rm CM}(\mathbf{x}^*), \quad (35)$$

where the constant β is denoted in Eq. (34).

Let us now discuss the case in the moving frame. The transformation from the moving frame to the center-of-mass frame can be expressed as $r^{*\mu} = \Lambda^\mu{}_\nu r^\nu$, where r is any position 4-vector and quantities without * stand for those of the moving frame. With the shorthand definition in Eq. (9), we have

$$r^{*0} = \gamma(r^0 + \mathbf{v}\cdot\mathbf{r}), \quad (36)$$

$$\mathbf{r}^* = \vec{\gamma}(\mathbf{r} + \mathbf{v}r^0), \quad (37)$$

where γ is a boost factor, and $\mathbf{v} = \mathbf{P}/P_0$ is the 3-velocity of the center of mass in the moving frame. We can rewrite $\mathbf{v}$ to a form for later use as

$$\mathbf{v} = \frac{2\pi}{LE_{\rm MF}}\mathbf{d} = \frac{2\pi}{\gamma L E_{\rm CM}}\mathbf{d}. \quad (38)$$

Using the Lorentz transformation in Eq. (19), the identity $P_\mu X^\mu = P_\mu^* X^{*\mu}$, and Eq. (30), the wave function in the moving frame can be expressed as

$$\psi_{\rm MF}(x, X) = e^{-iP_\mu X^\mu}\phi_{\rm MF}(x), \quad (39)$$

where

$$\phi_{\rm MF}(x) \equiv \phi_{\rm MF}(x^0, \mathbf{x}) = \phi_{\rm CM}(\gamma(x^0 + \mathbf{v}\cdot\mathbf{x}), \vec{\gamma}(\mathbf{x} + \mathbf{v}x^0)). \quad (40)$$

Therefore, the wave function $\phi_{\rm MF}$ depends on time separation $x^0 = x_1^0 - x_2^0$ explicitly. However, in the moving frame we only consider the case where two particles have equal time coordinate, namely, $x^0 = 0$. In the center-of-mass frame this corresponds to the tilted plane $(x^{*0}, \mathbf{x}^*) = (\gamma\mathbf{v}\cdot\mathbf{x}, \vec{\gamma}\mathbf{x})$. Since $\phi_{\rm CM}$ is dependent of the relative temporal separation x^{*0}, we can clearly observe the effect of the tilt to the wave function, and Eq. (40) takes the form

$$\phi_{\rm MF}(0, \mathbf{x}) = \phi_{\rm CM}(\gamma\mathbf{v}\cdot\mathbf{x}, \vec{\gamma}\mathbf{x}). \quad (41)$$

Using Eqs. (33) and (38), we can rewrite Eq. (41) as

$$\phi_{\rm MF}(0, \mathbf{x}) = e^{i\beta'\pi\mathbf{d}\cdot\mathbf{x}/L}\phi_{\rm CM}(\vec{\gamma}\mathbf{x}), \quad (42)$$

where β' is a constant, namely,

$$\beta' = \frac{m_2 - m_1}{m_1+m_2} + \frac{m_2^2 - m_1^2}{E_{\rm CM}^2}. \quad (43)$$

Equation (42) has a simple physical interpretation: the center-of-mass system watches the torus in the moving frame expanded by a boost factor γ to the direction of total momentum, while the length scales to the perpendicular directions are preserved. Equation (42) relates the moving frame wave function,

$$\psi_{\rm MF}(0, \mathbf{x}, t, \mathbf{X}) = e^{-iE_{\rm MF}t + i\mathbf{P}\cdot\mathbf{X}}\phi_{\rm MF}(0, \mathbf{x}), \quad (44)$$

to the center-of-mass frame wave function Eq. (35). The total energy of two-particle system from both frames is connected by identity $E_{\rm MF}^2 = E_{\rm CM}^2 + \mathbf{P}^2$. By inspecting Eqs. (31), (32), and (35), and after some manipulations, we finally achieve that the wave function $\phi_{\rm CM}$ satisfies the Helmholtz equation

$$(\nabla_{\mathbf{x}^*}^2 + k^{*2})\phi_{\rm CM}(\mathbf{x}^*) = 0, \quad (45)$$

where

$$k^{*2} = \frac{E_{\rm CM}^2}{4} + \frac{(m_1^2 - m_2^2)^2}{4E_{\rm CM}^2} - \frac{m_1^2 + m_2^2}{2}. \quad (46)$$

This result is consistent with the solution in Ref. [22].

The Eqs. (42) and (45) will be essentially important when we consider the wave functions of the system on a cubic box, and the boundary conditions imposed by the cubic box in the moving frame are transformed by Eq. (42) into the boundary conditions on the solutions in Eq. (45). Thus, Eq. (45) is an important result, which represents one of the main results of the present work. In the following discussions, we remove the superscript * from the quantities in the center-of-mass frame. We can easily check that if we take $m_1 = m_2$, all the corresponding results in Ref. [6] are restored.

B. The scattering wave function

For our concrete problem, we only suppose that the Klein-Gordon equation (20) in the center-of-mass frame still have a square integral solution even with the inclusion of the potential $V_\mu(\mathbf{x})$, which has a finite range [2], namely,

$$V_\mu(\mathbf{x}) = 0 \quad \text{for } |\mathbf{x}| > R, \tag{47}$$

where we assume that there exists R such that Eq. (47) is true both in the center-of-mass and moving frames. Then Klein-Gordon equation (22) hold true when $|\mathbf{x}| > R$, and the wave functions Eqs. (35) and (44) are connected by Eq. (42) in this region.

In the center-of-mass frame the interaction of the system is spherically symmetric. The wave function is usually expanded in spherical harmonics

$$\phi_{\mathrm{CM}}(\mathbf{x}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\theta,\varphi)\phi_{lm}(x), \tag{48}$$

where $\mathbf{x} = x(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. It is well known that the expansion of the two-particle scattering wave function in terms of spherical harmonics has a physical meaning only in the center-of-mass frame. This is especially relevant in the study of resonance scattering, where the resonance channel is an eigenstate of the angular momentum.

