Phase shift formulas for baryon-baryon scattering in elongated boxes

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We have established the relations between the baryon-baryon scattering phase shifts and the two-particle energy spectrum in the elongated box. We have studied the cases with both the periodic boundary condition and twisted boundary condition in the center of mass frame. The framework is also extended to the system of nonzero total momentum with periodic boundary condition in the moving frame. This will be helpful to extract the phase shifts in the continuum from lattice QCD data using asymmetric volumes.

I. INTRODUCTION

The phase shift for strong elastic scattering of two hadrons is encoded in the basic knowledge on the strong interaction which is one of the four elementary interactions in nature. The phase shift $\delta_l$ is related to the phase difference between the outgoing and the ingoing $l$ wave outside the interaction range, and parameterizes the complicated form of this interaction. The scattering length can be extracted from its effective range expansion. The knowledge from the phase shift also serves to study the resonance, such as in reference [1–8]. Among these references, the authors determined the masses, the widths of the resonances $K^*$ (892), $\rho$, and $a_0$ by calculating the scattering phase shifts of $\pi K$, $\eta K$ coupled channels, $\pi\pi$, $KK$ coupled channels, and $\pi\eta$, $KK$ coupled channels, and etc. A phase shift crossing through $\pi/2$ is often indicative of a resonance, while the sharpness of the rise allows to determine the property of resonance according to Breit-Wigner type functional form.

In the aspect of particle and nuclear physics, unraveling the origin of baryon forces based on the quantum chromodynamics (QCD) is one of the most challenging issues. The precise informations on nuclear and hyperon forces serve as the key ingredients to calculate properties of nuclei, dense matter and the structure of neutron stars [9–13]. According to the baryon-baryon scattering phase shifts that are measured in experiments, people established the relationships on realistic nuclear forces and the fundamental theories such as QCD. However, scattering experiments with hyperons are very difficult because of their short lives. Then, hyperon forces suffer from large uncertainties. Under these circumstances, it is most desirable to carry out the first-principles calculations of baryon forces by lattice QCD. By measuring appropriate correlation functions, energy eigenvalues of two-particle states in a finite box can be obtained. Lüscher found out a relation, now commonly known as Lüscher’s formula, which relates the energy of two-particle state in a finite box of size $L$, i.e., $E(L)$, to the elastic scattering phase-shift $\delta(E(L))$ of the two particles in the continuum [14–17].

Owing to the advent of Lüscher’s formula, various lattice studies, both quenched [18–25] and unquenched [26–35], have been performed over the years to investigate the scattering of hadrons. The original Lüscher’s formula was derived for systems of two identical spinless particles in center-of-mass (COM) frame with periodic boundary condition in cubic box. It restrains the applicability of the formalism to general hadron scattering. To overcome the difficulties, one can of course consider asymmetric volumes [36, 37], or boosting the system to a frame that is different from COM [38–42]. Both will enhance the energy resolution of the problem. Another possible generalization is to use the so-called twisted boundary conditions advocated in Refs. [43–46]. All these generalizations enable one to compute the scattering phases in the low-momentum range which benefits for studying the property of low energy hadron-hadron scattering. Then, generalizations to particles with spin [47–49] are also possible. For example, in Refs. [50, 51], Lüscher’s formulas have been extended to elastic scattering of baryons.

In a cubic box, the three momenta of a single particle are quantized according to $k = (2\pi/L)n$ with $n \in \mathbb{Z}^3$, where $\mathbb{Z}^3$ is the set of 3-tuples of integers. In real simulations, large values of $L$ is needed to control lattice artifacts because of these non-zero momentum modes. However, in the cubic lattice, many low momentum modes are energy degenerate such as modes $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$ since they are related to each another by the cubic symmetry. This means that the second lowest energy level of the particle with non-vanishing momentum corresponds to $n = (1,1,0)$. If one would like to measure these states on the lattice, even larger values of $L$ should be used. One way to remedy this is to use an elongated box. The technique of asymmetric box has first been applied to the calculation of pion-pion elastic scattering [52] and later used in the study of $D^{*+}D^0$ system [53]. In a recent comprehensive study, Frank X. Lee and Andrei Alexandru have derived Lüscher phase shift formulas for mesons and baryons in elongated boxes [54]. In their work, various scenarios, such as moving and zero-momentum states in cubic and elongated boxes, are systematically studied and relations between them are also clarified. The derived formulas are applicable to a wide set of meson-meson and meson-baryon elastic scattering
processes. Therefore they can be applied to investigate various resonances, such as $a_1$, $\Delta$, Roper and so on. In this paper, we would like to synthesize the above mentioned generalizations by trying to seek phase shift formulas that are applicable for baryon-baryon scattering in the elongated box which is a specific asymmetric box whose dimensions are $L \times L \times \eta L$, where $\eta$ is the elongation factor in the $z$-direction.

The organization of the paper is as follows. In Sec. II, we start out by discussing scattering phase shift using a quantum-mechanical model in COM frame in an elongated box. Then, in Sec. III, we generalize the scattering phase shift formulas in the elongated box: in subsection III A, we provide scattering phase shift formulas for baryon-baryon scattering in MF, and in subsection III B, we show the scattering phase shift formulas for baryon-baryon scattering in COM frame with twisted boundary condition. In Sec. IV, we obtain the results in a cubic box, and then perform the consistency checks and have confirmed the validation on the elongated results by comparing the two cases. In Sec. V, we give a brief summary, and also discuss the possible applications of our derived formulas in real lattice simulations.

II. PHASE SHIFT FORMULAS FOR BARYON-BARYON SCATTERING IN COM FRAME IN ELONGATED BOXES

In this section, we try to obtain phase shift formulas that are applicable for baryon-baryon scattering in COM frame in elongated boxes. Basically, we first derive the scattering phase shift formulas for baryon-baryon scattering in a cubic box in COM frame, and then we generalize the formulas to the case in elongated boxes.

