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# Two particle states and the $S$-matrix elements in multi-channel scattering*

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Abstract: Using a quantum mechanical model, the exact energy eigenstates for two-particle two-channel scattering are studied in a cubic box with periodic boundary conditions in all three directions. A relation between the exact energy eigenvalue in the box and the two-channel $S$-matrix elements in the continuum is obtained. This result can be viewed as a generalization of the well-known Lüscher's formula which establishes a similar relation in elastic scattering.

Keywords: Lattice Quantum Field Theory, Lattice Gauge Field Theories, Lattice QCD.

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## Contents



## 1. Introduction

Scattering experiments play an important role in the study of interactions among particles. In these experiments, scattering cross sections are measured. By a partial wave analysis, one obtains the experimental results on particle-particle scattering in terms scattering phase shifts in channels of definite quantum numbers. In the case of strong interaction, experimental results on hadron-hadron scattering phase shifts are available in the literature [1−5]. On the theoretical side, Quantum Chromodynamics (QCD) is believed to be the underlying theory of strong interactions. However, due to its non-perturbative nature, low-energy hadron-hadron scattering should be studied with a non-perturbative method. Lattice QCD provides a genuine non-perturbative method which can tackle these problems in principle, using numerical simulations. In a typical lattice calculation, energy eigenvalues of two-particle states with definite symmetry can be obtained by measuring appropriate correlation functions. Therefore, it would be desirable to relate these energy eigenvalues which are available through lattice calculations to the scattering phases which are obtained in the scattering experiment. This was accomplished in a series of papers by Lüscher [6−9] for a cubic box topology. In these references, especially ref. [8], Lüscher found a non-perturbative relation of the energy of a two-particle state in a cubic box (a torus) with the corresponding 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 [10], and also in quenched QCD [11−18]. 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 [17] using quenched Wilson fermions and recently also in two flavor full QCD [19].

For hadron scattering at low energies, usually the elastic scattering is dominant since the inelastic channels are not opened. However, when the energy of the scattering process exceeds some threshold, inelastic scattering starts to contribute and the scattering of the particles cannot be described by single channel elastic scattering anymore. In the case of pion-pion scattering, for example, the scattering process is elastic below the four pion and the two kaon threshold. If the center of mass energy exceeds the four pion threshold, inelastic effects starts to contribute. The inelastic effects become very important when the energy is getting close to the two kaon threshold. At this point, pion-pion can be scattered into kaon-kaon pair final state. Although the four pion threshold is in fact below the two kaon threshold, four pion final state will not contribute significantly due to its weak coupling to the two pion initial state. The fact that four pion states are coupled to the two pion state weakly in the low-energy limit is seen from the QCD chiral lagrangian. A six pion vertex in this lagrangian involves derivative coupling which is vanishing in the low-energy limit. Experimental investigations show that the contribution of four pion states would only make substantial contribution when the energy is well over 1GeV. Therefore, if the energy is not much higher than 1GeV, pion-pion scattering can be approximated rather well by a two-channel model. It is then interesting to study the relation between the multi-channel two particle states and the scattering phases, just as what we have done in the single channel case.

In this paper, we establish a relation between the energy of a two particle state in a finite cubic box and the scattering matrix parameters. It is a generalization of the famous Lüscher formula to the multi-channel situation. This relation is non-perturbative in nature and it is derived in a quantum mechanical model of two-channel scattering. The result can also be generalized to the case of asymmetric box. Further generalization to the case of massive field theory is under consideration.

## 2. The quantum mechanical model to two channel scattering

In this paper, we study a quantum mechanical model of two-channel scattering. Generalization to more channels can be done similarly. The model under investigation has the following hamiltonian:

$$H = \begin{pmatrix} -\frac{1}{2m_1}\nabla^2 & 0 \\ 0 & E_T - \frac{1}{2m_2}\nabla^2 \end{pmatrix} + \begin{pmatrix} V_1(r) & \Delta(r) \\ \Delta^*(r) & V_2(r) \end{pmatrix} . \tag{2.1}$$

We will also use the notation:

$$V(r) = \begin{pmatrix} V_1(r) & \Delta(r) \\ \Delta^*(r) & V_2(r) \end{pmatrix} \tag{2.2}$$

to denote the matrix valued potential whose matrix elements $V_1(r)$, $V_2(r)$ and $\Delta(r)$ all vanish for $r > R$. $E_T > 0$ designates a positive threshold energy of the second channel. That is to say, if the center of mass energy for the scatter process is less than $E_T$, there will be no asymptotic scattering states in the second channel.



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Energy eigenstates of the hamiltonian (2.1) with energy $E$ can be decomposed into spherical harmonics:

$$\Psi(\mathbf{r}) = \sum_{l,m} Y_{lm}(\hat{\mathbf{r}}) \begin{pmatrix} \psi_{1;lm}(r) \\ \psi_{2;lm}(r) \end{pmatrix} . \tag{2.3}$$

The radial wave-functions $\psi_{i;lm}(r)$ with $i = 1, 2$ satisfy the radial Schrödinger equation:

$$\begin{aligned} \left[\frac{1}{2m_1}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) + E - V_1(r)\right]\psi_1(r) &= \Delta(r)\psi_2(r)\,, \\ \left[\frac{1}{2m_2}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) + E' - V_2(r)\right]\psi_2(r) &= \Delta^*(r)\psi_1(r)\,, \end{aligned} \tag{2.4}$$

where $E' \equiv E - E_T$.

