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Two particle states in an asymmetric box ☆

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Abstract

The exact two-particle energy eigenstates in an asymmetric rectangular box with periodic boundary conditions in all three directions are studied. Their relation with the elastic scattering phases of the two particles in the continuum are obtained. These results can be viewed as a generalization of the corresponding formulae in a cubic box obtained by Lüscher before. In particular, the s-wave scattering length is related to the energy shift in the finite box. Possible applications of these formulae are also discussed.

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1. Introduction

In a series of papers, Lüscher obtained results [1–4] which relate the energy of a two-particle state in a cubic box (a torus) with the elastic scattering phases of the two particles in the continuum. This formula, now known as Lüscher's formula, has been utilized in a number of applications, e.g., linear sigma model in the broken phase [5], and also in quenched QCD [6–13]. Due to limited numerical computational power, the s-wave scattering length, which is related to the scattering phase shift at vanishing relative three momentum, is mostly studied in hadron scattering using quenched approximation. CP-PACS Collaboration calculated the scattering phases at non-zero momenta in pion–pion s-wave scattering in the $I = 2$ channel [12] using quenched Wilson fermions and recently also in two flavor full QCD [14]. In typical lattice QCD calculations, if one would like to probe for physical information concerning two-particle states with non-zero relative three momentum, large lattices have to be used which usually requires enormous amount of computing resource. One of the reasons for this is the following. In a cubic box, the three momenta of a single particle are quantized according to: $\mathbf{k} = (2\pi/L)\mathbf{n} \equiv (2\pi/L)(n_1, n_2, n_3)$, with $\mathbf{n} \in Z^3$.[1] In order to control lattice artifacts due to these non-zero momentum modes, one needs to have large values of L. One disad-

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[1] That is, n_1, n_2 and n_3 are integers.

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vantage of the cubic box is that the energy of a free particle with lowest non-zero momentum is degenerate. This means that the second lowest energy level of the particle with non-vanishing momentum corresponds to $\mathbf{n} = (1, 1, 0)$. 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 a three-dimensional box whose shape is not cubic. If we use a *generic* rectangular box of size $(\eta_1 L) \times (\eta_2 L) \times L$ with η_1 and η_2 other than unity, we would have three different low-lying one-particle energy with non-zero momenta corresponding to $\mathbf{n} = (1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$, respectively. This scenario is useful since it presents more available low momentum modes for a given lattice size, which is important in the study of hadron–hadron scattering phase shift. Similar situation also occurs in the study of K to $\pi\pi$ matrix element (see Ref. [15] for a review and references therein). There, one also needs to study two-particle states with non-vanishing relative three-momentum. Again, a cubic box yields too few available low-lying non-vanishing momenta and large value of L is needed to reach the physical interesting kinematic region. In these cases, one could try an asymmetric rectangular box with only one side being large while the other sides moderate. In an asymmetric rectangular box, the original formulae due to Lüscher, which give the relation between the energy eigenvalues in the finite box and the continuum scattering phases, have to be modified accordingly. The purpose of this Letter is to derive the equivalents of Lüscher's formulae in the case of a generic rectangular (not necessarily cubic) box.

We consider two-particle states in a box of size $(\eta_1 L) \times (\eta_2 L) \times L$ with periodic boundary conditions. For definiteness, we take $\eta_1 \geqslant 1$, $\eta_2 \geqslant 1$, which amounts to denoting the length of the smallest side of the rectangular box as L. The following derivation depends heavily on the previous results obtained in Ref. [3]. We will take over similar assumptions as in Ref. [3]. In particular, the relation between the energy eigenvalues and the scattering phases derived in the non-relativistic quantum mechanical model can be carried over to the case of relativistic, massive field theory under these assumptions, the same way as in the case of cubic box which was discussed in detail in Ref. [3]. For the quantum mechanical model, we assume that the range of the interaction, denoted by R, of the two-particle system is such that $R < L/2$.

The modifications which have to be implemented, as compared with Ref. [3], are mainly concerned with different symmetries of the box. In a cubic box, the representations of the rotational group are decomposed into irreducible representations of the cubic group. In a generic asymmetric box, the symmetry of the system is reduced. In the case of $\eta_1 = \eta_2 \neq 1$, the basic group becomes D_4; if $\eta_1 \neq \eta_2 \neq 1$, the symmetry is further reduced to D_2, modulo parity operation. Therefore, the final expression relating the energy eigenvalues of the system and the scattering phases will be different.