A. Brief review of the basic Lüscher's formula

In nonrelativistic quantum mechanics, after factoring out the center-of-mass motions, the asymptotic form of the wave function is written as

$$\psi_{s\nu}(r) \rightarrow \infty \left( \chi_{s\nu} e^{i \hat{k} \cdot \hat{r}} + \sum_{s'\nu'} \chi_{s'\nu'} M_{s'\nu';s\nu} \frac{e^{i kr}}{r} \right). \quad (1)$$

In the remote past, the wave function reduces to an incident plane wave with prescribed quantum numbers. Here $\chi_{s\nu}$ designates spin-wavefunction which is an eigenstate of spin angular momentum of $s^2$ and $\nu$ with the eigenvalues given by $s = 0, \nu = 0$ (singlet state), or $s = 1, \nu = 1, -1, 0$ (triplet state). $M_{s'\nu';s\nu}$ is the scattering amplitude. When one chooses the $z$-axis to coincide with $\hat{k}$, the scattering amplitudes introduced above is related to the $S$-matrix elements as [55]

$$M_{s'\nu';s\nu}(\hat{k} \cdot \hat{r}) = \frac{1}{2 \hat{k} r} \sum_{l=0}^{\infty} \sum_{J=-l}^{l} \sqrt{4\pi (2l+1)} i^{(l-l')} \langle J M | l' m'; s' \nu' \rangle \langle J M | l 0; s \nu \rangle Y_{l'}(\hat{r}). \quad (2)$$

From the Clebsch-Gordan coefficients $\langle J M | l' m'; s' \nu' \rangle$ and $\langle J M | l 0; s \nu \rangle$, we find $M = \nu$ and $m = M - \nu'$. In the previous equation, we have ignored the sum over $M$ and $m$ for a given pair of $\nu$ and $\nu'$. It is well-known that the phase shift enters via $S$-matrix. Lüscher obtained a relation, which relates the energy of two-particle state in a finite box of size $L$, i.e., $E(L)$, to the elastic scattering phase $\delta(E(L))$ of the two particles in the continuum. This inspires us that if one calculates two-particle scattering phase shifts, one should derive the corresponding Lüscher's formula firstly.

With the help of Eq. (1) and Eq. (2), we obtain the following asymptotic form of the wave function as

$$\psi_{s\nu}(r) = \sum_{s'JM} \sqrt{4\pi (2l+1)} W_{l'J}\langle J M | l 0; s \nu \rangle Y_{l'}(\hat{r}). \quad (3)$$

where $Y_{l'}(\hat{r})$ is the spin spherical harmonics whose explicit form is given by

$$Y_{l'm}(\hat{r}) = \sum_{m'} Y_{lm}(\hat{r}) c_{m'm}. \quad (4)$$

In Eq. (3), $W_{l'J}(r)$ is the radial wave function of the two-particle scattering state. In the large $r$ region, when the two-particle interaction is ignored and the potential vanishes, the wave function $W_{l'J}(r)$ has the following asymptotic form:

$$W_{l'J}(r) = \frac{1}{2ikr} i^{(l-l')} \left[ S_{l'J} e^{i kr} + (-1)^{l+1} e^{-ikr} \delta_{l're} \right]. \quad (5)$$

For baryon-baryon scattering, we enclose the two-particle system in a cubic box of size $L$ with periodic boundary condition. In the outer region where the potential vanishes, the wave function becomes

$$\psi(r) = \sum_{s'JM} \left[ F_{JMls} W_{l'J} \right] Y_{l'M}(\hat{r}). \quad (6)$$

Then, we can expand the wave function into a linear superposition of the singular periodic solutions, i.e., $G_{JMls}(r; k^2)$, of the Helmholtz equation in the outer region. Thus, one can get

$$\psi(r) = \sum_{s=0}^{\infty} \sum_{l=0}^{\infty} \sum_{J=-l}^{l} \sum_{M=-l}^{l} v_{JMls} G_{JMls} (r; k^2). \quad (7)$$

Here, $G_{JMls}(r; k^2)$ can be further expanded in terms of spherical harmonics

$$G_{JMls} = \frac{(-1)^J 4 \pi i^{l+1}}{4\pi} \left( Y_{l'M} n_l(kr) + \sum_{J'JM'lv} M_{JMl;JMl'} \langle k^2 \rangle Y_{l'M'}(kr) \right). \quad (8)$$
where the explicit form of $\mathcal{M}_{JM; J'}(q^2)$ with $k = (2\pi/L)q$ is written as

$$
\mathcal{M}_{JM; J'}(q^2) = \sum_{m,m'} \langle JM|lm; sv\rangle\langle J'M'|l'm'; sv\rangle
\times \mathcal{M}_{lm,l'm'}(q^2),
$$

with

$$
\mathcal{M}_{lm,l'm'}(q^2) = \sum_{t=|l-l'|} \frac{(-1)^{l+l'}\sqrt{2l+1}}{2\pi/2q^{l+1}}
\times Z_{tt}^c(q^2, \eta)(l00|l'0)\langle llmt_z|l'm'\rangle
\times \sqrt{(2l+1)(2l+1)}.(10)
$$

For convenience, we introduce the short-hand function

$$
\omega_{lm}(q^2) = \frac{Z_{lm}(q^2, \eta)}{\pi^{3/2} q^{l+1}}.
$$

Then the zeta function in cubic boxes is written as

$$
Z_{lm}(q^2) = \sum_n \frac{\gamma_{lm}(n)}{n^2 - q^2},
$$

B. Extension in elongated boxes in COM frame

In the following, we generalize the basic form of Lüscher’s formula to that in an elongated box. In this case, one can expand the wave function of the system in the outer region as a series of the modified matrix, whose element is $\mathcal{M}_{JM; J'}(q^2, \eta)$, i.e.,

$$
\mathcal{M}^{(s)}_{JM; J'}(q^2, \eta) = \sum_{m,m'} \langle JM|lm; sv\rangle\langle J'M'|l'm'; sv\rangle
\times \mathcal{M}_{lm,l'm'}(q^2, \eta),
$$

$$
\mathcal{M}_{lm,l'm'}(q^2, \eta) = \sum_{t=|l-l'|} \sqrt{2l+1}
\times Z_{tt}^c(q^2, \eta)(l00|l'0)\langle llmt_z|l'm'\rangle
\times \sqrt{(2l+1)(2l+1)}.(15)
$$