About the coupled differential equations (2.4), the following statement can be proven.

**Theorem.** *If the matrix valued potential (2.2) is such that every matrix element of* $r^2V(r)$ *is analytic around* $r = 0$ *and that* $\lim_{r\to 0} r^2V(r) = 0$*, then the coupled differential equations (2.4) has two finite, linearly independent solutions near* $r = 0$*:* $u^{(i)}_{l;j}(r)$*, with* $i = 1, 2$ *designating different solutions and* $j = 1, 2$ *denoting different component of the solution. Moreover, these solutions can be chosen such that:*

$$u^{(i)}_{l;j}(r) \sim r^l \delta_{ij}\,. \tag{2.5}$$

*Equations (2.4) has two further linear independent solutions* $v^{(i)}_{l;j}(r)$ *that are unbounded near* $r = 0$ *and satisfy:* $v^{(i)}_{l;j}(r) \sim r^{-l-1}\delta_{ij}$*.*

The proof of this theorem is quite similar to the proof in the single channel case. Details are provided in the appendix.

## 3. Two channel scattering and the $S$ matrix in infinite volume

In this section, we briefly describe the quantum mechanical treatment of inelastic scattering. We will concentrate on the two channel case, although the formalism can easily be generalized to more channels.

At large $r$ where the potential $V(r)$ vanishes, the wave function of the scattering state can be chosen to have the following form:

$$\Psi^{(1)}(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} \begin{pmatrix} e^{i\mathbf{k}_1\cdot\mathbf{r}} + f_{11}(\hat{\mathbf{k}}_1\cdot\hat{\mathbf{r}})\frac{e^{ik_1 r}}{r} \\ f_{21}(\hat{\mathbf{k}}_1\cdot\hat{\mathbf{r}})\sqrt{\frac{m_2}{m_1}}\frac{e^{ik_2 r}}{r} \end{pmatrix} . \tag{3.1}$$

This wave function has the property that in the remote past, it becomes an incident plane wave in the first channel with definite wave vector $\mathbf{k}_1$. It is an eigenstate of the full hamiltonian with energy: $E = \mathbf{k}_1^2/(2m_1)$. Similarly, if the energy $E > E_T$, one can also build an eigenstate of the hamiltonian which in the remote pase becomes an incident plane wave in the second channel:

$$\Psi^{(2)}(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} \begin{pmatrix} f_{12}(\hat{\mathbf{k}}_2\cdot\hat{\mathbf{r}})\sqrt{\frac{m_1}{m_2}}\frac{e^{ik_1 r}}{r} \\ e^{i\mathbf{k}_2\cdot\mathbf{r}} + f_{22}(\hat{\mathbf{k}}_2\cdot\hat{\mathbf{r}})\frac{e^{ik_2 r}}{r} \end{pmatrix} . \tag{3.2}$$

This state is also an eigenstate of the hamiltonian with energy $E = E_T + \mathbf{k}_2^2/(2m_2)$.



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In partial wave analysis, one decompose the coefficients: $f_{ij}$ appearing in the above construction into spherical harmonics:

$$f_{11}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{r}}) = \frac{1}{2ik_1} \sum_{l=0}^{\infty} (2l+1) \left[ S_{11}^{(l)}(k_1) - 1 \right] P_l(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{r}}) \,, \tag{3.3}$$

$$f_{21}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{r}}) = \frac{1}{2i\sqrt{k_1 k_2}} \sum_{l=0}^{\infty} (2l+1) S_{21}^{(l)}(k_1) P_l(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{r}}) \,, \tag{3.4}$$

and similar expressions for $f_{12}$ and $f_{22}$. With this we find the two scattering eigenstates in eq. (3.1) and eq. (3.2) can be expressed as:

$$\begin{aligned} \Psi^{(1)}(\mathbf{r}) &\stackrel{r\to\infty}{\longrightarrow} \sum_{lm} 4\pi Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^*(\hat{\mathbf{k}}_1) \begin{pmatrix} \frac{1}{2ik_1 r} \left[ S_{11}^{(l)} e^{ik_1 r} + (-)^{l+1} e^{-ik_1 r} \right] \\ \frac{1}{2i\sqrt{k_1 k_2} r} \sqrt{\frac{m_2}{m_1}} S_{21}^{(l)} e^{ik_2 r} \end{pmatrix} , \\ \Psi^{(2)}(\mathbf{r}) &\stackrel{r\to\infty}{\longrightarrow} \sum_{lm} 4\pi Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^*(\hat{\mathbf{k}}_2) \begin{pmatrix} \frac{1}{2i\sqrt{k_1 k_2} r} \sqrt{\frac{m_1}{m_2}} S_{12}^{(l)} e^{ik_1 r} \\ \frac{1}{2ik_2 r} \left[ S_{22}^{(l)} e^{ik_2 r} + (-)^{l+1} e^{-ik_2 r} \right] \end{pmatrix} . \end{aligned} \tag{3.5}$$