When $x > R$, ϕ_{CM} is a solution of Eq. (45), and the functions ϕ_{lm} satisfy the radial differential equation

$$\left[\frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx} - \frac{l(l+1)}{x^2} + k^2\right]\phi_{lm}(x) = 0, \tag{49}$$

where

$$k^2 = \frac{E_{\mathrm{CM}}^2}{4} + \frac{(m_1^2 - m_2^2)^2}{4E_{\mathrm{CM}}^2} - \frac{m_1^2 + m_2^2}{2}. \tag{50}$$

The solutions of Eq. (49) can be expressed as linear combinations of the spherical Bessel functions

$$\phi_{lm}(x) = c_{lm}[a_l(k)j_l(kx) + b_l(k)n_l(kx)]. \tag{51}$$

Although in the region $x < R$ the form of the radial equation is unknown. By comparing the wave functions defined in Eqs. (48) and (51), we obtain the well-known connection between the scattering phase shift and the coefficients a_l and b_l [2], namely,

$$e^{i2\delta_l(k)} = \frac{a_l(k) + ib_l(k)}{a_l(k) - ib_l(k)}. \tag{52}$$

Since a_l and b_l can be taken real-valued when $k > 0$, $\delta_l(k)$ is a real analytic function. Now, for a given l sector, the phase shift $\delta_l(k)$ can be expressed in terms of the moving frame energy E_{MF} through the relation

$$k^2 = \frac{E_{\mathrm{MF}}^2 - \mathbf{P}^2}{4} + \frac{1}{4}\frac{(m_1^2 - m_2^2)^2}{E_{\mathrm{MF}}^2 - \mathbf{P}^2} - \frac{m_1^2 + m_2^2}{2}. \tag{53}$$

C. Eigenstates on a cubic box

In the moving frame, we now investigate two generic particles enclosed in a cubic box of size $L \times L \times L$ with periodic boundary conditions. The temporal direction of the box is chosen to be infinite. The moving frame wave functions ψ_{MF} should be periodic with respect to the position of each particle, namely,

$$\psi_{\mathrm{MF}}(\mathbf{x}_1, \mathbf{x}_2) = \psi_{\mathrm{MF}}(\mathbf{x}_1 + \boldsymbol{l}L, \mathbf{x}_2 + \mathbf{m}L), \qquad \boldsymbol{l}, \mathbf{m} \in \mathbb{Z}^3. \tag{54}$$

The form of the wave function ψ_{MF} is given by Eq. (44)

$$\psi_{\mathrm{MF}}(\mathbf{x}_1, \mathbf{x}_2) = \exp\left(i\frac{\mathbf{P}\cdot(m_1\mathbf{x}_1 + m_2\mathbf{x}_2)}{m_1 + m_2}\right)\phi_{\mathrm{MF}}(\mathbf{x}_1 - \mathbf{x}_2). \tag{55}$$

Combining Eqs. (54) and (55) yields

$$\mathbf{P} = \frac{2\pi}{L}\mathbf{d}, \tag{56}$$

$$\phi_{\mathrm{MF}}(\mathbf{x}) = e^{i\pi(2m_1/(m_1+m_2))\mathbf{d}\cdot\mathbf{n}}\phi_{\mathrm{MF}}(\mathbf{x} + \mathbf{n}L), \tag{57}$$

where $\mathbf{n} = \boldsymbol{l} - \mathbf{m}$, $\mathbf{d}$, $\mathbf{n} \in \mathbb{Z}^3$ and $\mathbf{P}$ is the total momentum.[1] The quantization rule (57) separates the wave functions into the discrete total momentum sectors, which we can categorize by the 3-vector $\mathbf{d}$. In the current study, we are naturally interested in sectors $\mathbf{d} = (0, 0, 1)$ and $\mathbf{d} = (0, 1, 1)$ (and its permutations).

Now we are in the position to employ Eq. (42) to get the corresponding periodicity rule for the center-of-mass wave function. For a chosen vector $\mathbf{d}$, we have

$$\phi_{\mathrm{CM}}(\mathbf{x}) = e^{i\pi\mathbf{d}\cdot\mathbf{n}(1+((m_2^2-m_1^2)/E_{\mathrm{CM}}^2))}\phi_{\mathrm{CM}}(\mathbf{x} + \vec{\gamma}\mathbf{n}L), \quad \mathbf{n} \in \mathbb{Z}^3. \tag{58}$$

For compactness, we refer to the functions obeying the periodicity rule (58) as modified $\mathbf{d}$-periodic functions. As we see later, the modified $\mathbf{d}$-periodic rule (58) is a milestone in this work.

In the center-of-mass frame, the interaction of the system holds the same period as the wave function. Assuming that $L > 2R$, we can denote the "exterior" region

$$\Omega_{\mathrm{CM}} = \{\mathbf{r} \in \mathbb{R}^3 | |\mathbf{r} - \vec{\gamma}\mathbf{n}L| > R, \mathbf{n} \in \mathbb{R}^3\}, \tag{59}$$

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[1] Equation (57) can also be written as

$$\phi_{\mathrm{MF}}(\mathbf{x}) = e^{-i\pi(2m_2/(m_1+m_2))\mathbf{d}\cdot\mathbf{n}}\phi_{\mathrm{MF}}(\mathbf{x} + \mathbf{n}L).$$

Following the almost same procedures and addressing the corresponding formulae, we can arrive at the same final numerical results. For our case, $\mathbf{d}\cdot\mathbf{n}$ is an integer.

where the potential V_L disappears. In this region the wave function ϕ_{CM} satisfies the Helmholtz in Eq. (45). In the region $R < r < L/2$ the solution for ϕ_{CM} of the Helmholtz equation can be expanded in spherical harmonics and spherical Bessel functions. Following Sec. III B, it is easily verified that there exists a unique solution of the full interacting equations of motion in $\mathbb{R}^3$ which coincides with ϕ_{CM} in the external region.

Now the major task for us is to combine the boundary condition in Eq. (58) and the spherical components given by Eq. (48). We accomplish this by looking the general form of the Helmholtz equation and expanding it in spherical harmonics and Bessel functions in the region $R < r < L/2$ [6].

D. Singular *d*-periodic solutions of the Helmholtz equation

In this subsection we derive the general solutions of the Helmholtz equation obeying the modified periodicity rule (58). Except the modified **d**-periodicity, our derivation follows the works in Sec. 4.4 of Ref. [6].