Hereafter for convenience, we introduce the short-hand function $\omega_{lm}(q^2, \eta)$ for zeta function as follows:

$$
\omega_{lm}(q^2, \eta) = \frac{Z_{lm}(q^2, \eta)}{\pi^{3/2} q^{l+1}}.
$$

Then the generalized zeta function for $z$-elongated boxes is given by

$$
Z_{lm}(q^2, \eta) = \sum_n \frac{\gamma_{lm}(\mathbf{n})}{\mathbf{n}^2 - q^2}.
$$

where $\gamma_{lm}(\mathbf{n}) = \mathbf{n}^2 \gamma_{lm}(\theta, \phi)$. Here, the modified index $\mathbf{n}$ is $\mathbf{n} = (n_x, n_y, n_z)$. Apart from the above-mentioned substitutions, the extra attention should also be paid to the difference in symmetry. In order to discuss Lüscher’s formula in the elongated box, the symmetry of two-particle system is no longer $O_h$ but reduces to $D_{4h}$ group. This group contains 16 elements that can be divided into the following ten conjugate classes: $A^+_1, A^+_2, B^+_1, B^+_2$, and $E^\pm$. For instance, for $J = 0, 1, 2$ when the cutoff momentum $\Lambda = 2$, the decomposition into irreducible representation is given by $0^\pm = A^\pm_1$, $1\pm = A^\pm_2 \oplus E^\pm$, $2^\pm = A^\pm_3 \oplus B^\pm_1 \oplus B^\pm_2 \oplus E^\pm$, respectively [54]. In a definite irreducible representation of the $D_{4h}$ group, the basis vectors are labeled as $|\Gamma, \xi, J, l, s, n\rangle$, where $\Gamma$ denotes the representation; $\xi$ runs from 1 to the number of the dimensions, and $n$ runs from 1 to the multiplicity of the representation. This basis can be expressed by linear combinations of $|JM\rangle$. The corresponding matrix $\mathcal{M}$ is diagonal with respect to $\Gamma$ and $\xi$ by Schur’s lemma [16]. If there is no multiplicity, the labels $n = 1$ and $n' = 1$ can be dropped. Therefore, in a definite symmetry sector $\Gamma$, the explicit form of Lüscher’s formula is given by Eq. (18).
Before writing out the explicit form of the phase shift formula, one should exploit the symmetry properties to simplify the $\mathcal{M}$ matrix and the parity of the two-particle system. On the one hand, the matrix is hermitian which constrains half of the off-diagonal elements. Furthermore, a lot of short-hand functions $\omega_{lm}(q^2, \eta)$ vanish to satisfy certain constraints, which can be traced back to how the zeta function behaves under the symmetry operations in the elongated box. The properties follow Ref. [54]. On the other hand, the total angular momentum for two scattering particles with spin $s_1$ and $s_2$ is $J = s_1 + s_2 + l$ with $l$ the relative orbital angular momentum dubbed “partial waves”. For the asymptotic states, the two particles are far away from each other so that they are not interacting. Then, we can label the states with $s$, $s_1$, and $s_2$, where $s = s_1 + s_2$ is the total spin. The total angular momentum $J$ is conserved during the scattering process, but both $l$ and $s$ will change. For the baryon-baryon scattering considered in this paper, the total spin $s$ can take 0 (singlet state) or 1 (triplet states). Moreover, the orbital angular momentum also remains fixed for our cases: In the case with $s = 0$ we have $l = J$ which is conserved, and the parity is simply $(-1)^J$. When $s = 1$ for a given $J$, $l$ takes three different values, i.e., $l = J + 1$, $J - 1$, $J$. The first two have the same parity $(-1)^{J+1}$, and the parity for third one is $(-1)^J$. The total parity of the two-particle state is equal to $P_{\text{tot}} = P_1 P_2 (-1)^l$, where $P_1$ and $P_2$ are the intrinsic parities of the two scattering particles. For simplicity we assume that the intrinsic parity $P_1 P_2$ is positive, then the total parity is $(-1)^l$. For parity-conserving theories like QCD, there is no scattering between states with opposite parity. Then we divide Lüscher’s formulas into the case A and case B corresponding to the states with parity $(-1)^{J+1}$ and parity $(-1)^J$ respectively.

C. Application to case A

In this case ($s = s' = 1$, $l = J \pm 1$), Lüscher’s formula becomes

\[
\sum_{l''} (S_{l'';l}^J - \delta_{l''} \delta_{s''}) \mathcal{M}_{J,l'';J,l''}(\Gamma) - i \delta_{J,J'} (S_{l'';l}^J + \delta_{l''} \delta_{s''}) = 0. \tag{18}
\]

According to non-zero matrix elements $\omega_{lm}$ are given in Tab. I, one can obtain phase shift in the definite symmetry. Then we list the phase shift with different irreducible representations of the $D_{4h}$ group.

If we consider the explicit parity and also suppose that the cutoff angular momentum is $\Lambda = 2$, the decomposition in this case becomes $0^- = A_1^-$, $1^+ = A_2^+ \oplus E^+$, $2^- = A_1^- \oplus B_1^- \oplus B_2^- \oplus E^-$. For instance, in the $A_1^-$ representation, the phase shift formula is Eq. (20).

\[
\left| \cot \delta_{01} - (\omega_{00} - 2\sqrt{30} \omega_{22}) \right| - \frac{\sqrt{10}}{5} \omega_{20} - \frac{2\sqrt{15}}{15} \omega_{22} \cot \delta_{21} - (\omega_{00} + \frac{\sqrt{5}}{5} \omega_{20} - \frac{\sqrt{30}}{15} \omega_{22}) = 0. \tag{20}
\]

If we ignore the mixing with $J = 2$, one can extract phase shift $\delta_{01}$ from

\[
\cot \delta_{01} = \omega_{00} - \frac{2\sqrt{30}}{15} \omega_{22}. \tag{21}
\]

Next, if we want to calculate phaseshift $\delta_{21}$, we can consider representation $B_1^-, B_2^-$, and $E^-$. The phase shift formula in these three representations are written as

\[
\begin{align*}
\cot \delta_{21} &= \omega_{00} - \frac{\sqrt{5}}{5} \omega_{20} - \frac{\sqrt{30}}{5} \omega_{22} \\
\cot \delta_{21} &= \omega_{00} - \frac{\sqrt{5}}{5} \omega_{20} + \frac{\sqrt{30}}{5} \omega_{22} . \\
\cot \delta_{21} &= \omega_{00} + \frac{\sqrt{5}}{10} \omega_{20}
\end{align*}
\]