2. Energy eigenstates and singular periodic solutions of Helmholtz equation

As discussed in Ref. [3], the energy eigenstates in a box is intimately related to the singular periodic solutions of the Helmholtz equation:

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = 0. \tag{1}$$

These solutions are periodic: $\psi(\mathbf{r} + \hat{\mathbf{n}}L) = \psi(\mathbf{r})$ and are bounded by certain powers of $r = |\mathbf{r}|$ near $r = 0$. The momentum modes in the rectangular box are quantized as: $\mathbf{k} = (2\pi/L)\tilde{\mathbf{n}}$. Here we introduce the notations: $\tilde{\mathbf{n}} \equiv (n_1/\eta_1, n_2/\eta_2, n_3)$ and $\hat{\mathbf{n}} \equiv (n_1\eta_1, \eta_2 n_2, n_3)$ with $\mathbf{n} = (n_1, n_2, n_3) \in Z^3$. For regular values of k,[2] the singular periodic solutions of Helmholtz equation can be obtained from the Green's function:

$$G\left(\mathbf{r}; k^2\right) = \frac{1}{\eta_1\eta_2 L^3}\sum_{\mathbf{p}} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\mathbf{p}^2 - k^2}. \tag{2}$$

We define: $\mathcal{Y}_{lm}(\mathbf{r}) \equiv r^l Y_{lm}(\Omega_{\mathbf{r}})$, where $\Omega_{\mathbf{r}}$ represents the solid angle parameters (θ, ϕ) of $\mathbf{r}$ in spherical coordinates; Y_{lm} are the usual spherical harmonic functions. It is well known that $\mathcal{Y}_{lm}(\mathbf{r})$ consist of all linear independent, homogeneous functions in (x, y, z) of degree l that transform irreducibly under the rotational group. We then define

$$G_{lm}\left(\mathbf{r}; k^2\right) = \mathcal{Y}_{lm}(\nabla) G\left(\mathbf{r}; k^2\right), \tag{3}$$

which form a complete, linear independent set of functions of singular periodic solutions to Helmholtz

[2] This means that $|k| \neq (2\pi/L)|\tilde{\mathbf{n}}|$ for any $\mathbf{n} \in Z^3$.

equation. The functions $G_{lm}(\mathbf{r};k^2)$ may be expanded into spherical harmonics:

$$G_{lm}\big(\mathbf{r};k^2\big) = \frac{(-)^l k^{l+1}}{4\pi}\Bigg[Y_{lm}(\Omega_{\mathbf{r}})n_l(kr) + \sum_{l'm'}\mathcal{M}_{lm;l'm'}Y_{l'm'}(\Omega_{\mathbf{r}})j_{l'}(kr)\Bigg]. \tag{4}$$

Here, j_l and n_l are the usual spherical Bessel functions and the matrix $\mathcal{M}_{lm;l'm'}$ is related to the *modified* zeta function via

$$\mathcal{M}_{lm;js} = \sum_{l'm'}\frac{(-)^s i^{j-l}\mathcal{Z}_{l'm'}(1,q^2;\eta_1,\eta_2)}{\eta_1\eta_2\pi^{3/2}q^{l'+1}} \times\sqrt{(2l+1)(2l'+1)(2j+1)} \times\begin{pmatrix} l & l' & j\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l & l' & j\\ m & m' & -s\end{pmatrix}. \tag{5}$$

In this formula, the Wigner $3j$-symbols can be related to the Clebcsh–Gordan coefficients in the usual way. For a given angular momentum cutoff Λ, the quantity $\mathcal{M}_{lm;l'm'}$ can be viewed as the matrix element of a linear operator $\hat{M}$ in a vector space $\mathcal{H}_\Lambda$, which is spanned by all harmonic polynomials of degree $l \leqslant \Lambda$. The modified zeta function is formally defined by

$$\mathcal{Z}_{lm}\big(s,q^2;\eta_1,\eta_2\big) = \sum_{\mathbf{n}}\frac{\mathcal{Y}_{lm}(\tilde{\mathbf{n}})}{(\tilde{\mathbf{n}}^2-q^2)^s}. \tag{6}$$