We will call a function ϕ a singular modified **d**-periodic solution of the Helmholtz equation, when it is a smooth function defined for all $\mathbf{x} \neq \vec{\gamma}\mathbf{n}L$, $\mathbf{n} \in \mathbb{Z}^3$, and it satisfies the Helmholtz equation, namely,

$$(\nabla^2 + k^2)\phi(\mathbf{x}) = 0, \qquad (60)$$

for some value of $k > 0$, and obeys the modified **d**-periodicity rule, namely,

$$\phi(\mathbf{x}) = e^{i\alpha\pi\mathbf{d}\cdot\mathbf{n}}\phi(\mathbf{x} + \vec{\gamma}\mathbf{n}L), \qquad \mathbf{n} \in \mathbb{Z}^3, \qquad (61)$$

here and hereafter, for compactness, we defined a factor α, namely,

$$\alpha \equiv 1 + \frac{m_2^2 - m_1^2}{E_{CM}^2}. \qquad (62)$$

When $m_1 = m_2$, $\alpha = 1$, this is the case Rummukainen and Gottlieb studied in Ref. [6]. Moreover, we require that the wave function is bounded by a power of $1/|\mathbf{x}|$ near the origin:

$$\lim_{\mathbf{x}\to 0}|\mathbf{x}^{\Lambda+1}\phi(\mathbf{x})| < \infty \qquad (63)$$

for some positive integer Λ, which is the degree of ϕ. For our purpose, it suffices to study the regular values of k, namely,

$$k \neq \frac{2\pi}{L}\left|\vec{\gamma}^{-1}\left(\mathbf{n} + \frac{\alpha}{2}\mathbf{d}\right)\right|, \qquad \mathbf{n} \in \mathbb{Z}^3. \qquad (64)$$

We can now denote the Green function

$$G^{\mathbf{d}}(\mathbf{x}; k) = \gamma^{-1}L^{-3}\sum_{\mathbf{p}\in\Gamma}\frac{e^{i\mathbf{p}\cdot\mathbf{x}}}{\mathbf{p}^2 - k^2}, \qquad (65)$$

where summation over $\mathbf{p}$ is over the momentum lattice

$$\Gamma = \left\{\mathbf{p} \in \mathbb{R}^3 \,\middle|\, \mathbf{p} = \frac{2\pi}{L}\vec{\gamma}^{-1}\left(\mathbf{n} + \frac{\alpha}{2}\mathbf{d}\right), \mathbf{n} \in \mathbb{Z}^3\right\}. \qquad (66)$$

Equation (65) is well defined since k is nonsingular. If now we select $\mathbf{k} = (2\pi/L)\vec{\gamma}^{-1}(\mathbf{m} + \frac{\alpha}{2}\mathbf{d})$ for some $\mathbf{m} \in \mathbb{Z}^3$, then

$$\mathbf{k}\cdot(\mathbf{x} + \vec{\gamma}\mathbf{n}L) = \mathbf{k}\cdot\mathbf{x} + \alpha\pi\mathbf{d}\cdot\mathbf{n} + 2\pi\mathbf{m}\cdot\mathbf{n}, \qquad (67)$$

where $\mathbf{n} \in \mathbb{Z}^3$, and the function $G^{\mathbf{d}}(\mathbf{x}; k)$ meets clearly the modified **d**-periodicity rule, as we expected. Furthermore, it satisfies

$$(\nabla^2 + k^2)G^{\mathbf{d}}(\mathbf{x}; k) = -\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\alpha\pi\mathbf{d}\cdot\mathbf{n}}\delta(\mathbf{x} + \vec{\gamma}\mathbf{n}L). \qquad (68)$$

We can easily check that the function $G^{\mathbf{d}}(\mathbf{x}; k)$ is a singular modified **d**-periodic solution of Helmholtz equation with degree 1. More singular periodic solution can be obtained by differentiating $G^{\mathbf{d}}$ with respect to $\mathbf{x}$. Let us denote functions

$$G^{\mathbf{d}}_{lm}(\mathbf{x}; k) = \mathcal{Y}_{lm}(\nabla)G^{\mathbf{d}}(\mathbf{x}; k), \qquad (69)$$

where we introduce the harmonic polynomials $\mathcal{Y}_{lm}(\mathbf{x}) = x^l Y_{lm}(\theta, \varphi)$. Since $\mathcal{Y}_{lm}(\nabla)$ commutes with ∇^2, the functions $G^{\mathbf{d}}_{lm}$ are singular modified **d**-periodic solutions of the Helmholtz equation. We can show that the functions $G^{\mathbf{d}}_{lm}$ form a complete set of solutions, and any singular modified **d**-periodic solution of degree Λ is a linear combination of the functions $G^{\mathbf{d}}_{lm}(\mathbf{x}; p)$ with $l \leq \Lambda$ [2]. When $0 < x < L/2$ the functions $G^{\mathbf{d}}_{lm}$ can be expanded in usual spherical harmonics. The expansion takes the form

$$G^{\mathbf{d}}_{lm}(\mathbf{x}; k) = \frac{(-1)^l k^{l+1}}{4\pi}\left[n_l(kx)Y_{lm}(\theta, \varphi) + \sum_{l'=0}^{\infty}\sum_{m'=-l}^{l}\mathcal{M}^{\mathbf{d}}_{lm,l'm'}(k)j_{l'}(kx)Y_{l'm'}(\theta, \varphi)\right], \qquad (70)$$

where the singular part at $\mathbf{x} = 0$ is directly computable from the action of $\mathcal{Y}_{lm}(\nabla)$ to the function $n_0(kx)$. The regular part contains coefficients $\mathcal{M}^{\mathbf{d}}_{lm,l'm'}(k)$. In practice we need only the first few of them, for completeness, we provide the general expression:

$$\mathcal{M}^{\mathbf{d}}_{lm,l'm'}(k) = \frac{(-1)^l}{\gamma\pi^{3/2}}\sum_{j=|l-l'|}^{l+l'}\sum_{s=-j}^{j}\frac{i^j}{q^{j+1}}Z^{\mathbf{d}}_{js}(1; q^2)C_{lm,js,l'm'}, \qquad (71)$$

where $q = kL/(2\pi)$. The tensor $C_{lm,js,l'm'}$ can be expressed in terms of Wigner $3j$ symbols [23]

$$C_{lm,js,l'm'} = (-1)^{m'} i^{l-j+l'} \sqrt{(2l+1)(2j+1)(2l'+1)} \times \begin{pmatrix} l & j & l' \\ m & s & -m' \end{pmatrix} \begin{pmatrix} l & j & l' \\ 0 & 0 & 0 \end{pmatrix}. \quad (72)$$

The modified zeta function is formally denoted by

$$\mathcal{Z}^{\mathbf{d}}_{lm}(s; q^2) = \sum_{\mathbf{r} \in P_{\mathbf{d}}} \frac{\mathcal{Y}_{lm}(\mathbf{r})}{(\mathbf{r}^2 - q^2)^s}, \quad (73)$$

where the summation is over the set

$$P_{\mathbf{d}} = \left\{ \mathbf{r} \in \mathbf{R}^3 | \mathbf{r} = \vec{\gamma}^{-1}\left(\mathbf{n} + \frac{\alpha}{2}\mathbf{d}\right), \mathbf{n} \in \mathbb{Z}^3 \right\}. \quad (74)$$

The sum in Eq. (73) converges when $\mathrm{Re}2s > l + 3$, and can be analytically continued to the whole complex plane.