Finally, let us discuss the quantum number $J^P$ of the two-particle state which is $1^+$ in $A_2^+$ and $E^+$ representations, i.e., the total angular momentum $J$ is fixed for 1. There is a mixing with $l = J - 1 = 0$ (S-wave) and $l = J + 1 = 2$ (D-wave). To proceed, we need to param-
TABLE I: \(D_{4h}\) symmetry group for angular momentum up to \(J = 2\) and \(l = 2\). The results are separated according to parity \((-1)^{J+1}\).

| \(\Gamma\) | \(J\) | \(J'\) | \(M^{(1)}(\Gamma)\) |
|---|---|---|---|
| \(A_1^+\) | 01 | 01 | \(\omega_{00} = \frac{2\sqrt{10}}{3} \omega_{22}\) |
| | | 01 | \(-\frac{2}{5} \omega_{20} - \frac{2\sqrt{10}}{3} \omega_{22}\) |
| | | 21 | \(\omega_{00} + \frac{\sqrt{10}}{3} \omega_{20} - \frac{\omega_{22}}{2}\) |
| \(A_2^+\) | 10 | 10 | \(\omega_{00}\) |
| | | 12 | \(\frac{\sqrt{10}}{3} \omega_{20}\) |
| \(B_1^+\) | 21 | 21 | \(\omega_{00} - \frac{\sqrt{10}}{3} \omega_{20} - \frac{2\sqrt{10}}{3} \omega_{22}\) |
| \(B_2^+\) | 21 | 21 | \(\omega_{00} - \frac{\sqrt{10}}{3} \omega_{20} + \frac{2\sqrt{10}}{3} \omega_{22}\) |
| \(E^+\) | 10 | 10 | \(\omega_{00}\) |
| | | 12 | \(-\frac{2\sqrt{10}}{3} \omega_{20} - \frac{\omega_{22}}{3}\) |
| \(E^-\) | 21 | 21 | \(\omega_{00} + \frac{\sqrt{10}}{3} \omega_{20}\) |

where \(I_{2 \times 2}\) is a \(2 \times 2\) unit matrix. In \(E^+\) representation, we should substitute \(M^{(1)}_{Jll'}\) according to Tab. I with Eq. (23).

D. Application to case B

For this case \((l = l' = l'' = J, s = 0, 1)\), the Lüscher’s formula can be expressed as shown in Eq. (24).

\[
\sum_{l''} (S_{l''s';ls} - \delta_{l''l} \delta_{ss'}) M^{(s')}_{Jll'';Jl''} - i \delta_{JJ'} (S_{ls';ls} + \delta_{ss'}) = 0 .
\] (24)

If we consider the explicit parity and also suppose that the cutoff angular momentum is \(\Lambda = 2\), the decompo-
The matrix again using the "eigenphase convention" of Blatt and Biedenharn [56], whose explicit form is similar to Eq. (22). Thus, \( \delta_\alpha \) and \( \delta_\beta \) are the scattering phase shifts corresponding to two eigenstates of the S-matrix called \( \alpha \) and \( \beta \) waves respectively. At low energies, however, the \( \alpha \)-wave is predominantly \( s = 0 \) with a small admixture of the \( s = 1 \), while the \( \beta \)-wave is predominantly \( s = 1 \) with a small admixture of the \( s = 0 \). According to the non-zero matrix elements, one can obtain phase shift formula in a definite symmetry. For example, if we focus on the \( A_1^+ \) representation with positive parity that corresponds \( J = 0 \) and ignoring the index \( l \) and \( l' \), both of which are unity, the phase shift formula is Eq. (25).

\[
S_{2 \times 2} = \begin{pmatrix}
\cos \epsilon & -\sin \epsilon \\
\sin \epsilon & \cos \epsilon \\
\end{pmatrix} \begin{pmatrix}
\epsilon^{2i\delta_\alpha} & 0 \\
0 & \epsilon^{2i\delta_\beta} \\
\end{pmatrix} \begin{pmatrix}
\cos \epsilon & \sin \epsilon \\
-\sin \epsilon & \cos \epsilon \\
\end{pmatrix}
\]

In the above discussion, we have not taken into account the possibility for the identical nature of the two scattering particles, and thus the singlet-triplet transition within the same parity is allowed. However, for the two identical particles, the singlet-triplet transition is forbidden since the singlet state has an antisymmetric spin wave function which then requires a symmetric spatial one that necessarily has positive parity while the triplet state has the opposite parity. Below, we list Lüscher formulas for \( s = s' = 0 \) and \( s = s' = 1 \) cases respectively:

\[
\sum_{l'\nu'} (S_{l'0;0} - \delta_{l'\nu'}) \mathcal{M}_{Jl';Jl'}^{(0)} - i \delta_{J'l'} (S_{l0;0} + 1) = 0 .
\]

(27)

\[
\sum_{l'\nu'} (S_{l'1;1} - \delta_{l'\nu'}) \mathcal{M}_{Jl';Jl'}^{(1)} - i \delta_{J'l'} (S_{l1;1} + 1) = 0 .
\]

(28)

The formula in \( E^- \) representation is similar to Eq. (26) expect that the matrix \( \mathcal{M}_{Jl'Jl'}^{(s')} \) in the equation is replaced by the corresponding one according to Tab. II and Tab. III.

In particular, Lüscher's formula for \( s = s' = 0 \) is same with the meson-meson scattering case. Then, we only discuss the case for \( s = s' = 1 \). In this case, we denote phase shift as \( \delta_J \) (we have ignored the index \( l \) due to \( J = l \) in this case) in the definite representation. According to the non-zero matrix elements listed in Tab. II, one can obtain phase shift \( \delta_J \) in the definite representation.