The two component wave-functions appearing in the above formulae are in fact the radial wave functions of the Schrödinger equation (2.4) in the large $r$ region:[1]

$$\begin{aligned} w_l^{(1)}(r) &\simeq \begin{pmatrix} \frac{1}{2ik_1 r} \left[ S_{11}^{(l)} e^{ik_1 r} + (-)^{l+1} e^{-ik_1 r} \right] \\ \frac{1}{2i\sqrt{k_1 k_2} r} \sqrt{\frac{m_2}{m_1}} S_{21}^{(l)} e^{ik_2 r} \end{pmatrix} , \\ w_l^{(2)}(r) &\simeq \begin{pmatrix} \frac{1}{2i\sqrt{k_1 k_2} r} \sqrt{\frac{m_1}{m_2}} S_{12}^{(l)} e^{ik_1 r} \\ \frac{1}{2ik_2 r} \left[ S_{22}^{(l)} e^{ik_2 r} + (-)^{l+1} e^{-ik_2 r} \right] \end{pmatrix} . \end{aligned} \tag{3.6}$$

It is obvious that the two radial wave functions $w_l^{(1)}(r)$ and $w_l^{(2)}(r)$ are linearly independent. Therefore, according to the theorem stated in the previous section, they are linear superpositions of the general solutions: $u_l^{(1)}(r)$ and $u_l^{(2)}(r)$. The converse is also true. The radial wave functions $u_l^{(1)}(r)$ and $u_l^{(2)}(r)$ defined via eq. (2.5) can be expressed as linear superpositions of the two radial wave functions in eq. (3.6). In other words, there exists a non-singular $2 \times 2$ matrix $C$ such that:

$$w_l^{(i)}(r) = \sum_j C_{ij} u_l^{(j)}(r) \,, \qquad u_l^{(i)}(r) = \sum_j C_{ij}^{-1} w_l^{(j)}(r) \,. \tag{3.7}$$

Another important physical property of the wave-function (3.5) is that the matrix elements which enter the expansion, namely $S_{ij}^{(l)}$, form a $2 \times 2$ unitary matrix which is nothing but the $S$-matrix in the subspace with orbital angular momentum $l$. This unitarity condition comes directly from the probability conservation law of quantum mechanics. We have, for example:

$$|S_{11}^{(l)}|^2 + |S_{21}^{(l)}|^2 = 1 \,, \qquad |S_{12}^{(l)}|^2 + |S_{22}^{(l)}|^2 = 1 \,. \tag{3.8}$$

[1] In fact, if we use the corresponding spherical Bessel's function $j_l$ and $n_l$, we can get an expression for $w_l^{(1)}(r)$ and $w_l^{(2)}(r)$ for $r > R$. eq. (3.6) is the asymptotic form when $r \to \infty$.



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In practice, if the theory has $CP$ symmetry which is the case in QCD, the two-channel $S$-matrix is usually parameterized as:[2]

$$S^{(l)}(E) = \begin{pmatrix} \eta_l e^{2i\delta_1^l} & i\sqrt{1-\eta_l^2}e^{i(\delta_1^l+\delta_2^l)} \\ i\sqrt{1-\eta_l^2}e^{i(\delta_1^l+\delta_2^l)} & \eta_l e^{2i\delta_2^l} \end{pmatrix}, \tag{3.9}$$

where the real parameters: $\delta_1^l(E)$, $\delta_2^l(E)$ and $\eta_l(E)$ are all functions of the energy $E$. We will assume in the following that the $S$-matrix of the scattering problem has this form.

## 4. Energy eigenfunctions on a torus

Now we enclose the system discussed above in a cubic, periodic box with finite extension $L$ in every spatial direction. The Schrödinger equation for the system now takes a similar form as in the infinite volume except that the potential is periodically extended and the (two-component) eigenfunction has to satisfy the periodic boundary condition:

$$[H_0 + V_L(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \qquad \psi(\mathbf{r}+L\mathbf{n}) = \psi(\mathbf{r}). \tag{4.1}$$

where the free hamiltonian is given by:

$$H_0 = \begin{pmatrix} -\frac{1}{2m_1}\nabla^2 & 0 \\ 0 & E_T - \frac{1}{2m_2}\nabla^2 \end{pmatrix} \tag{4.2}$$

and the periodically extended potential is:

$$V_L(\mathbf{r}) \equiv \sum_{\mathbf{n}} V(\mathbf{r}+L\mathbf{n}). \tag{4.3}$$

The eigenvalue equation (4.1) now has discrete spectrum and the corresponding eigenfunctions are smooth.

It is convenient to partition the whole space into two regions. In the inner region, every point satisfies the condition: $|\mathbf{r}| < R$, $mod(L)$. In the outer region:

$$\Omega = \{\mathbf{r} : |\mathbf{r}| > R, \mathrm{mod}\,(L)\}. \tag{4.4}$$

Note that in the outer region $\Omega$, the interaction potential $V_L(\mathbf{r}) = 0$ and the Schrödinger equation (4.1) reduces to two *decoupled* Helmholtz equations:

$$(\nabla^2 + k_i^2)\psi_i(\mathbf{r}) = 0, \qquad \text{i=1,2}, \tag{4.5}$$

where the energy eigenvalue $E$ is given by:

$$E = \frac{k_1^2}{2m_1} = E_T + \frac{k_2^2}{2m_2}. \tag{4.6}$$

For energy $0 < E < E_T$, $k_1$ is real and $k_2$ takes purely imaginary values; for energy $E < 0$, both $k_1$ and $k_2$ are purely imaginary.; for $E > E_T$, which is the case of two channel scattering above the threshold, both $k_1$ and $k_2$ are real numbers.

[2]For the potential models, we assume that the potential is invariant under time reversal and parity. Then, one has $S_{fi} = S_{i^*f^*}$, where $i^*$ and $f^*$ denotes the time-reversed state of $i$ and $f$. With this in mind, it is easily seen that eq. (3.9) is the most general $2 \times 2$ unitary matrix for the scattering matrix of spinless particles.