In Table I we summarized the expressions of $\mathcal{M}^{\mathbf{d}}_{lm,l'm'}$ for l, $l' \le 3$. For compactness, we denoted

$$w_{lm} = \frac{1}{\pi^{3/2}\sqrt{2l+1}} \gamma^{-1} q^{-l-1} \mathcal{Z}^{\mathbf{d}}_{lm}(1; q^2). \quad (75)$$

The necessary Wigner $3j$-symbol values can be obtained in Ref. [23]. Matrix elements missing from the Table I are either zero, or can be obtained through the symmetry relations.

We can easily verify that, if we set $m_1 = m_2$, all of the above definitions and formulae nicely reduce to the those obtained in Ref. [6], as we expected. Of course, if we select $\mathbf{d} = 0$, the moving frame and the center-of-mass frame coincide, $\gamma \to 1$ and $P_{\mathbf{d}} \to \mathbb{Z}^3$, and they further neatly reduce to the forms given in Ref. [2]. Table I can be compared with Table 3 in Ref. [6], which summaries the matrix elements for $m_1 = m_2$. The major difference is the appearance of functions w_{10}, w_{30}, and w_{50} in Table I. If we set $m_1 = m_2$, then $w_{10} \to 0$, $w_{30} \to 0$, and $w_{50} \to 0$, and Rummukainen-Gottlieb's results are immediately restored.

E. Construction of energy eigenstates

The general form of the solutions of the equations of motion in the region $R < |\mathbf{x}| < L/2$ was given in Eqs. (48) and (51). Thus, the functions $G^{\mathbf{d}}_{lm}(\mathbf{x}, k^2)$ [6] form a com-

TABLE I. Matrix elements $\mathcal{M}^{\mathbf{d}}_{lm,l'm'}$ for $\mathbf{d} = (0, 0, 1)$, $m_1 \neq m_2$ and for l, $l' \le 3$.

l	m	l'	m'	$M^{\mathbf{d}}_{lm,l'm'}$								
0	0	0	0	w_{00}								
1	0	0	0		iw_{10}							
1	0	1	0	w_{00}		$+2w_{20}$						
1	1	1	1	w_{00}		$-w_{20}$						
2	0	0	0			$-\sqrt{5}w_{20}$						
2	0	1	0		$i\sqrt{\frac{4}{5}}w_{10}$		$i\sqrt{\frac{27}{35}}w_{30}$					
2	1	1	1		$i\sqrt{\frac{1}{5}}w_{10}$		$i\sqrt{\frac{18}{35}}w_{30}$					
2	0	2	0	w_{00}		$+\frac{10}{7}w_{20}$		$+\frac{18}{7}w_{40}$				
2	1	2	1	w_{00}		$+\frac{5}{7}w_{20}$		$-\frac{12}{7}w_{40}$				
2	2	2	-2					$\frac{3}{7}\sqrt{70}w_{44}$				
2	2	2	2	w_{00}		$-\frac{10}{7}w_{20}$		$+\frac{3}{7}w_{40}$				
3	0	0	0				$-iw_{30}$					
3	0	1	0			$-\frac{3}{7}\sqrt{21}w_{20}$		$-\frac{4}{7}\sqrt{21}w_{40}$				
3	1	1	1			$-\frac{3}{7}\sqrt{14}w_{20}$		$+\frac{3}{7}\sqrt{14}w_{40}$				
3	3	1	-1						$2\sqrt{3}w_{44}$			
3	0	2	0		$-i3\sqrt{\frac{3}{35}}w_{10}$		$-i\frac{4}{3}\sqrt{\frac{1}{5}}w_{30}$			$-i\frac{10}{9}\sqrt{\frac{1}{111}}w_{50}$		
3	1	2	1		$-i2\sqrt{\frac{6}{35}}w_{10}$		$-i\sqrt{\frac{2}{105}}w_{30}$			$-i\frac{5}{9}\sqrt{\frac{2}{111}}w_{50}$		
3	2	2	2		$i\sqrt{\frac{3}{7}}w_{10}$		$i\frac{2}{3}w_{30}$			$i\frac{1}{3}\sqrt{\frac{5}{11}}w_{50}$		
3	0	3	0	w_{00}		$+\frac{4}{3}w_{20}$		$+\frac{18}{11}w_{40}$			$+\frac{100}{33}w_{60}$	
3	1	3	1	w_{00}		$+w_{20}$		$+\frac{3}{11}w_{40}$			$-\frac{25}{11}w_{60}$	
3	2	3	-2						$\frac{3}{11}\sqrt{70}w_{44}$			$+\frac{10}{11}\sqrt{14}w_{64}$
3	2	3	2	w_{00}				$-\frac{21}{11}w_{40}$			$+\frac{10}{11}w_{60}$	
3	3	3	-1						$\frac{3}{11}\sqrt{42}w_{44}$			$-\frac{5}{33}\sqrt{210}w_{64}$
3	3	3	3	w_{00}		$-\frac{5}{3}w_{20}$		$+\frac{9}{11}w_{40}$			$-\frac{5}{33}w_{60}$	

plete set of singular modified **d**-periodic solutions when $l \leq \Lambda$, where Λ is the degree of the function. If we require that these functions are equal, we have

$$\sum_{l=0}^{\Lambda}\sum_{m=-l}^{l} v_{lm} G_{lm}^{\mathbf{d}}(\mathbf{x}, k^2) = \sum_{l=0}^{\Lambda}\sum_{m=-l}^{l} c_{lm}[a_l(k)j_l(kx) + b_l(k)n_l(kx)]Y_{lm}(\theta, \varphi) \quad (76)$$

for some constants c_{lm} and v_{lm}. Using the Eq. (70), we can remove v_{lm} and obtain

$$c_{lm}a_l(k) = \sum_{l'=0}^{\Lambda}\sum_{m'=-l'}^{l'} c_{l'm'}b_{l'}(k)\mathcal{M}^{\mathbf{d}}_{l'm',lm}(k). \quad (77)$$

The matrix elements $\mathcal{M}_{l'm',lm}$ can be viewed as the matrix element of an operator M. If the determinant of a matrix is zero, we can obtain a nontrivial solution for the vector c_{lm}. We rewrite Eq. (77) as a matrix equation,

$$C(A - BM) = 0,$$

where matrix $A_{(lm),(l'm')} = a_l(p)\delta_{l,l'}\delta_{m,m'}$ (similar for B). Since A and B are diagonal and all the diagonal elements of $A - iB$ are nonzero, we can denote the phase shift matrix [2,6],

$$e^{2i\delta} = \frac{A + iB}{A - iB}. \quad (78)$$

The determinant condition requires that [6]

$$\det[e^{2i\delta}(M - i) - (M + i)] = 0. \quad (79)$$

This relation is equal to Eq. (4.10) in Ref. [2].