If we focus on phase shift \( \delta_2 \), one can consider \( A_1^+ \), \( B_1^+ \), \( B_2^+ \), and \( E^+ \) representations. The phase shift formulas in these representations are similar with each other expect that the matrix \( \mathcal{M}_{Jl'Jl'}^{(s')} \) is different. We list the explicit form of these matrix in Tab. II. For instance, we take \( A_1^+ \) representation as an example, where the phase shift formula is

\[
\cot \delta_2 = \omega_0 - \frac{4}{7} \omega_{40} - \frac{\sqrt{5}}{7} \omega_{20} + \frac{\sqrt{30}}{7} \omega_{22} + \frac{2\sqrt{10}}{7} \omega_{42} .
\]

(29)

Then, if one wants to obtain \( \delta_1 \), one should consider \( A_2^- \) and \( E^- \) representations. Here, we take \( A_2^- \) representation as an example. In this case, the phase shift \( \delta_1 \) is
TABLE II: $D_{4h}$ symmetry group for angular momentum up to $J = 2$ and $l = 2$. The results are separated according to parity $(-1)^s, s=s' = 1$

| $\Gamma$ | $JlJ'\ell'\mathcal{M}_{JlJ'\ell'}^{ij}(\Gamma)$ |
|--------|--------------------------------------------------|
| $A^+_1$ | $222 \quad \omega_{00} - \sqrt{2} \omega_{20} + \sqrt{6} \omega_{22}$ |
| $A^-_2$ | $11 \quad \omega_{00} - \sqrt{2} \omega_{20} + \sqrt{6} \omega_{22}$ |
| $B^+_1$ | $222 \quad \omega_{00} - \sqrt{2} \omega_{20} - \sqrt{6} \omega_{22}$ |
| $B^-_2$ | $222 \quad \omega_{00} - \sqrt{2} \omega_{20} - \sqrt{6} \omega_{22}$ |
| $E^+_1$ | $111 \quad \omega_{00} - \frac{1}{2} \omega_{20}$ |
| $E^-_3$ | $222 \quad \omega_{00} + \frac{1}{2} \omega_{20} + \frac{4}{\sqrt{3}} \omega_{22}$ |

TABLE III: $D_{4h}$ symmetry group for angular momentum up to $J = 2$ and $l = 2$. The results are separated according to parity $(-1)^s, s=s' = 0$

| $\Gamma$ | $JlJ'\ell'\mathcal{M}_{JlJ'\ell'}^{ij}(\Gamma)$ |
|--------|--------------------------------------------------|
| $A^+_1$ | $222 \quad \omega_{00} + \frac{1}{2} \omega_{20} + \frac{2}{\sqrt{3}} \omega_{22}$ |
| $A^-_2$ | $111 \quad \omega_{00} + \frac{1}{2} \omega_{20} + \frac{2}{\sqrt{3}} \omega_{22}$ |
| $B^+_1$ | $222 \quad \omega_{00} + \frac{1}{2} \omega_{20} - \frac{2}{\sqrt{3}} \omega_{22}$ |
| $B^-_2$ | $222 \quad \omega_{00} + \frac{1}{2} \omega_{20} - \frac{2}{\sqrt{3}} \omega_{22}$ |
| $E^+_1$ | $111 \quad \omega_{00} - \frac{1}{2} \omega_{20}$ |
| $E^-_3$ | $222 \quad \omega_{00} + \frac{1}{2} \omega_{20} - \frac{4}{\sqrt{3}} \omega_{22}$ |

\[
\cot \delta_1 = \omega_{00} - \frac{\sqrt{5}}{5} \omega_{20} + \frac{\sqrt{30}}{5} \omega_{22}. \quad (30)
\]

III. SOME GENERALIZATIONS OF PHASE SHIFT FORMULAS FOR BARYON-BARYON SCATTERING IN ELONGATED BOXES

A. Phase shift formulas for baryon-baryon scattering in MF

In this subsection, we extend the phase shift formula that has been obtained in the previous subsection for baryon-baryon scattering to moving frames (MF) in an elongated box. We will follow the notations in Ref. [38] below. We denote the four momenta of the two particles with periodic boundary conditions in the lab frame by

\[
\mathbf{k} = (E_1, \mathbf{k}), \quad \mathbf{P} - \mathbf{k} = (E_2, \mathbf{P} - \mathbf{k}), \quad (31)
\]

where $E_1 = \sqrt{k^2 + m_1^2}$ and $E_2 = \sqrt{(\mathbf{P} - \mathbf{k})^2 + m_2^2}$ are energies of the two particles respectively, $m_1$ and $m_2$ are the mass values of the two baryons respectively. The total three momentum $\mathbf{P} \neq 0$ of the two-particle system is quantized by the condition $\mathbf{P} = (2\pi/L)\mathbf{d}$ with $\mathbf{d} \in \mathbb{Z}^3$. The COM frame is then moving relative to the lab frame with a velocity

\[
\mathbf{v} = \mathbf{P}/(E_1 + E_2). \quad (32)
\]

Then, we denote the momenta of the two particles with $\mathbf{k}^*$ and $(-\mathbf{k}^*)$ for the two scattering particles. Thus, $\mathbf{k}^*$ is related to $\mathbf{k}$ by conventional Lorentz boost:

\[
\mathbf{k}^* = \gamma(\mathbf{k}^\parallel - \mathbf{v} E_1), \quad \mathbf{k}^\perp = \mathbf{k}^\perp, \quad (33)
\]

where the symbol $\parallel$ and $\perp$ designate the components of the corresponding vector perpendicular and parallel to $\mathbf{v}$, respectively. For simplicity, the above relation is also denoted by the shorthand notation: $\mathbf{k}^* = \frac{\mathbf{v}}{c} \mathbf{k}$. A similar transformation relation holds for the other particles.