According to this definition, the modified zeta function at the right-hand side of Eq. (5) is formally divergent and needs to be analytically continued. Following similar discussions as in Ref. [3], one could obtain a finite expression for the modified zeta function which is suitable for numerical evaluation. It is also obvious from the symmetry of D_4 or D_2 that, for $l \leqslant 4$, the only non-vanishing zeta functions at $s = 1$ are: $\mathcal{Z}_{00}$, $\mathcal{Z}_{20}$, $\mathcal{Z}_{2\pm2}$, $\mathcal{Z}_{40}$, $\mathcal{Z}_{4\pm2}$ and $\mathcal{Z}_{4\pm4}$. One easily verifies that, if $\eta_1 = \eta_2 = 1$, all of the above definitions and formulae reduce to the those obtained in Ref. [3].

The energy eigenstates of the two-particle system may be expanded in terms of singular periodic solutions of Helmholtz equation. This solution in the region where the interaction is vanishing can be expressed in terms of ordinary spherical Bessel functions, which is related to the scattering phases in the usual way. For the two-particle eigenstate in the symmetry sector Γ in a box of particular symmetry (either D_4 or D_2), the energy eigenvalue, $E = k^2/2\mu$ with μ being the reduced mass of the two particles, is determined by

$$\det\big[e^{2i\delta} - \hat{U}(\Gamma)\big] = 0,$$
$$\hat{U}(\Gamma) = \big(\hat{M}(\Gamma)+i\big)/\big(\hat{M}(\Gamma)-i\big). \tag{7}$$

Here Γ denotes a particular representation of the group D_4 or D_2. $\hat{M}(\Gamma)$ represents a linear operator in the vector space $\mathcal{H}_\Lambda(\Gamma)$. This vector space is spanned by all complex vectors whose components are v_{ln}, with $l \leqslant \Lambda$, and n runs from 1 to the number of occurrence of Γ in the decomposition of representation with angular momentum l, see Ref. [3] for details. To write out more explicit formulae, one therefore has to consider decompositions of the rotational group representations under appropriate symmetries.

3. Symmetry of an asymmetric box

As mentioned in the beginning of this Letter, modifications have to be made since the symmetry of an asymmetric box is different from that of a cubic one. We first describe the case $\eta_1 = \eta_2$. The symmetry group is D_4, which has 4 one-dimensional representations: A_1, A_2, B_1, B_2 and a two-dimensional irreducible representation E. The representations of the rotational group are decomposed according to

$$\mathbf{0} = A_1^+,\qquad \mathbf{1} = A_2^- + E^-,$$
$$\mathbf{2} = A_1^+ + B_1^+ + B_2^+ + E^+, \tag{8}$$

as is seen, in the A_1^+ sector, up to $l \leqslant 2$ both s-wave and d-wave contribute. This corresponds to *two* linearly independent, homogeneous polynomials with degrees not more than 2, which are invariant under D_4. These two polynomials can be identified as $\mathcal{Y}_{00}$ and $\mathcal{Y}_{20} \propto (x^2+y^2-2z^2)$. Therefore, we can write out the reduced matrix element $\mathcal{M}(A_1^+)_{ll'} = m_{ll'}$ in this sector:

$$m_{00} = \mathcal{W}_{00},\qquad m_{20} = m_{02} = -\mathcal{W}_{20},$$
$$m_{22} = \mathcal{W}_{00} + \frac{2\sqrt{5}}{7}\mathcal{W}_{20} + \frac{6}{7}\mathcal{W}_{40}, \tag{9}$$

where we have introduced the notation

$$\mathcal{W}_{lm}\big(1, q^2; \eta_1, \eta_2\big) \equiv \frac{\mathcal{Z}_{lm}(1, q^2; \eta_1, \eta_2)}{\pi^{3/2}\eta_1\eta_2 q^{l+1}}. \tag{10}$$

We find that, in the case of D_4 symmetry, Eq. (7) becomes

$$\left(1 + \frac{m_{02}^2}{m_{00}}\frac{\tan\delta_2}{1 - m_{22}\tan\delta_2}\right)\tan\delta_0 = \frac{1}{m_{00}}. \tag{11}$$

Similar formula also appears in the case of cubic box except that the mixing with s-wave comes in at $l = 4$, not at $l = 2$.

