Extraction of Hadron Interactions above Inelastic Threshold in Lattice QCD

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We propose a new method to extract hadron interactions above inelastic threshold from the Nambu-Bethe-Salpter amplitude in lattice QCD. We consider the scattering such as $A+B \to C+D$, where A, B, C, D are names of different 1-particle states. An extension to cases where particle productions occur during scatterings is also discussed.
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§1. Introduction

The origin of the nuclear force is one of the major unsolved problems in particle and nuclear physics even after the establishment of the quantum chromodynamics (QCD). Recently, three of the present authors proposed a new approach to extract the NN interactions below inelastic threshold in lattice QCD.[1),2),3)] Through the Nambu-Bethe-Salpeter (NBS) wave function, the energy-independent but non-local potential $U(\boldsymbol{r}, \boldsymbol{r}')$ is so defined that the NBS wave function obeys the Schrödinger type equation in finite volume. Since $U(\boldsymbol{r}, \boldsymbol{r}')$ is localized in its spatial coordinates due to confinement of quarks and gluons, the potential receives finite volume effect only weakly in a large box. Therefore, once U is determined and is appropriately extrapolated to $L \to \infty$, one may simply use the Schrödinger equation in the infinite space to calculate the scattering phase shifts and bound state spectra, which can be compared with experimental data. With this approach we successfully extract not only the nucleon potential[1),2),3),4)] but also the hyperon potential[5),6)] below inelastic threshold in QCD.

Although this method is shown to be quite successful in order to describe elastic

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hadron interactions, the hadron interactions generally leads to inelastic scatterings as the total energy of the system increases. In this paper, we extend our method to such inelastic scatterings in order to extract hadron interactions in general. In Sec. 2, we briefly summarize our method previously used to extract the potential in the elastic scattering. In Sec. 3, we present our main idea to analyze the inelastic scattering from lattice QCD in the finite volume. We here discuss the scattering such as $A + B \to C + D$ scattering, where A, B, C, D represent some 1-particle states. This is a simplified version of the baryon scattering in the strangeness $S = -2$ and isospin $I = 0$ channel, where $\Lambda\Lambda$, $N\Xi$ and $\Sigma\Sigma$ appear as asymptotic states if the total energy is larger than $2m_\Sigma$. In Sec. 4, we discuss the extension of our proposal to the scattering with particle productions such as $A + B \to A + B + C$. In Sec. 5 we summarize this paper together with recent applications of our method in lattice QCD. A preliminary account of these results is given in Ref.7).

§2. Hadron interactions below threshold: elastic scattering

In this section, we summarize our strategy, previously used to extract the potential between two hadrons below inelastic threshold in lattice QCD.

2.1. *Nambu-Bethe-Salpeter wave function*

A key quantity in our method is the equal-time Nambu-Bethe-Salpter (NBS) amplitude, which we call the "NBS wave function" throughout this paper. Let us consider the following NBS wave function for a particle A and a particle B in QCD with total energy W in the center of mass system (*i.e.* the total three-momentum $\boldsymbol{P} = 0$) in the infinite box;

$$\psi^W_{AB}(\boldsymbol{r})e^{-Wt} = \lim_{\delta\to 0^+} \langle 0|T\{\varphi_A(\boldsymbol{y}, t+\delta)\varphi_B(\boldsymbol{x}, t)\}|AB; W, \boldsymbol{P} = 0\rangle \qquad (2\cdot1)$$

where the relative coordinate is denoted as $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{y}$. Here the local operators for the A and the B, which might be composite, are denoted by $\varphi_A(\boldsymbol{x}, t)$ and $\varphi_B(\boldsymbol{y}, t)$ with possible indices such as spinor or flavor being suppressed for simplicity. The QCD vacuum is denoted by $|0\rangle$, while the state $|AB; W, \boldsymbol{P} = 0\rangle$ is a QCD eigenstate with the same quantum numbers as the AB system. Note that $|AB; W, \boldsymbol{P} = 0\rangle$ can be taken as a product of 1-particle asymptotic state $|A\rangle_{\rm in} \otimes |B\rangle_{\rm in}$ in the infinite box, while this is not true in the finite box.