IV. SYMMETRY DISCUSSIONS

When the moving frame and center-of-mass frame coincide, the two-particle system exhibits a cubic symmetry and the wave functions transform under the representations of the cubic group O_h. However, if the two frames are not equivalent, the Lorentz translation boost from the moving frame to the center-of-mass frame in effect "deforms" the cubical volume and only some subgroups of the original O_h group survive [6].

According to Eq. (42), the deformations caused by the Lorentz boost are like this: the length scales to the direction of the boost are multiplied by γ, while the perpendicular length scales are preserved. Depending on the orientation of the boost with respect to the directions defined by the periodicity of the moving frame torus, some different subgroups of the cubic symmetry survive. In this work, we mainly consider a boost along one of the coordinate axes, namely $\mathbf{d} = (0, 0, 1)$. The geometry of the box changes $(1, 1, 1) \rightarrow (1, 1, \gamma)$, and the relevant symmetry group is tetragonal point group C_{4v}. This group has 8 elements: 4 rotations through an angle $(n\pi/2)$, where $n = 0, 1, 2, 3,$ around the x_3 axis; and all four of the above multiplied by the reflection with respect to the (1,3) plane.

TABLE II. The classification of the Lorentz boosts on a torus and the reduction of the cubic symmetry. The first column displays the direction of the boost (modulo permutations); a is taken to be a nonzero real number. The notation used for the groups is the Schoenflies notation [24].

d	Point group	Classification	N_{elements}
(0, 0, 0)	O_h	Cubic	48
(0, 0, a)	C_{4v}	Tetragonal	8
(0, a, a)	C_{2v}	Orthorhombic	4

The relevant point groups and the boost vectors are classified in Table II. We should bear in mind that only O_h group contains the parity transformation $\mathbf{x} \rightarrow -\mathbf{x}$.

In this paper we are mainly interested in the three lowest total momentum sectors, $|\mathbf{d}| = 0$, 1 and 2 due to the reasons discussed in Ref. [6]. Therefore, in the following we mainly discuss the cubic and tetragonal symmetry groups O_h, C_{4v}, and C_{2v}.

Generally speaking, the energy eigenvalues will belong to some irreducible representation of the corresponding symmetry group of the generic two-particle system. The tetragonal group C_{4v} has four one-dimensional representations A_1, A_2, B_1, B_2, and one two-dimensional representation E [24]. The representations of the rotational group are reduced into irreducible representations of C_{4v} as

$$\Gamma^{(0)} = A_1, \qquad \Gamma^{(1)} = A_1 \oplus E, \qquad \Gamma^{(2)} = A_1 \oplus B_1 \oplus B_2 \oplus E. \quad (80)$$

The representations can be obtained through using the character tables [24] or by enumerating harmonic polynomials of degree l which transform under the representations of C_{4v}. The basis polynomials for the corresponding representations are summarized in Table III for $l \leq 2$, and the polynomials are the linear combinations of the harmonic polynomials $\mathcal{Y}_{lm}(\mathbf{x})$ for each l sector.

The tetragonal group C_{2v} has four one-dimensional representations A_1, A_2, B_1, B_2 [24]. The representations of the rotational group are further reduced into irreducible representations of C_{2v} as

TABLE III. The basis polynomials of the irreducible representations of C_{4v}.

Representation	$l = 0$	$l = 1$	$l = 2$	Indices
A_1	1	x_3	$x_3^2 - \frac{1}{3}x^2$	
A_2				
B_1			$x_1^2 - x_2^2$	
B_2			x_1x_2	
E		x_i	x_ix_3	$i = 1, 2$

TABLE IV. The basis polynomials of the irreducible representations of C_{2v}.

Representation	$l=0$	$l=1$	$l=2$
A_1	1	x_3	$x_3^2 - \frac{1}{3}x^2$
A_2			x_1x_2
B_1		x_1	x_1x_3
B_2		x_2	x_2x_3

$$\Gamma^{(0)} = A_1, \quad \Gamma^{(1)} = A_1 \oplus B_1 \oplus B_2, \quad \Gamma^{(2)} = A_1 \oplus A_2 \oplus B_1 \oplus B_2. \tag{81}$$

Similarly, we can obtain the basis polynomials for the C_{2v} representation, which are summarized in Table IV for $l \le 2$, and the polynomials are the linear combinations of the harmonic polynomials $\mathcal{Y}_{lm}(\mathbf{x})$ for each l sector.

In a typical lattice calculation, the symmetry sector that is easiest to investigate is the sector: A_1. We will therefore concentrate on this particular symmetry sector. As is seen, up to $l \le 2$, s wave, p wave, and d wave contribute to this sector. The other symmetry sectors can be easily worked out in the same way.

First, let us consider the case where the angular momentum cutoff $\Lambda = 0$. From the reduction relations (80) and (81) and Tables III and IV, we note that only $\mathcal{M}^{\mathbf{d}}_{00,00}$ belongs to this sector, and Eq. (79) is one dimensional. It can be written to the form

$$\tan\delta_0(k) = \frac{1}{\mathcal{M}^{\mathbf{d}}_{00,00}} = \frac{\gamma q \pi^{3/2}}{\mathcal{Z}^{\mathbf{d}}_{00}(1; q^2)}, \qquad q = \frac{L}{2\pi}k. \tag{82}$$

This is our essential result for the generic two-particle system.

If $\Lambda = 1$, then the sector $l = 1$ is included, and the matrix in Eq. (79) is two dimensional. Hence the determinant condition contains both phase shifts δ_0 and δ_1, corresponding to the infinite volume $l = 0$ scalar and $l = 1$ vector scattering channels:

$$\begin{aligned}&[e^{2i\delta_0}(m_{00} - i) - (m_{00} + i)][e^{2i\delta_1}(m_{11} - i) - (m_{11} + i)] \\ &\quad = m_{10}^2(e^{2i\delta_0} - 1)(e^{2i\delta_1} - 1),\end{aligned} \tag{83}$$

where we denote $m_{ab} \equiv \mathcal{M}^{\mathbf{d}}_{a0,b0}$. If δ_1 vanishes, namely, $\delta_1 = 0 \pmod{\pi}$, as what we expected, Eq. (83) reduces immediately to Eq. (82). Let us now discuss the case where the δ_1 does not disappear, namely, $\delta_1 \neq 0$. Normally we can reasonably suppose that the low-energy scattering phase is dominated by the lowest l channel and that the scattering phases at higher l channels are relative small. This is particularly right in low-energy elastic scattering [2,6]. It is well known that for small scattering momentum k, the leading low-energy behavior of the scattering phases $\delta_l(k)$ looks like

$$\delta_l(k) = n_l\pi + a_l k^{2l+1} + \mathcal{O}(k^{2l+3}), \tag{84}$$

for some integer n_l [2]. Therefore, in the low-energy limit, It is a good approximation to treat the p-wave and d-wave scattering phases as small perturbations.