For the case $\eta_1 \neq \eta_2$, the symmetry group becomes D_2 which has only 4 one-dimensional representations: A, B_1, B_2 and B_3. The decomposition (8) is replaced by

$$\begin{aligned}&\mathbf{0} = A^+, \qquad \mathbf{1} = B_1^- + B_2^- + B_3^-,\\ &\mathbf{2} = A^+ + A^+ + B_1^+ + B_2^+ + B_3^+.\end{aligned} \tag{12}$$

So, up to $l \leqslant 2$, A^+ occurs *three* times: once in $l = 0$ and twice in $l = 2$. The corresponding basis polynomials can be taken as: $\mathcal{Y}_{00}$, $\mathcal{Y}_{20}$ and $(\mathcal{Y}_{22} + \mathcal{Y}_{2-2})/\sqrt{2}$. If we denote the above three states as: 0, 2 and $\bar{2}$, the reduced matrix $\hat{M}(A^+)$ is three-dimensional with matrix elements m_{00}, $m_{02} = m_{20}$ and m_{22} given in Eq. (9) and the rest are given by

$$\begin{aligned}
m_{0\bar{2}} &= m_{\bar{2}0} = -\frac{1}{\sqrt{2}}(\mathcal{W}_{22} + \mathcal{W}_{2-2}),\\
m_{2\bar{2}} &= m_{\bar{2}2} = -\frac{\sqrt{10}}{7}(\mathcal{W}_{22} + \mathcal{W}_{2-2})\\
&\qquad + \frac{\sqrt{30}}{14}(\mathcal{W}_{42} + \mathcal{W}_{4-2}),\\
m_{\bar{2}\bar{2}} &= \mathcal{W}_{00} - \frac{2\sqrt{5}}{7}\mathcal{W}_{20} + \frac{1}{7}\mathcal{W}_{40}\\
&\qquad + \sqrt{\frac{5}{14}}(\mathcal{W}_{44} + \mathcal{W}_{4-4}).
\end{aligned} \tag{13}$$

Similar to Eq. (11), the relation between the energy eigenvalue and the scattering phases now reads

$$\begin{aligned}
&\left(\frac{1}{m_{00}}\cot\delta_0 - 1\right)\begin{vmatrix} 1 - m_{22}\tan\delta_2 & m_{2\bar{2}}\tan\delta_2 \\ m_{2\bar{2}}\tan\delta_2 & 1 - m_{\bar{2}\bar{2}}\tan\delta_2 \end{vmatrix}\\
&\quad = \frac{m_{02}\tan^2\delta_2}{m_{00}}\begin{vmatrix} m_{02} & m_{2\bar{2}} \\ m_{0\bar{2}} & (\cot\delta_2 - m_{\bar{2}\bar{2}}) \end{vmatrix}\\
&\qquad - \frac{m_{0\bar{2}}\tan^2\delta_2}{m_{00}}\begin{vmatrix} m_{02} & (\cot\delta_2 - m_{22}) \\ m_{0\bar{2}} & m_{2\bar{2}} \end{vmatrix}.
\end{aligned} \tag{14}$$

If the d-wave phase shift were small enough, it is easy to check that both Eqs. (11) and (14) simplifies to

$$\cot\delta_0(k) = m_{00} = \frac{\mathcal{Z}_{00}(1, q^2; \eta_1, \eta_2)}{\pi^{3/2}\eta_1\eta_2 q}. \tag{15}$$

For the general case, Eqs. (11) and (14) offer the desired relation between the energy eigenvalues in the A_1^+ sector and the scattering phases for the cases $\eta_1 = \eta_2$ and $\eta_1 \neq \eta_2$, respectively.

4. Large volume expansion of the scattering length

It is known that in low-energy scattering processes, the scattering phases $\delta_l(k)$ behaves like: $\tan\delta_l(k) \sim k^{2l+1}$ for small k, where k is the relative momentum of the two particles being scattered. It is easy to verify that both m_{00} and m_{02} behave like $1/q^3$ as $q \sim 0$. Since $\tan\delta_2(q)$ goes to zero like q^5, we see that the effects due to d-wave phase shift in Eqs. (11) and (14) are negligible as long as the relative momentum q is small enough. Therefore, in both cases, the s-wave scattering length a_0 will be determined by the zero momentum limit of Eq. (15).