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It is easy to see that:

$$\Psi(\mathbf{r};E)=\sum_{lm}\left[\sum_{i=1}^{2}b^{(i)}_{lm}u^{(i)}_l(r)\right]Y_{lm}(\mathbf{n})\,. \tag{4.7}$$

solves the Schrödinger equation in the inner region for $|\mathbf{r}|<R$. In the outer region $\Omega$, for a given value of energy $E$, the corresponding eigenfunction must be superposition of the free Schrödinger equation, which in the outer region decouples to two independent Helmholtz equations. Since there are two linear independent radial wave functions, the eigenfunction must be some linear combination of the two:

$$\Psi(\mathbf{r};E)=\sum_{lm}\left[\sum_{i}c^{(i)}_{lm}w^{(i)}_l(r)\right]Y_{lm}(\mathbf{n})\,,\ \text{for } r>R\,, \tag{4.8}$$

with $c^{(j)}_{lm}=\sum_i b^{(i)}_{lm}C_{ij}$ being non-vanishing coefficients. Note that when the system is enclosed in a finite periodic box, the exact energy eigenvalues become discrete. The degeneracy in the radial wave-function in general is then lifted. That is to say, for a given value of energy, there exists only one radial wave-function, unlike in the infinite volume where there are two such wave-functions for a given energy.

On the other hand, in the region $\Omega$, the solution must be linear superposition of the singular periodic solutions of Helmholtz equation:

$$\Psi(\mathbf{r};E)=\begin{pmatrix}\sum_{lm}v^{(1)}_{lm}G_{lm}(\mathbf{r};k_1^2)\\ \sum_{lm}v^{(2)}_{lm}G_{lm}(\mathbf{r};k_2^2)\end{pmatrix}. \tag{4.9}$$

Combining eq. (4.9) and eq. (4.8), using the basic expansion of $G_{lm}(\mathbf{r})$:

$$G_{lm}(\mathbf{r};k^2)=\frac{(-)^lk^{l+1}}{4\pi}\left[Y_{lm}(\Omega_{\mathbf{r}})n_l(kr)+\sum_{l'm'}\mathcal{M}_{lm;l'm'}Y_{l'm'}(\Omega_{\mathbf{r}})j_{l'}(kr)\right], \tag{4.10}$$

we arrive at the following set of linear equations:

$$\begin{aligned}
c^{(1)}_{lm}(S^{(l)}_{11}+1)+c^{(2)}_{lm}\sqrt{\frac{k_1m_1}{k_2m_2}}S^{(l)}_{12} &= \sum_{l'm'}\frac{(-)^{l'}k_1^{l'+1}}{4\pi}v^{(1)}_{l'm'}\mathcal{M}^{(1)}_{l'm';lm}\,,\\
-ic^{(1)}_{lm}(S^{(l)}_{11}-1)-ic^{(2)}_{lm}\sqrt{\frac{k_1m_1}{k_2m_2}}S^{(l)}_{12} &= \frac{(-)^lk_1^{l+1}}{4\pi}v^{(1)}_{lm}\,,\\
c^{(2)}_{lm}(S^{(l)}_{22}+1)+c^{(1)}_{lm}\sqrt{\frac{k_2m_2}{k_1m_1}}S^{(l)}_{21} &= \sum_{l'm'}\frac{(-)^{l'}k_2^{l'+1}}{4\pi}v^{(2)}_{l'm'}\mathcal{M}^{(2)}_{l'm';lm}\,,\\
-ic^{(2)}_{lm}(S^{(l)}_{22}-1)-ic^{(1)}_{lm}\sqrt{\frac{k_2m_2}{k_1m_1}}S^{(l)}_{21} &= \frac{(-)^lk_2^{l+1}}{4\pi}v^{(2)}_{lm}\,.
\end{aligned} \tag{4.11}$$

In these equations, the symbol $\mathcal{M}^{(i)}_{l'm';lm}$ represents $\mathcal{M}_{l'm';lm}(k_i^2)$ for $i=1,2$, respectively. The explicit expression for for $\mathcal{M}_{l'm';lm}(k_i^2)$ are given in ref. [8] which we quote here:

$$\begin{aligned}
\mathcal{M}_{lm;js}(k^2)=&\sum_{l'm'}\frac{(-)^si^{j-l}\mathcal{Z}_{l'm'}(1,q^2)}{\pi^{3/2}q^{l'+1}}\sqrt{(2l+1)(2l'+1)(2j+1)}\\
&\times\begin{pmatrix}l & l' & j\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l & l' & j\\ m & m' & -s\end{pmatrix}.
\end{aligned} \tag{4.12}$$

Here we have used the Wigner's $3j$-symbols and $q = kL/(2\pi)$. The zeta function $\mathcal{Z}_{lm}(s, q^2)$ is defined as:

$$\mathcal{Z}_{lm}(s, q^2) = \sum_{\mathbf{n}} \frac{\mathcal{Y}_{lm}(\mathbf{n})}{(\mathbf{n}^2 - q^2)^s} \,. \tag{4.13}$$

According to this definition, the summation at the right-hand side of eq. (4.13) is formally divergent for $s = 1$ and needs to be analytically continued. Following similar discussions as in ref. [8], one could obtain a finite expression for the zeta function which is suitable for numerical evaluation [20, 21]. From the analytically continued formula, it is obvious from the symmetry of $O(Z)$ that, for $l \leq 4$, the only non-vanishing zeta functions at $s = 1$ are: $\mathcal{Z}_{00}$, and $\mathcal{Z}_{40}$.