If we expand $\delta_0 = \delta_0^0 + \Delta_0$, where δ_0^0 satisfies Eq. (82) and Δ_0 is a perturbative term, we can work out the first order correction due to Eq. (83) as

$$\Delta_0(k) = \sigma(k)\delta_1(k). \tag{85}$$

The function $\sigma(k)$ represents the sensitivity of higher scattering phases. For C_{4v} symmetry, it is given by

$$\sigma(k) = -\frac{m_{10}^2}{m_{00}^2 + 1}, \tag{86}$$

which is not naturally small and there is no "built-in" mechanism which would automatically decouple the $l = 1$ channel and the $l = 0$ channel. In order for the Eq. (82) to be a good approximation, the phase shift $\delta_1(k)(\mathrm{mod}\,\pi)$ has to be small. Luckily, the case is usually so: the scattering of two particles is dominated by the lowest allowed angular momentum channel.

The sensitivity function $\sigma(q^2)$ can be calculated using the matrix elements given in Eq. (75), and in Appendices A and B, we give a detailed procedure to evaluate the zeta function. The sensitivity function $\sigma(q^2)$ versus q^2 for C_{4v} symmetry with $\alpha = 1.15$ and $\gamma = 1.177$ is illustrated in Fig. 1, here γ is a boost factor, and α factor is defined in Eq. (62), which are typical values we used in Ref. [20]. The lower panel in Fig. 1 is simply the same function as in the upper panel with the scale of the vertical axis being

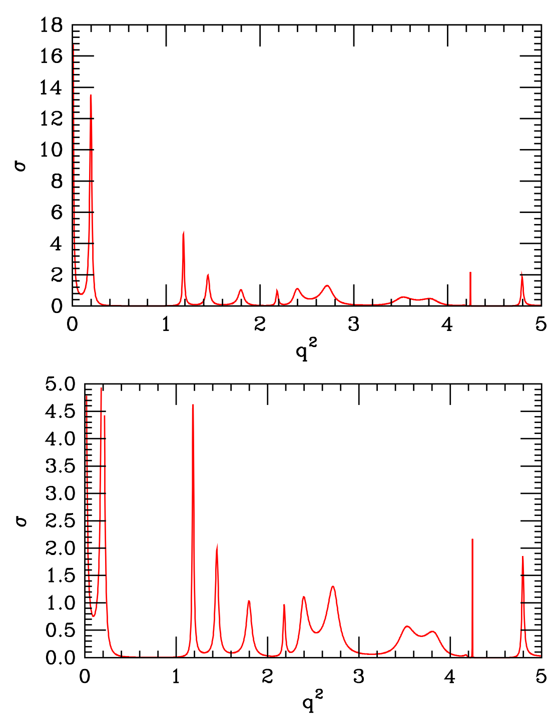

FIG. 1 (color online). The sensitivity $\sigma(q^2)$ as a function of q^2 for C_{4v} symmetry with parameters $\alpha = 1.15$ and $\gamma = 1.177$.

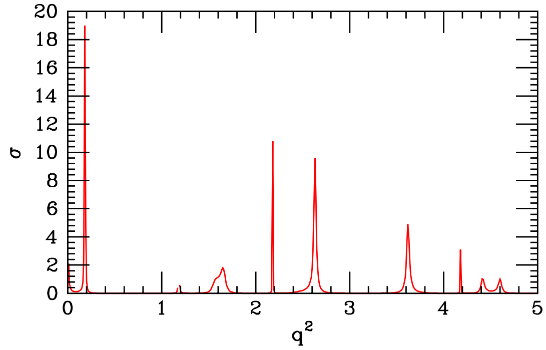

FIG. 2 (color online). The sensitivity $\sigma(q^2)$ as a function of q^2 for C_{4v} symmetry with parameters $\alpha = 1.05$ and $\gamma = 1.177$.

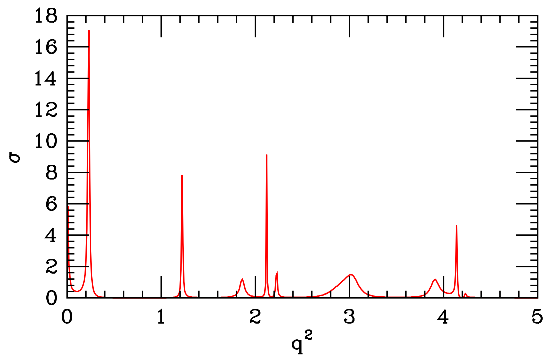

FIG. 3 (color online). The sensitivity $\sigma(q^2)$ as a function of q^2 for C_{4v} symmetry with parameters $\alpha = 1.1$ and $\gamma = 1.067$.

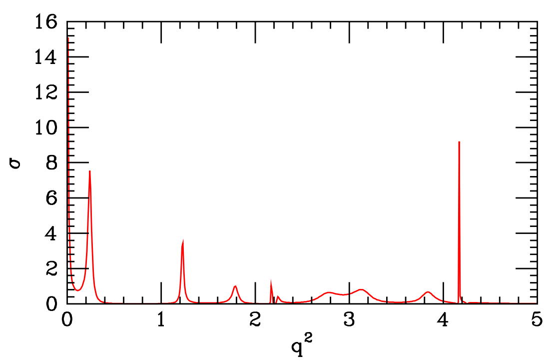

FIG. 4 (color online). The sensitivity $\sigma(q^2)$ as a function of q^2 for C_{4v} symmetry with parameters $\alpha = 1.15$ and $\gamma = 1.067$.

magnified, in order to show the detailed variation of the sensitivity function.

In the work, we also calculate the sensitivity function $\sigma(q^2)$ using the typical α and γ with various values, we found it mostly varies in the range 0–20, in Figs. 2–4, we plotted just three of them. It is seen that the sensitivity function $\sigma(q^2)$ is finite for all $q^2 > 0$. For some special values of q^2, however, the sensitivity function $\sigma(q^2)$ has a sharp peak. This is because of the almost coincidence of singularities of matrix elements m_{00} and matrix elements m_{01} for some choices of α and γ. For all other values of q^2 away from these values, the sensitivity $\sigma(p^2)$ is quite moderate. These characteristics of sensitivity function $\sigma(q^2)$ is somewhat similar to that of the sensitivity function $\sigma_2(q^2)$ in Ref. [7].

We also notice that, when $q \to 0$, the sensitivity function $\sigma(q^2)$ is usually large. However, this does not normally cause any problem because it is nicely canceled out by δ_1 which is of small q^3 order at small q. Therefore, for the range $0 < q^2 < 1.1$ (except some special q^2 values), the Eq. (82) can be reasonably considered to be a good approximation. In fact, this is the range which are usually used to study the elastic scattering [20].