Following similar steps listed in Sec. II, we obtained the Lüscher’s formula in this case. Lüscher’s formula takes exactly the same form as Eq. (13) except that all matrix elements are replaced with the modified matrix elements $\mathcal{M}_{JlJ'\ell'}(\mathbf{k}^2, \eta)$. The explicit form for the matrix element is written as

\[
\mathcal{M}_{JlJ'\ell'}(\mathbf{k}^2, \eta) = \sum_{m'm'} \langle JM|lm; sv\rangle \langle J'M'|l'm'; sv\rangle \times \mathcal{M}^{d(s)}_{JlJ'\ell'l'm'}(\mathbf{k}^2, \eta) \quad (34)
\]

with $\mathbf{k} = \mathbf{k}/(2\pi)$. The reduction matrix in moving frames has been obtained in Ref. [38, 41], whose explicit
form is given by
\[
\mathcal{M}_{lm;lm'}^d(\kappa^2, \eta) = \sum_{t'=l-l'} \sum_{t=|l-l'|} \frac{(-1)^{l+l'+t}}{\gamma \pi^{3/2} \eta^{l+1}} [t \rangle \langle t' | \langle 000 | [t'] \langle lmm' | [l'] \langle m't | s \rangle s \rangle \\
\times Z_{tt'}^d(\kappa^2, \eta) \langle 000 | [t] \langle t' | lmm' \rangle \langle l' m' | s \rangle s \rangle \right].
\]

(35)

where \(\gamma\) is the Lorentz factor of the boost, and the modified zeta function \(Z_{tt'}^d(\kappa^2, \eta)\) is defined via
\[
Z_{tt'}^d(\kappa^2, \eta) = \sum_{\hat{n} \in \mathcal{P}_d} \frac{Y_{tt'}(\hat{n})}{\hat{n}^2 - \kappa^2}.
\]

(36)

In the above formula, \(\mathcal{P}_d\) is the following set,
\[
\mathcal{P}_d = \left\{ \hat{n} \in \mathbb{R}^3 | \hat{n} = \gamma(n + \frac{1}{2} d) \in \mathbb{Z}^3 \right\},
\]

(37)

where \(d = (L/2 \pi) \mathbf{P},\) \(\alpha = 1 + \frac{w_i^2 - w_2^2}{w_3^2},\) and \(w_i^2 = m_i^2 + k^2\) with \(i = 1, 2\) being the energy for the two scattering particles. We will also use \(E^*\) to denote the total energy in the center of mass frame and introduce the short-hand

\[
\phi_{lm}^d(\kappa^2, \eta) = \frac{Z_{lm}^d(\kappa^2, \eta)}{\gamma \pi^{3/2} \eta^{l+1}}.
\]

(38)

In addition, an extra attention should also be paid to the difference in symmetries. In order to discuss phase shift formula in MF, we should introduce the space group \(G,\) which is a semi-direct product of lattice translational group \(T\) and the cubic group \(O.\) The representations are characterized by the little group \(\Gamma\) and the corresponding total momentum \(P.\) For example, for the case with \(\mathbf{P} = \frac{2\pi}{L} \mathbf{e}_3,\) the corresponding little group is \(C_{4v}.\) Then, following similar steps as in the COM frame, one can readily obtain the explicit formulas for the little group \(C_{4v}.\) Before giving the explicit form of phase shift, we should calculate non-vanished matrix of \(\mathcal{M}_{lm;lm'}^d,\) with the \(C_{4v}\) group that is listed in Tab. IV and Tab. V. Then, following similar steps as in Sec. II, one can readily obtain the phase shift formulas in the moving frame. Here, we take phase shift formula in Case A, where \(l = j + 1\) as an example. For instance, in the \(A_1\) representation, the phase shift formula is given by Eq. (39) if we ignore the mixing with \(l = 2.\)

\[
\begin{align*}
\cot \delta_{01} - (\omega_{00} - \frac{2 \sqrt{2} \omega_{22}}{\sqrt{3}}) &+ \sqrt{\frac{2}{3}} \omega_{11} + \sqrt{\frac{2}{3}} \omega_{10} \\
\cot \delta_{02} &+ \sqrt{\frac{2}{3}} \omega_{12} \\
\cot \delta_{10} &- \omega_{00} \\
\cot \delta_{21} - (\omega_{00} + \frac{2 \sqrt{2} \omega_{22}}{\sqrt{3}}) &+ \sqrt{\frac{2}{3}} \omega_{11} - \sqrt{\frac{2}{3}} \omega_{12} \\
\end{align*}
\]

(39)

We note that there is mixing between odd and even \(J\) due to lack of parity in the boosted two-particle state.

B. Phase shift formulas for baryon-baryon scattering in COM frame with twisted boundary condition

In this subsection, we impose the twisted boundary condition for the two-particle system in the COM frame.

The quantized momentum is \(k = \frac{2\pi}{L}(n + \frac{d}{2L})\) with \(n\) the three-dimensional vector and \(\theta\) is the twist angle. By adjusting the twist angle, one can gain more moments for the two-particle energy levels. Lüscher’s formula takes exactly the same form as shown in Eq. (13) except that all the labels of \(\mathcal{M}_{JML;J'M'L'}^{(s)}\) are replaced by \(\mathcal{M}_{JML;J'M'L'}^{(s)}\).

The explicit form of \(\mathcal{M}_{JML;J'M'L'}^{(s)}\) is given by
\[
\mathcal{M}_{JML;J'M'L'}^{(s)}(q^2, \eta) = \sum_{m'm'} \langle JM|lm; sv\rangle \langle J'M'|l'm'; sv\rangle \\
\times \phi_{lm;lm'}^{(s)}(q^2, \eta),
\]

(40)

where
\[
\begin{align*}
\phi_{lm;lm'}^{(s)}(q^2, \eta) &+ \sum_{t'=l-l'} \sum_{t=|l-l'|} \frac{(-1)^{l+l'+t}}{\gamma \pi^{3/2} \eta^{l+1}} [t \rangle \langle t' | \langle 000 | [t] \langle t' | lmm' \rangle \langle l' m' | s \rangle s \rangle \\
\times Z_{tt'}^{(s)}(q^2, \eta) \langle 000 | [t] \langle t' | lmm' \rangle \langle l' m' | s \rangle s \rangle \right].
\end{align*}
\]

(41)

Here, \(\Gamma = \{ \hat{n} \in \mathbb{R}^3 | \hat{n} = n + (2\pi)^{-1} \phi, n \in \mathbb{Z}^3 \},\) and \(\mathbb{R}^3\) is the set of real 3-tuples. The short-hand function for zeta function is
\[
\omega_{lm;lm'}^{(s)}(q^2, \eta) = \frac{Z_{lm}^{(s)}(q^2, \eta)}{\pi^{3/2} q q^{l+1}}.
\]