Eliminating the coefficients $v^{(1)}_{lm}$ and $v^{(2)}_{lm}$ from the set of equations (4.11) , one obtains a homogeneous linear equation for the coefficients $c^{(1)}_{lm}$ and $c^{(2)}_{lm}$. In order to have non-trivial solutions for the coefficients $c^{(1)}_{lm}$ and $c^{(2)}_{lm}$, the corresponding matrix has to be singular. This condition then gives:

$$\begin{vmatrix} \mathcal{M}^{(1)+}_{l'm';lm} - S^{(l')}_{11}\mathcal{M}^{(1)-}_{l'm';lm} & \sqrt{\frac{k_2 m_2}{k_1 m_1}} S^{(l')}_{21}\mathcal{M}^{(2)-}_{l'm';lm} \\ \sqrt{\frac{k_1 m_1}{k_2 m_2}} S^{(l')}_{12}\mathcal{M}^{(1)-}_{l'm';lm} & \mathcal{M}^{(2)+}_{l'm';lm} - S^{(l')}_{22}\mathcal{M}^{(2)-}_{l'm';lm} \end{vmatrix} = 0 \,, \tag{4.14}$$

where the matrix elements $\mathcal{M}^{(i)\pm}_{l'm';lm}$ are defined as:

$$\mathcal{M}^{(i)\pm}_{l'm';lm}(k_i^2) = \mathcal{M}^{(i)}_{l'm';lm}(k_i^2) \pm i\delta_{l'l}\delta_{m'm} \,, \tag{4.15}$$

with the parameter $k_i^2$ related to the exact energy eigenvalue via eq. (4.6). Now if we further assume that the matrices: $\mathcal{M}^{(i)-}_{l'm';lm}(k_i^2)$ are non-singular, eq. (4.14) may be expressed as:

$$\begin{vmatrix} U^{(1)}_{l'm';lm} - S^{(l)}_{11}\delta_{l'l}\delta_{m'm} & \sqrt{\frac{k_2 m_2}{k_1 m_1}} S^{(l)}_{21}\delta_{l'l}\delta_{m'm} \\ \sqrt{\frac{k_1 m_1}{k_2 m_2}} S^{(l)}_{12}\delta_{l'l}\delta_{m'm} & U^{(2)}_{l'm';lm} - S^{(l)}_{22}\delta_{l'l}\delta_{m'm} \end{vmatrix} = 0 \,, \tag{4.16}$$

where the unitary matrices $U^{(i)}$ are defined as:

$$U^{(i)}_{l'm';lm} = \left(\frac{\mathcal{M}^{(i)} + i}{\mathcal{M}^{(i)} - i}\right)_{l'm';lm} \,. \tag{4.17}$$

This is the general relation we are looking for in the case of two-channel scattering. Obviously, when the off-diagonal matrix elements of the $S$-matrix, i.e. $S^{(l)}_{12}$ and $S^{(l)}_{21}$ vanish, eq. (4.14) reduces to the famous Lüscher's formula [8] for the single-channel elastic scattering.

## 5. Eigenstates with definite cubic symmetry

The general result (4.16) obtained in the previous section can be further simplified when we consider irreducible representations of the symmetry group of the cubic box. We know that energy eigenstates in a box can be characterized by their transformation properties under

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the symmetry group of the box. For this purpose, one has to decompose the representations of the rotational group with angular momentum $l$ into irreducible representations of the corresponding symmetry group of the box. For a symmetric cubic box, the relevant symmetry group is the cubic group $O(Z)$.

In a given symmetry sector, denoted by the irreducible representation $\Gamma$, the representation of the rotational group with angular momentum $l$ is decomposed into irreducible representations of $O(Z)$. This decomposition may contain the irreducible representation $\Gamma$. We may pick our basis of the representation as: $|\Gamma, \alpha; l, n\rangle$. Here $\alpha$ runs from 1 to $dim(\Gamma)$, the dimension of the irreducible representation $\Gamma$. Label $n$ runs from 1 to the total number of occurrence of $\Gamma$ in the decomposition of rotational group representation with angular momentum $l$. The matrix $\hat{M}$ is diagonal with respect to $\Gamma$ and $\alpha$ by Schur's lemma.

For the two-particle eigenstates in the symmetry sector $\Gamma$, the general formula (4.16) reduces to:

$$\begin{vmatrix} U^{(1)}(\Gamma) - S^{(l)}_{11} & \sqrt{\frac{k_2 m_2}{k_1 m_1}} S^{(l)}_{21} \\ \sqrt{\frac{k_1 m_1}{k_2 m_2}} S^{(l)}_{12} & U^{(2)}(\Gamma) - S^{(l)}_{22} \end{vmatrix} = 0\,. \tag{5.1}$$

Here $\hat{U}(\Gamma)$ represents a linear operator in the vector space $\mathcal{H}_\Lambda(\Gamma)$.[3] This vector space is spanned by all complex vectors whose components are $v_{ln}$, with $l \leq \Lambda$, and $n$ runs from 1 to the number of occurrence of $\Gamma$ in the decomposition of representation with angular momentum $l$ [8]. To write out more explicit formulae, one therefore has to consider decompositions of the rotational group representations under appropriate cubic symmetries.