We should bear in mind that if $\delta_1(k)$ is not small, it is very difficult to extract the phase shift functions from the energy spectrum: there are two unknown functions $\delta_0(k)$ and $\delta_1(k)$ but only one Eq. (83). In principle, we still can extract the s-wave scattering phase shift from Eq. (83) through dividing the p-wave phase shift by lattice simulations at various energy, since the corrections due to scattering phases with higher l can be estimated from lattice calculations as well. For example, from Table III, it is obviously seen that, for lattices with C_{4v} symmetry, by inspecting energy eigenstate with E symmetry on the lattice, one can obtain a rough estimate for the p-wave scattering phase δ_1 which dominates this symmetry sector. It seems to be too difficult, but naturally, it is still possible to compute the energy spectrum; this is our future task.

If we choose the sector $\mathbf{d} = 0$, the moving frame and the center-of-mass frame coincide, $\gamma \to 1$ and $P_{\mathbf{d}} \to \mathbb{Z}^3$, and Eq. (83) immediately reduces to the form given in Ref. [2]. Of course, if we select $m_1 = m_2$ and $P_{\mathbf{d}} \to \{\mathbf{r} \in \mathbf{R}^3 | \mathbf{r} = \vec{\gamma}^{-1}(\mathbf{n} + \mathbf{d}/2)\}$, $\mathbf{n} \in \mathbb{Z}^3$, and Eq. (83) nicely reduces to the form presented in Ref. [6]. These are what we expected.

As for $\Lambda = 2$ or higher, it is quite complicated. See the relevant discussion in Ref. [7]. Bearing in mind that this work is an exploratory study for some systems like the πK system, the main purpose is to present some conceptual and theoretical issues, we think that it is enough justified these above assumptions and simplifications.

V. CONCLUSION

In this paper, we strictly investigated the generic two-particle scattering states with periodic boundary conditions, and the best-efforts are paid to derive the modified **d**-periodic rule which is crucial to the modification of the original Rummukainen-Gottlieb formula. The expressions of the energy eigenvalues and the scattering phases in the continuum, which can be regarded as a direct generalization of the famous Rummukainen-Gottlieb formulae to the generic two-particle system in the moving frame, are developed. In particular, we show that the s-wave scattering phase is related to the energy shift by a pretty simple formula, which is just a small alteration of the corresponding formula. We also checked that all of Rummukainen-

Gottlieb's results in Ref. [6] are nicely restored if we set $m_1 = m_2$.

Since the so-called κ meson is a low-lying scalar meson with strangeness, a study of κ meson decay is an explicit exploration of the three-flavor structure of the low-energy hadronic interactions, which is not directly probed in $\pi\pi$ scattering, therefore, it is a significant step for us understanding the dynamical aspect of hadron reactions with QCD. Moreover, the BES Collaboration recently carried out some experimental measurements [25,26] to investigate κ resonance mass and its decay width. With the modified formula in Eq. (82) and our strict discussion of this formula from theoretical aspects, now it will be possible to compute the resonance masses and perhaps its decay widths of some resonances, including possible exotic hadrons as well as traditional hadrons like κ and vector kaon K^*, etc., directly from lattice simulation in a correct manner. We have already used these formulae to preliminarily analyze our πK scattering at the $I = 1/2$ channel [20], and the reasonable results of our lattice simulation data supports these formula.

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APPENDIX A: THE CALCULATION OF ZETA FUNCTION

The method for evaluating the zeta function when $\mathbf{d} = 0$ has been discussed by Lüscher in Ref. [2]. Rummukainen and Gottlieb extended this discussion in the moving frame for $\mathbf{d} \neq 0$, $\alpha = 1$ [6]. The formalism used here is further adapted to the case of $\mathbf{d} \neq 0$, $\alpha \neq 1$, and we just present the essential formulae for numerically calculating zeta function without detailed derivation.

We first denoted the heat kernel of the Laplace operator on a modified $\mathbf{d}$-periodic torus in Eq. (58), namely,

$$K_{\mathbf{d}}(t, \mathbf{x}) = \frac{1}{(2\pi)^3} \sum_{\mathbf{r} \in P_{\mathbf{d}}} e^{i\mathbf{r}\cdot\mathbf{x} - t\mathbf{r}^2}, \tag{A1}$$

where the summation for $\mathbf{r}$ is carried out over the set

$$P_{\mathbf{d}} = \left\{\mathbf{r} | \mathbf{r} = \vec{\gamma}^{-1}\left(\mathbf{n} + \frac{\alpha}{2}\mathbf{d}\right), \mathbf{n} \in \mathbb{Z}^3\right\}, \tag{A2}$$

here the factor α is denoted in Eq. (62), and the operation $\vec{\gamma}^{-1}$ is defined in Eq. (9). Following Poisson's identity, we can rewrite the heat kernel as

$$K_{\mathbf{d}}(t, \mathbf{x}) = \gamma \frac{1}{(4\pi t)^{3/2}} e^{i1/2\alpha\mathbf{d}\cdot\mathbf{x}} \sum_{\mathbf{n}\in\mathbb{Z}^3} e^{-i\alpha\pi\mathbf{d}\cdot\mathbf{n}} \times \exp\left[-\frac{1}{4t}(\mathbf{x} - 2\pi\vec{\gamma}\mathbf{n})^2\right]. \tag{A3}$$

The expression in Eq. (A1) is fast convergent when t is large, and the expression in Eq. (A3) is useful when t is small. We denote the truncated heat kernel $K^{\lambda}_{\mathbf{d}}(t, \mathbf{x})$ as

$$K^{\lambda}_{\mathbf{d}}(t, \mathbf{x}) = K_{\mathbf{d}}(t, \mathbf{x}) - \sum_{\mathbf{r}\in P_{\mathbf{d}}, |\mathbf{r}|<\lambda} \exp(i\mathbf{r}\cdot\mathbf{x} - t\mathbf{r}^2). \tag{A4}$$

We apply the operator $\mathcal{Y}_{lm}(-i\nabla_{\mathbf{x}})$ to the heat kernels as

$$\mathcal{K}^{\lambda}_{\mathbf{d},lm}(t, \mathbf{x}) = \mathcal{Y}_{lm}(-i\nabla_{\mathbf{x}})\mathcal{K}^{\lambda}_{\mathbf{d}}(t, \mathbf{x}). \tag{A5}$$

It can be shown that the zeta function has a rapidly convergent integral expression

$$\mathcal{Z}^{\mathbf{d}}_{lm}(1; q^2) = \sum_{\mathbf{r}\in P_{\mathbf{d}}, |\mathbf{r}|<\lambda} \frac{\mathcal{Y}_{lm}(\mathbf{r})}{\mathbf{r}^2 - q^2} + (2\pi)^3 \int_0^{\infty} dt \left(e^{tq^2} K^{\lambda}_{\mathbf{d},lm}(t, \mathbf{0}) - \frac{\gamma\delta_{l,0}\delta_{m,0}}{16\pi^2 t^{3/2}}\right). \tag{A6}$$

This is our desired integral representation. To calculate the integrand, we use the kernel expression (A1) when $t \geq 1$, and the kernel expression (A3) in the case of $t < 1$. The cutoff λ is chosen so that $\lambda^2 > \mathrm{Re}q^2$. We can easily verify that, when $m_1 = m_2$ (or equivalently $\alpha = 1$), Rummukainen-Gottlieb's result in Ref. [6] is restored.