If the total energy $W = E^A_k + E^B_k = \sqrt{m_A^2 + \boldsymbol{k}^2} + \sqrt{m_B^2 + \boldsymbol{k}^2}$ is smaller than the inelastic threshold E_{th}, $\psi^W_{AB}(\boldsymbol{r})$ satisfies

$$\psi^W_{AB}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\boldsymbol{p}\cdot\boldsymbol{r}}}{(\boldsymbol{p}^2 - \boldsymbol{k}^2 - i\epsilon)} \frac{E^A_p + E^A_k}{4WE^A_p} T_{AB,AB}(p_A, p_B; k_A, k_B) + \mathcal{I}(\boldsymbol{r}) \qquad (2\cdot2)$$

where $p_A = (E^A_p, \boldsymbol{p})$, $k_A = (E^A_k, \boldsymbol{k})$, $k_B = (E^B_k, -\boldsymbol{k})$ are on-shell 4 momenta, while $p_B = (W - E^A_p, -\boldsymbol{p})$ is generally off-shell. Therefore $T_{AB,AB}(q_1, q_2, q_3, q_4)$ is in general off-shell T-matrix, defined through the connected four-point Green's function

$G^{(c)}_{AB,AB}(p_1, p_2; p_3, p_4)$ as

$$G^{(c)}_{AB,AB}(p_1, p_2; p_3, p_4) = (2\pi)^4 \delta^4(p_1 + p_2 - p_3 - p_4) \times iD_A(p_1) iD_B(p_2) iT_{AB,AB}(p_1, p_2; p_3, p_4) iD_A(p_3) iD_B(p_4) \quad (2\cdot3)$$

where $D_{A(B)}(p)$ is the free propagator for a particle $A(B)$ in the momentum space, which does not contain the negative energy part (*i.e.* the contribution of the corresponding anti-particle). In the above expression, $\mathcal{I}(\mathbf{r})$, which is exponentially suppressed for large $r = |\boldsymbol{r}|$ as e^{-cr} with $c \propto \sqrt{E_{th}^2 - W^2} > 0$, represents contributions from other than elastic scattering $A + B \to A + B$.

With the partial wave decomposition that

$$\psi^W_{AB}(\boldsymbol{r}) = 4\pi \sum_{l,m} i^l \psi^W_{AB,l}(r,k) Y_{lm}(\Omega_{\boldsymbol{r}}) \overline{Y_{lm}(\Omega_{\boldsymbol{k}})} \quad (2\cdot4)$$

where $k = |\boldsymbol{k}|$, Y_{lm} is the spherical harmonic function and $\Omega_{\boldsymbol{r}}$ is the solid angle of the vector $\boldsymbol{r}$, one can show for the large r that

$$\psi^W_{AB,l}(r,k) \to A_l \frac{\sin(kr - l\pi/2 + \delta_l(k))}{kr}, \quad (2\cdot5)$$

where the "phase shift" $\delta_l(k)$ is the phase of the S-matrix of the $A + B \to A + B$ scattering for the partial wave l. Therefore the NBS wave function is indeed the "wave function" which describes the $AB \to AB$ elastic scattering.[8),9),10),3)]

In the finite volume, restricted values of k denoted by k_n can be realized to satisfy the boundary condition. From the energy of two particle W_L in the finite volume, one can determine the phase shift $\delta_l(k_n)$ through Lüscher's formula,[11)] where k_n is determined from $W_L = E^A_{k_n} + E^B_{k_n}$.

2.2. *Strategy to define the potential*

In this subsection, we summarize our strategy to define the "potential" in QCD.