(43)

For the case with \(\phi = (0, 0, 0)\), the corresponding little group is written as \(C_{4v}.\) Taking the phase shift formula
TABLE IV: $C_{4v}$ symmetry group for angular momentum up to $J = 2$ and $l = 2$. The results are separated according to parity $(-1)^{J±1}.s = s′ = 1$

| $\Gamma$ | $Jl$ | $J′l′$ | $M_{00}^{d(1)}(\Gamma)$ |
|---------|------|--------|------------------|
| $A_1$   | 01   | 01     | $\omega_{00} = \frac{2\sqrt{10}}{\omega_{12}}$ |
|         | 01   | 10     | $\omega_{00} + \frac{\sqrt{10}}{\omega_{12}}$ |
|         | 12   |        | $\omega_{00} - \frac{\sqrt{10}}{\omega_{12}}$ |
|         | 21   |        | $\omega_{00} + \frac{\sqrt{10}}{\omega_{12}}$ |
| $B_1$   | 21   | 21     | $\omega_{00} - \frac{\sqrt{10}}{\omega_{12}}$ |
|         | 21   | 10     | $\omega_{00} + \frac{\sqrt{10}}{\omega_{12}}$ |
| $E$     | 10   | 10     | $\omega_{00} = \frac{\sqrt{10}}{\omega_{12}}$ |

TABLE V: $C_{4v}$ symmetry group for angular momentum up to $J = 2$ and $l = 2$. The results are separated according to parity $(-1)^{J±1}.s = s′ = 1$

| $\Gamma$ | $Jl$ | $J′l′$ | $M_{00}^{d(1)}(\Gamma)$ |
|---------|------|--------|------------------|
| $A_1$   | 11   | 11     | $\omega_{00} - \frac{\sqrt{10}}{\omega_{12}}$ |
|         | 11   | 22     | $\omega_{00} + \frac{\sqrt{10}}{\omega_{12}}$ |
|         | 22   | 22     | $\omega_{00} = \frac{\sqrt{10}}{\omega_{12}}$ |
| $B_1$   | 22   | 22     | $\omega_{00} - \frac{\sqrt{10}}{\omega_{12}}$ |
|         | 22   | 11     | $\omega_{00} + \frac{\sqrt{10}}{\omega_{12}}$ |
| $E$     | 11   | 11     | $\omega_{00} = \frac{\sqrt{10}}{\omega_{12}}$ |

IV. PHASE SHIFT FORMULAS FOR BARYON-BARYON SCATTERING IN COM FRAME IN CUBIC BOX

In this section, we briefly discuss phase shift formulas for baryon-baryon scattering in COM frame in cubic box.

On the one hand, we can perform the consistency checks and validation on the elongated results by comparing the two cases. On the other hand, this can serve as a basis for exploring the relationship between the two cases, providing valuable insight into how the results transform from one to the other.

Lüscher’s formula takes the form given in Eq. (13). To write out a more explicit formula, we should consider the definite cubic symmetries. For the case of integer total momentum $J$, we need to consider the group of $O_h$, which contains 48 elements and can be divided into 10 conjugate classes: $A_1^+, A_2^+, E^+, T^+_1$ and $T^+_2$. For instance, for $J = 0, 1, 2, \Lambda = 2$, the decomposition into irreducible representation is given by $0^+ = A_1^+, 1^+ = T^+_1$, $2^+ = T^+_2 \oplus E^+$ respectively [54]. Then, we take Lüscher’s formula in Case $A(s = s′ = 1, l = J ± 1)$ as an exam-
ple. Before writing out the explicit phase formula in this case, we list non-vanished matrix elements \( M_{J,l;J';l'}^{(s)}(\Gamma) \) in Tab. VI. According to the non-zero matrix elements, one can obtain phase shift formula in the definite symmetry. If we focus in \( A_1 \) representation, the phase shift formula is Eq. (44).

\[
\cot \delta_{01} - (\omega_{00} - 2\sqrt{30}/3 \omega_{22}) = 0
\]

(44)

If we consider D-wave resonance, we can give the phase shift formulas in \( E^- \) and \( T_2^- \) representations respectively, i.e.,

\[
\cot \delta_{21} = \omega_{00} - 2\sqrt{30}/15 \omega_{22},
\]

(46)

\[
\cot \delta_{21} = \omega_{00} + \sqrt{30}/15 \omega_{22}.
\]

(47)

Finally, for the \( T_1^+ \) representation with \( O_h \) group, the phase shift formula is given by Eq. (48).

\[
\left| S_{2\times2} - I_{2\times2} \right| \left( \begin{array}{c}
\omega_{00} - 2\sqrt{30}/15 \omega_{22} \\
-2\sqrt{30}/15 \omega_{22} - \omega_{00} + 2\sqrt{30}/15 \omega_{22}
\end{array} \right) - i \left( S_{2\times2} + I_{2\times2} \right) = 0
\]

(48)

Then, let us discuss the relationship of two-particle scattering L"uscher’s formula between the cubic case and the elongated case. In Tab. VII, we listed the symmetry relationship between \( O_h \) and \( D_{4h} \). By using the relationship in Tab. VII, one can readily obtain the following relationships. For \( J = J' = 0 \), the \( A_1 \) has one-to-one correspondence:

\[
M_{01:01}^{(1)}(A_1^*) = M_{01:01}^{(1)}(A_1^-).
\]

(49)

Then, for \( J = J' = 2 \), the \( E^- \) splits into \( A_1^- \) and \( B_1^- \), i.e.,

\[
M_{21:21}^{(1)}(E^-) = \frac{1}{2} M_{21:21}(A_1^-) + \frac{1}{2} M_{21:21}(B_1^-).
\]

(50)

Next, for \( J = J' = 1 \), the \( T_1^+ \) is divided into \( A_2^+ \) and \( E^+ \) so that

\[
\begin{align*}
M_{10:10}^{(1)}(T_1^+) &= \frac{1}{3} M_{10:10}(A_2^+) + \frac{2}{3} M_{10:10}(E^+) \\
M_{10:12}^{(1)}(T_1^+) &= \frac{1}{3} M_{10:12}(A_2^+) + \frac{2}{3} M_{10:12}(E^+) \\
M_{12:12}^{(1)}(T_1^+) &= \frac{1}{3} M_{12:12}(A_2^+) + \frac{2}{3} M_{12:12}(E^+)
\end{align*}
\]