For a large box, a large L expansion of the formulae can be deduced. Using Eq. (15), we find that the s-wave scattering length a_0 is related to the energy difference in a generic rectangular box via[3]

$$\begin{aligned}\delta E = -\frac{2\pi a_0}{\eta_1\eta_2\mu L^3}\bigg[1 &+ c_1(\eta_1, \eta_2)\left(\frac{a_0}{L}\right)\\ &+ c_2(\eta_1, \eta_2)\left(\frac{a_0}{L}\right)^2 + \cdots\bigg].\end{aligned} \tag{16}$$

Here, μ designates the reduced mass of the two particles whose mass values are m_1 and m_2, respectively. Energy shift $\delta E \equiv E - m_1 - m_2$ where E is the energy eigenvalue of the two-particle state. Functions

[3] For low relative momenta, the d-wave scattering phase behaves like: $\tan\delta_2(q) \sim a_2 k^5 = a_2(2\pi/L)^5 q^5$, with a_2 being the d-wave scattering length. If we treat the effects due to $\tan\delta_2$ perturbatively, we see from Eqs. (11) and (14) that, in Eq. (16), functions c_1 and c_2 receive contributions that are proportional to (a_2/L^5), which is of higher order in $1/L$ for large L.

Table 1
Numerical values for the subtracted zeta functions and the coefficients $c_1(\eta_1, \eta_2)$ and $c_2(\eta_1, \eta_2)$ under some typical topology. The three-dimensional rectangular box has a size $L_1 = \eta_1 L$, $L_2 = \eta_2 L$ and $L_3 = L$

$L_1 : L_2 : L_3$	η_1	η_2	$\hat{Z}_{00}(1, 0; \eta_1, \eta_2)$	$\hat{Z}_{00}(2, 0; \eta_1, \eta_2)$	$c_1(\eta_1, \eta_2)$	$c_2(\eta_1, \eta_2)$
1 : 1 : 1	1	1	−8.913633	16.532316	−2.837297	6.375183
6 : 5 : 4	1.5	1.25	−12.964476	41.526870	−2.200918	3.647224
4 : 3 : 2	2	1.5	−16.015122	91.235227	−1.699257	1.860357
3 : 2 : 2	1.5	1	−10.974332	32.259457	−2.328826	3.970732
2 : 1 : 1	2	1	−11.346631	63.015304	−1.805872	1.664979
3 : 3 : 2	1.5	1.5	−14.430365	53.784051	−2.041479	3.091200
2 : 2 : 1	2	2	−18.430516	137.771800	−1.466654	1.278623

$c_1(\eta_1, \eta_2)$ and $c_2(\eta_1, \eta_2)$ are given by

$$c_1(\eta_1, \eta_2) = \frac{\hat{Z}_{00}(1, 0; \eta_1, \eta_2)}{\pi \eta_1 \eta_2},$$
$$c_2(\eta_1, \eta_2) = \frac{\hat{Z}_{00}^2(1, 0; \eta_1, \eta_2) - \hat{Z}_{00}(2, 0; \eta_1, \eta_2)}{(\pi \eta_1 \eta_2)^2}, \tag{17}$$

where the subtracted zeta function is defined as

$$\hat{Z}_{00}\big(s, q^2; \eta_1, \eta_2\big) = \sum_{|\tilde{\mathbf{n}}|^2 \neq q^2} \frac{1}{(\tilde{\mathbf{n}}^2 - q^2)^s}. \tag{18}$$

In Table 1, we have listed numerical values for the coefficients $c_1(\eta_1, \eta_2)$ and $c_2(\eta_1, \eta_2)$ under some typical topology. In the first column of Table 1, we tabulated the ratio for the three sides of the box: $\eta_1 : \eta_2 : 1$. Note that for $\eta_1 = \eta_2 = 1$, these two functions reduce to the old numerical values for the cubic box which had been used in earlier scattering length calculations.

5. Conclusions

In this Letter, we have studied two-particle scattering states in a generic rectangular box with periodic boundary conditions. The relations of the energy eigenvalues and the scattering phases in the continuum are found. These can be viewed as a generalization of the well-known Lüscher's formula. In particular, we show that the s-wave scattering length is related to the energy shift by a simple formula, which is a direct generalization of the corresponding formula in the case of cubic box. We argued that this asymmetric topology might be useful in practice since it provides more available low-lying momentum modes in a finite box, which will be advantageous in the study of scattering phase shifts at non-zero three momenta in hadron–hadron scattering and possibly also in other applications.

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