APPENDIX B: THE EVALUATION OF THE ZETA FUNCTION $\mathcal{Z}_{10}(s; q^2)$

In this appendix we briefly discuss one useful method for numerical evaluation of zeta function $\mathcal{Z}_{10}(s; q^2)$. Here we follow the methods and notations in Ref. [11].

The definition of zeta function $\mathcal{Z}^{\mathbf{d}}_{10}(s; q^2)$ in Eq. (73) is

$$\sqrt{\frac{4\pi}{3}} \cdot \mathcal{Z}^{\mathbf{d}}_{10}(s; q^2) = \sum_{\mathbf{r}\in P_{\mathbf{d}}} \frac{r_3}{(r^2 - q^2)^s}, \tag{B1}$$

where the summation for $\mathbf{r}$ is carried out over the set

$$P_{\mathbf{d}} = \left\{\mathbf{r} | \mathbf{r} = \vec{\gamma}^{-1}\left(\mathbf{n} + \frac{\alpha}{2}\mathbf{d}\right), \mathbf{n} \in \mathbb{Z}^3\right\}, \tag{B2}$$

here the factor α is denoted in Eq. (62). The operation $\vec{\gamma}^{-1}$ is defined in Eq. (9). Without loss of generality, we consider that the value q^2 can be a positive or negative.

First we consider the case of $q^2 > 0$, and we separate the summation in $\mathcal{Z}^{\mathbf{d}}_{10}(s; q^2)$ into two parts as

$$\sum_{\mathbf{r}\in P_{\mathbf{d}}} \frac{r_3}{(r^2 - q^2)^s} = \sum_{r^2<q^2} \frac{r_3}{(r^2 - q^2)^s} + \sum_{r^2>q^2} \frac{r_3}{(r^2 - q^2)^s}. \tag{B3}$$

The second term can be written in an integral form,

$$\sum_{r^2>q^2}\frac{r_3}{(r^2-q^2)^s}=\frac{1}{\Gamma(s)}\sum_{r^2>q^2}r_3\bigg[\int_0^1 dt t^{s-1}e^{-t(r^2-q^2)}+\int_1^\infty dt t^{s-1}e^{-t(r^2-q^2)}\bigg]=\frac{1}{\Gamma(s)}\int_0^1 dt t^{s-1}e^{q^2t}\sum_{\mathbf{r}}r_3e^{-r^2t}-\sum_{r^2<q^2}\frac{r_3}{(r^2-q^2)^s}+\sum_{\mathbf{r}}r_3\frac{e^{-(r^2-q^2)}}{(r^2-q^2)^s}. \tag{B4}$$

The second term neatly cancels out the first term in Eq. (B3). With Poisson's resummation formula we can rewrite the first term in Eq. (B4) as

$$\frac{1}{\Gamma(s)}\int_0^1 dt t^{s-1}e^{tq^2}\sum_{\mathbf{r}}r_3e^{-r^2t}=\frac{\sqrt{\pi}}{\Gamma(s)}\int_0^1 dt t^{s-1}e^{tq^2}\bigg(\frac{\pi}{t}\bigg)^2\sum_{\mathbf{n}\in\mathbb{Z}^3}in_3e^{-i\alpha\pi\mathbf{n}\cdot\mathbf{d}}e^{-(\pi\vec{\gamma}\mathbf{n})^2/t}=\frac{\sqrt{\pi}}{\Gamma(s)}\int_0^1 dt t^{s-1}e^{tq^2}\bigg(\frac{\pi}{t}\bigg)^2\sum_{\mathbf{n}\in\mathbb{Z}^3}n_3\sin(\alpha\pi\mathbf{n}\cdot\mathbf{d})e^{-(\pi\vec{\gamma}\mathbf{n})^2/t}, \tag{B5}$$

where the imaginary parts are neatly canceled out.

After gathering all of the terms, we obtain the representation of the zeta function at $s=1$,

$$\sqrt{\frac{4\pi}{3}}\cdot\mathcal{Z}_{10}^{\mathbf{d}}(1;q^2)=\sum_{\mathbf{r}\in P_{\mathbf{d}}}r_3\frac{e^{-(r^2-q^2)}}{r^2-q^2}+\sqrt{\pi}\int_0^1 dte^{tq^2}\bigg(\frac{\pi}{t}\bigg)^2\times\sum_{\mathbf{n}\in\mathbb{Z}^3}n_3\sin(\alpha\pi\mathbf{n}\cdot\mathbf{d})e^{-(\pi\vec{\gamma}\mathbf{n})^2/t}. \tag{B6}$$

When $\alpha=1$, we can prove that this equation should be zero, then Rummukainen-Gottlieb's result is restored.

For the case of $q^2\le 0$, it is not necessary for us to separate the summation in $\mathcal{Z}_{10}(s;q^2)$, and it can be also written in an integral form. Following the same procedures, we arrive at the same expression in Eq. (B6). Hence, Eq. (B6) can be applied for both cases.

Substituting $\mathbf{d}=(0,0,1)$ into Eq. (B6) we obtain the representation of the zeta function that appeared in Eq. (73)

$$\sqrt{\frac{4\pi}{3}}\cdot\mathcal{Z}_{10}^{\mathbf{d}}(1;q^2)=\sum_{\mathbf{r}\in P_{\mathbf{d}}}r_3\frac{e^{-(r^2-q^2)}}{r^2-q^2}+\sqrt{\pi}\int_0^1 dte^{tq^2}\bigg(\frac{\pi}{t}\bigg)^2\times\sum_{\mathbf{n}\in\mathbb{Z}^3}n_3\sin(\alpha\pi n_3)e^{-(\pi\vec{\gamma}\mathbf{n})^2/t}. \tag{B7}$$

We can easily verify that, if $m_1=m_2$ (or equivalently $\alpha=1$), zeta function $\mathcal{Z}_{10}(1;q^2)\to 0$, Rummukainen-Gottlieb's result is recovered.

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