(51)

Then, for \( J = J' = 2 \), the \( T_2^- \) splits into \( B_2^- \) and \( E^- \), and we have

\[
M_{21:21}^{(1)}(T_2^-) = \frac{1}{3} M_{21:21}(B_2^-) + \frac{2}{3} M_{21:21}(E^-)
\]

(52)

Finally, we discuss the relationship of phase shift formulas between the cubic boxes and the elongated boxes. Here, we take \( T_2^- \) representation in cubic boxes as an example. From the elongated box to the cubic symmetry, the matrix elements \( M_{21:21}(B_2^-) \) and \( M_{21:21}(E^-) \) will individually approach \( M_{21:21}(T_2^-) \) in the limit \( \eta = 1 \). From Eq. (52), one can see how to follow this limit by subduction rule in this particular channel. The relationship translates directly into one for the phase shift as follows:

\[
\cot \delta_{21}(T_2^-) = \frac{1}{3} \cot \delta_{21}(B_2^-) + \frac{2}{3} \cot \delta_{21}(E^-).
\]

(53)

V. DISCUSSIONS AND CONCLUSIONS

In this paper, we have derived L"uscher phase shift formulas for baryon-baryon elastic scattering in elongated boxes. We show the cases where the baryon-baryon state
TABLE VI: \(O_h\) symmetry group for angular momentum up to \(J = 2\) and \(l = 2\). The results are separated according to parity \((-1)^{J/2+1}\).

| \(\Gamma\) | \(J_l J^{I'}\) | \(\mathcal{M}^{(J_l, J^{I'})}_{\Gamma, I} (\Gamma)\) |
|-----------|----------------|--------------------------------------------------|
| \(A_1^+\) | 01 01          | \(\omega_{00} - \frac{2\sqrt{3}}{15} \omega_{22}\) |
|           | 01 21          | \(- \frac{2\eta}{5} \omega_{00} - \frac{2\sqrt{3}}{15} \omega_{22}\) |
|           | 21 21          | \(\omega_{00} + \frac{2\eta}{5} \omega_{00} - \frac{2\sqrt{3}}{15} \omega_{22}\) |
| \(E^+\)   | 21 21          | \(\omega_{00} - \frac{2\sqrt{3}}{15} \omega_{22}\) |
| \(T^+_1\) | 10 10          | \(\omega_{00}\) |
|           | 10 12          | \(- \frac{2\eta}{5} \omega_{22}\) |
|           | 12 12          | \(\omega_{00} - \frac{2\eta}{5} \omega_{22}\) |
| \(T^+_2\) | 21 21          | \(\omega_{00} + \frac{2\eta}{5} \omega_{22}\) |

TABLE VII: Subduction rules in the descent in symmetry in the group from cubic box \((O_h)\) to the elongated box \((D_{4h})\).

| \(O_h\) | \(A_1^+\) | \(A_2^+\) | \(E^+\) | \(T^+_1\) | \(T^+_2\) | \(A_1^-\) | \(A_2^-\) | \(E^-\) | \(T^-_1\) | \(T^-_2\) |
|--------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| \(D_{4h}\) | \(A_1^+\) | \(B_1^+\) | \(A_2^+\) | \(B_1^+\) | \(A_2^+ \oplus E^+\) | \(B_2^+ \oplus E^+\) | \(A_1^-\) | \(B_1^-\) | \(A_2^- \oplus B_1^-\) | \(A_2^- \oplus E^-\) | \(B_2^- \oplus E^-\) |

is in COM frame with respect to the box, or moving, or with twisted boundary condition along the elongated direction. As a consistency check and validation on the elongated results, we have also derived the results in the cubic box by using the same approach. There are two differences between these two cases. One is the symmetry of the two-particle system and the other is the matrix \(\mathcal{M}\). We take the two-baryon scattering in COM frame as an example. In the cubic case, the symmetry group is \(O_h\) and in the elongated case, the symmetry group becomes \(D_{4h}\). In addition, the factor of \(\eta\) in matrix \(\mathcal{M}\) in the elongated box is equal to 1 for the cubic case. Our interest in elongated boxes stems from the fact that they allow us to vary the geometry of the box, and consequently the kinematics, with minimal amount of computer resources. On the other hand, elongated boxes have a different symmetry group than the cubic case and this has to be taken into account when designing interpolators and connecting the infinite volume phase-shifts with the two-body energies.

Let us discuss some possible applications of phase shift formula derived in this paper. Some typical examples for scattering with two spin-1/2 particles are listed here, and all examples are highly relevant in the study of the composition of dense nuclear matter which forms the neutron stars. One typical example is the \(\Lambda - \Lambda\), \(N - \Xi\), \(\Sigma - \Sigma\) scattering, where the existence of \(H\) dibaryon state has been discussed as the remaining of bound state in flavor singlet channel. Another example is \(\Lambda - N\) and \(\Sigma - N\) scattering which is useful to study properties of hyperonic matters inside the neutron stars. \(\Xi - \Xi\), \(N - N\) and \(N \Sigma\) scattering and \(N A\) scattering follow. These examples have been studied by using HAL QCD method in Refs. [57–60]. In principle, these issues can also be studied with Lüscher’s formulas in detail by using lattice QCD simulations in elongated boxes.

To summarize, in this paper we have generalized two-particle scattering phase shift formulas to the case of particles with spin 1/2, below the inelastic threshold in the COM frame and MF in the elongated box and COM frame in cubic box, respectively. Using a quantum mechanical model, a relation between the energy of the two-particle system and phase shift is established. It is verified that the phase shift formulas in elongated box in the limit \(\eta = 1\) and cubic box are consistent. Although we focus on the scattering between two particles with all of the spin being 1/2, there are not essential difficulties in generalizing it to cases with arbitrary spin in any number of channels. We expect that these relations will be helpful for the study of baryon-baryon scattering in lattice QCD simulations.

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