The basic symmetry group for a cubic box is the group $O(Z)$, which has 2 one-dimensional (irreducible) representations $A_1$ and $A_2$, a two-dimensional irreducible representation $E$, and 2 three-dimensional representations $T_1$ and $T_2$.[4] Up to angular momentum $l = 4$, the representations of the rotational group are decomposed according to:

$$\begin{aligned} \mathbf{0} &= A_1^+\,, \\ \mathbf{1} &= T_1^-\,, \\ \mathbf{2} &= T_2^+ + E^+\,, \\ \mathbf{3} &= A_2^- + T_1^- + T_2^-\,, \\ \mathbf{4} &= A_1^+ + E^+ + T_1^+ + T_2^+\,. \end{aligned} \tag{5.2}$$

In most lattice calculations, the symmetry sector that is easiest to investigate is the invariant sector: $A_1^+$. We therefore focus on this particular symmetry sector. We see from eq. (5.2) that, up to $l \leq 4$, only $s$-wave and $g$-wave contribute to this sector. This corresponds to *two* linearly independent, homogeneous polynomials with degrees not more than 4 which are invariant under $O(Z)$. The two basis polynomials can be identified as $\mathcal{Y}_{00}$ and $\mathcal{Y}_{40}$.[5]

[3]Please refer to ref. [8] for details.

[4]The notations of the irreducible representations of group $O(Z)$ that we adopt here follow those in ref. [8].

[5]Our conventions for the spherical harmonics are taken from ref. [22].

In the first order approximation, if we neglect the mixing between the $s$-wave and $g$-wave, we have for the $A_1^+$ sector:

$$\det \begin{pmatrix} e^{2i\Delta_1} - \eta_0 e^{2i\delta_1^0} & i\sqrt{\frac{k_2 m_2}{k_1 m_1}}\sqrt{1-\eta_0^2}e^{i\delta_1^0+i\delta_2^0} \\ i\sqrt{\frac{k_1 m_1}{k_2 m_2}}\sqrt{1-\eta_0^2}e^{i\delta_1^0+i\delta_2^0} & e^{2i\Delta_2} - \eta_0 e^{2i\delta_2^0} \end{pmatrix} = 0\,. \tag{5.3}$$

where we have also used the special parametrization (3.9) for the $s$-wave $S$-matrix elements and we have defined:

$$e^{2i\Delta_i} \equiv \frac{\mathcal{M}_{00}(k_i^2) + i}{\mathcal{M}_{00}(k_i^2) - i}\,, \tag{5.4}$$

which may also be expressed as:

$$\cot \Delta_i = \mathcal{M}_{00}(k_i^2) = \frac{\mathcal{Z}_{00}(1, q_i^2)}{\pi^{3/2} q_i}\,. \tag{5.5}$$

Note that the quantities appearing above, namely $\delta_1^0$, $\delta_2^0$, $\eta_0$, $\Delta_1$ and $\Delta_2$, are all functions of the energy: $E = k_1^2/(2m_1) = E_T + k_2^2/(2m_2)$. Expanding eq. (5.3) we get, after some algebra:

$$\cos(\Delta_1 + \Delta_2 - \delta_1^0 - \delta_2^0) = \eta_0 \cos(\Delta_1 - \Delta_2 - \delta_1^0 + \delta_2^0)\,. \tag{5.6}$$

This is the simplified formula for the $s$-wave $S$-matrix elements. Another equivalent way of writing the same formula is:

$$\tan(\Delta_1 - \delta_1^0)\tan(\Delta_2 - \delta_2^0) = \frac{1-\eta_0}{1+\eta_0}\,. \tag{5.7}$$

Therefore, if we neglect contaminations from higher angular momentum (mainly from $l = 4$), the parameters in the two-channel $S$-matrix elements, namely $\eta_0$, $\delta_1^0$, $\delta_2^0$ and the exact two-particle energy $E$ satisfy a relation given by (5.6). Unlike the single channel case, where the $S$-matrix has only one parameter (phase shift) and it is related to the exact energy in a one-to-one fashion, the two channel $S$-matrix now has 3 real parameters and these parameters are related to the exact energy $E$ by one relation. This relation is helpful since it provides a constraint on the four physical quantities. For example, if we can measure the exact energy $E$ in lattice calculations, and if we know the values of $\delta_1^0$ and $\delta_2^0$ from experimental data (e.g. by partial wave analysis), we in principle can infer information about the parameter $\eta_0$ which is difficult to measure in the experiment. If the experimental information is inadequate, say both $\delta_2^0$ and $\eta_0$ are poorly determined, our result (5.6) still helps to setup a constraint between the two poorly determined physical quantities. This is more or less the situation in $\pi\pi$ scattering just above the $KK$ threshold. Note that above the two-particle inelastic threshold, the number of states within a particular energy interval is roughly twice as many as in the single-channel case and every energy eigenvalue satisfies eq. (5.6).

It is instructive to discuss the situation just above the inelastic threshold. Assuming that the inelastic scattering only occurs in the $s$-wave, the total reaction cross section just above the threshold is given by:

$$\sigma_r^{l=0} \simeq A\sqrt{E - E_T}\,. \tag{5.8}$$

for very small $(E - E_T) > 0$ where $A$ is some proportionality constant. This means that the parameter $\eta_0$ behaves like:

$$\eta_0 \simeq 1 - \frac{A m_1 E_T}{\pi} \sqrt{E - E_T} \,, \tag{5.9}$$

just above the threshold. On the other hand, since the physical quantity $\delta^0_2$ vanishes at the threshold, we may parameterize it as:

$$\tan \delta^0_2 \simeq k_2 a^{(2)}_0 \,. \tag{5.10}$$

Quantity $a^{(2)}_0$ might be called the scattering length in the second channel. Substituting these into our general formula (5.7), we get:[6]

$$a^{(2)}_0 = \frac{m_1 E_T A}{2\pi\sqrt{2m_2}} \cot \left[\delta^0_1(E_T) - \Delta_1(E_T)\right] . \tag{5.11}$$

If we consider the mixing of the $g$-wave, the formula obtained above becomes more complicated. We can write out the four-dimensional reduced matrix $\mathcal{M}(A^+_1)$ whose matrix elements are denoted as: $\mathcal{M}(A^+_1)_{ll'} = m_{ll'} = m_{l'l}$, with $l$ and $l'$ takes values in 0 and 4, respectively. Using the general formula (4.12), it is straightforward to work out these reduced matrix elements in terms of matrix elements $\mathcal{M}_{lm;l'm'}$. We find that, in the case of cubic symmetry, eq. (5.1) becomes:

$$\begin{vmatrix} u^{(1)}_{00} - S^{(0)}_{11} & \sqrt{\frac{k_2 m_2}{k_1 m_1}} S^{(0)}_{21} & u^{(1)}_{04} & 0 \\ \sqrt{\frac{k_1 m_1}{k_2 m_2}} S^{(0)}_{12} & u^{(2)}_{00} - S^{(0)}_{22} & 0 & u^{(2)}_{04} \\ u^{(1)}_{04} & 0 & u^{(1)}_{44} - S^{(4)}_{11} & \sqrt{\frac{k_2 m_2}{k_1 m_1}} S^{(4)}_{21} \\ 0 & u^{(2)}_{04} & \sqrt{\frac{k_1 m_1}{k_2 m_2}} S^{(4)}_{12} & u^{(2)}_{44} - S^{(4)}_{22} \end{vmatrix} = 0 \,. \tag{5.12}$$

Here matrix $U$ is defined as in eq. (4.17) and $u_{ll'}$ are the corresponding matrix elements. At this level, so many parameters enter the relation and it seems that the formula is useful only when other information is available.

We also would like to remark that, although we worked out the formulae in a cubic box, similar relations can also be obtained for general rectangular box following the strategies outlined in ref. [20, 21]. Such topologies might be useful for the calculations of scattering phases. It is also clear that the results obtained in this paper can easily generalized to more than two channels as long as the initial and final states in the scattering are still two-particle states.

Finally, let us speculate about possible extension to the case of massive field theory. In the case of single channel scattering, it was shown in ref. [8] that the result obtained in the quantum-mechanical model can be carried over literally to the case of massive quantum field theory as long as the non-relativistic dispersion relations of the particles are replaced by relativistic ones and the polarization effects and other effects (exponentially small) are small enough. For the case of multi-channel scattering, we expect that a similar conclusion

[6]Note that $\Delta_2 \sim q_2/\mathcal{Z}_{00}(1, q^2_2) \sim k^3_2$ for small $k_2$, so $\tan(\Delta_2 - \delta^0_2) \sim -\tan\delta^0_2$.



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to hold although a proof is still lacking. If this turned out to be true, it means that the results obtained in this paper can also be generalized to the case of massive field theory apart from corrections that are exponentially small in the large volume limit.

In the case of field theory, another complication arises since in the framework of field theory, particle numbers are not conserved. One therefore has to specify what one means by two-particle states [8] in a finite volume. Generally speaking, two-particle states for elastic scattering are the discrete (but quasi-continuum) spectrum states above the lowest two-particle threshold. When the energy is increased, we may encounter another threshold where the inelastic channel is opened. In the case of pion-pion scattering, the lowest two-particle threshold is the two-pion threshold. The next lowest threshold is the four-pion threshold which is below the two-kaon threshold. It is clear that the formulae obtained in this paper would be applicable only when the coupling between the four pion states and the two particle (two pion and two kaon) states becomes negligible. If this were the case, then when we calculate the correlation function matrix among appropriate two-particle operators, two-particle states dominate the correlation function matrix. The energy eigenstates thus obtained are also mainly composed of two-particle states. As we have said in the introduction, the weakness of interaction of four pion states with two pion states can be seen from the chiral lagrangian in which they are coupled via derivative couplings. In a lattice QCD simulation, the validity of this assumption might also be checked numerically by investigating the volume dependence of the energy eigenstates obtained from the corresponding correlation functions. This is due to the fact that the density of state for single particle, two-particle and four-particle states have rather different volume dependence. Using this technique, for example, the authors in ref. [23] were able to argue that the energy eigenstates they obtained are in fact $KN$ scattering states (two-particle states) and not a single-particle penta-quark state. Similar technique can in principle be applied to distinguish the two-particle states from the four-particle states in a finite volume. Of course the feasibility of this can only be checked in a real numerical simulation. Here we can only point out this possibility.

## 6. Conclusions

In this paper, we have studied two-particle two-channel scattering states in a cubic box with periodic boundary conditions. Assuming that energy eigenstates are only two-particle states, the relation of the exact energy eigenvalues in the box and the physical parameters in the coupled channel $S$-matrix elements in the continuum is found. This formula can be viewed as a generalization of the well-known Lüscher's formula to the coupled channel situation (inelastic scattering). In particular, we show that the two-channel $S$-matrix elements in the $s$-wave are related to the energy of the two-particle system by a simple identity, if contaminations from higher angular momentum sectors are neglected. This relation is non-perturbative in nature and it will help us to establish connections between the $S$-matrix parameters in the multi-channel scattering with the energy eigenvalues which are in principle accessible in lattice calculations.

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## A. Proof of the theorem

In this appendix, the proof of the theorem concerning the structure of the solution to the radial Schrödinger equation is provided. In particular, we consider the coupled differential equations:

$$\frac{d^2\Psi(z)}{dz^2} + \frac{2}{z}\frac{d\Psi(z)}{dz} + Q(z)\Psi(z) = 0\,, \tag{A.1}$$

where $\Psi(z)$ is the two-component wave-function and the matrix $Q(z)$ is given by:

$$Q(z) = -\frac{l(l+1)}{z^2} + \begin{pmatrix} 2m_1[E - V_1(z)] & 2m_1\Delta(z) \\ 2m_2\Delta^*(z) & 2m_2[E' - V_2(z)] \end{pmatrix}. \tag{A.2}$$

We would like to study the structure of the solutions to eq. (A.1) near $z = 0$.

Using standard transformation:

$$\Psi(z) = z^{-1/2}\Phi(z)\,, \tag{A.3}$$

we find that eq. (A.1) reduces to:

$$\frac{d^2\Phi(z)}{dz^2} + \frac{1}{z}\frac{d\Phi(z)}{dz} + \tilde{Q}(z)\Phi(z) = 0\,, \tag{A.4}$$

with $\tilde{Q}(z)$ given by:

$$\tilde{Q}(z) = -\frac{(l+1/2)^2}{z^2} + \begin{pmatrix} 2m_1[E - V_1(z)] & 2m_1\Delta(z) \\ 2m_2\Delta^*(z) & 2m_2[E' - V_2(z)] \end{pmatrix}. \tag{A.5}$$

We now proceed to find canonical solutions of the type:

$$\Phi(z) = z^\rho \sum_{n=0}^{\infty} \chi_n z^n\,, \tag{A.6}$$

where $\chi_n$ are two-component coefficients, $\rho$ is the index of the canonical solution. Assuming $z^2 V(z)$ is analytic near $z = 0$ and $\lim_{z\to 0}[z^2 V(z)] = 0$, we have:

$$z^2\tilde{Q}(z) = \sum_{n=0}^{\infty} Q_n z^n\,, \qquad Q_0 = -(l+1/2)^2\,. \tag{A.7}$$

Comparing the coefficients of each order we get:

$$[(\rho+n)^2) - (l+1/2)^2]\chi_n + \sum_{k=1}^{n} Q_k\chi_{n-k} = 0\,. \tag{A.8}$$

In particular, when $n = 0$ the above equation gives the index equation satisfied by $\rho$:

$$\rho^2 - (l + 1/2)^2 = 0\,. \tag{A.9}$$

This equation yields two solutions: $\rho = \pm(l + 1/2)$. Note that $\chi_0$ is non-vanishing, this shows that the solutions near $z = 0$ are categorized into two classes. In one class, the solutions behave like: $\Phi(z) \sim z^{l+1/2}$; in the other class the solutions behave like: $\Phi(z) \sim z^{-(l+1/2)}$. Or in terms of the solution $\Psi(z)$, these two cases behave like $\Psi(z) \sim z^l$ and $\Psi(z) \sim z^{-(l+1)}$ respectively. Also note that when the index $\rho$ take the values of $\pm(l+1/2)$, the matrix $Q_0$ becomes identically zero. Obviously, we can find two linearly independent solutions $\chi_0$ for each $\rho$. Therefore, we have shown that the canonical solutions indeed have the properties as indicated in the theorem. Since the coefficients $\chi_n$ are fully determined by the recursion relation (A.8), all what remains to be shown is that the series solution (A.6) converges uniformly and absolutely in the neighborhood of $z = 0$.

To show the convergence of the series solution, we see from eq. (A.8) that:

$$\chi_n = \mp \frac{1}{n(2l+1)} \sum_{k=1}^{n} Q_k \chi_{n-k}\,. \tag{A.10}$$

Note that $z^2 \tilde{Q}(z)$ is analytic near $z = 0$, therefore we can always find two real numbers $M \geq 1$ and $R > 0$ such that:

$$||Q_k|| \leq M R^{-k}\,, \tag{A.11}$$

where $||\cdot||$ indicates a matrix norm.[7] Let us assume that:

$$|\chi_\nu| \leq M^\nu R^{-\nu} |\chi_0|\,, \qquad \nu = 1, 2, \cdots, (n-1)\,. \tag{A.12}$$

we now show that the above inequality then holds for $\nu = n$. This is seen by:

$$\begin{aligned} |\chi_n| &\leq \frac{1}{n(2l+1)} \sum_{k=1}^{n} ||Q_k|| |\chi_{n-k}| \\ &\leq \frac{|\chi_0| R^{-n}}{n(2l+1)} \sum_{k=1}^{n} M^{n-k+1} \leq M^n R^{-n} |\chi_0|\,. \end{aligned} \tag{A.13}$$

Therefore, by induction, the inequality $|\chi_n| \leq M^n R^{-n} |\chi_0|$ is true for any integer $n$. It then follows trivially that the series (A.6) is absolutely and uniformly convergent in a small neighborhood around $z = 0$ which completes our proof of the theorem.

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