(1) We choose the field operator φ_A and φ_B. If these operators are composite, there are many choices to create the same one-particle state. For example, we take the local operator for nucleon in our previous calculations for the nucleon potential.[1),2),3)]

(2) We then measure the NBS wave function, defined by

$$\psi^W_{AB}(\boldsymbol{r}) = \lim_{\delta \to 0^+} \langle 0 | T\{\varphi_A(\boldsymbol{x} + \boldsymbol{r}, \delta) \varphi_B(\boldsymbol{x}, 0)\} | AB; W, \boldsymbol{P} = 0 \rangle. \quad (2\cdot6)$$

(3) Motivated by the fact that the NBS wave function describes the elastic scattering in the large r, we define the non-local potential as

$$\left[E^{AB}_k - H^{AB}_0\right] \psi^W_{AB}(\boldsymbol{x}) = \int d^3y \, U(\boldsymbol{x}; \boldsymbol{y}) \psi^W_{AB}(\boldsymbol{y}), \quad (2\cdot7)$$

$$E^{AB}_k = \frac{k^2}{2\mu_{AB}}, \quad H^{AB}_0 = \frac{-\nabla^2}{2\mu_{AB}},$$

where $k = |\boldsymbol{k}|$ and the reduced mass μ_{AB} is defined by $1/\mu_{AB} = 1/m_A + 1/m_B$.

(4) We then perform the velocity (or derivative) expansion that $U(\boldsymbol{x};\boldsymbol{y}) = V(\boldsymbol{x},\nabla)\delta^3(\boldsymbol{x}-\boldsymbol{y})$. In the case of the NN scattering, for example, we have[12)]

$$V(\boldsymbol{r},\nabla) = V_0(r) + V_\sigma(r)(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2) + V_T(r)S_{12} + V_{\rm LS}(r)\boldsymbol{L}\cdot\boldsymbol{S} + O(\nabla^2) \quad (2\cdot8)$$

where $\boldsymbol{\sigma}_i$ is the spin operator of i-th particle, S_{12} is the tensor operator given by

$$S_{12} = \frac{3}{r^2}(\boldsymbol{\sigma}_1\cdot\boldsymbol{r})(\boldsymbol{\sigma}_2\cdot\boldsymbol{r}) - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2). \quad (2\cdot9)$$

In the above expansion, the first three terms are of the leading order (LO), which do not contain derivatives, while the 4-th term is of the next leading order (NLO) with one derivative.

(5) Once we obtain the potentials, we solve the Schrödinger equation with these potentials in the *infinite* volume to obtain physical observables such as the phase shift and binding energy. Note that the exact value of the scattering phase shift $\delta(k)$ is obtained from this Schrödinger equation, while $\delta(k')$ at $k'\neq k$ is approximated one as long as the derivative expansion for the potential is truncated at the finite order.

In order to extract the NBS wave function on the lattice, we evaluate the 4-point correlation function as

$$\begin{aligned}\mathcal{G}_{AB}(\boldsymbol{x},\boldsymbol{y},t-t_0;J^P) &\equiv \langle 0|T\{\varphi_A(\boldsymbol{x},t)\varphi_B(\boldsymbol{y},t)\}\overline{\mathcal{J}}_{AB}(t_0;J^P)|0\rangle && (2\cdot10)\\ &= \sum_n A_n\langle 0|T\{\varphi_A(\boldsymbol{x},0)\varphi_B(\boldsymbol{y},0)\}|W_n\rangle e^{-W_n(t-t_0)} && (2\cdot11)\\ &\to A_0\psi_{AB}^{W_0}(\boldsymbol{r}=\boldsymbol{x}-\boldsymbol{y};J^P)e^{-W_0(t-t_0)}, \quad t-t_0\to\infty && (2\cdot12)\end{aligned}$$

where $A_n = \langle W_n|\overline{\mathcal{J}}_{AB}(t_0;J^P)|0\rangle$, and $\overline{\mathcal{J}}_{AB}(t_0;J^P)$ is some source operator which create 2-particle states of AB at t_0 with fixed total angular momentum J and parity P.[1),2),3)]

2.3. *Frequently Asked Questions*

There exist some questions to the definition of the potential in the previous subsection.

(1) Does the potential depend on the choice of operators φ_A,φ_B ?
Yes. The potential of course depends on the operators φ_A,φ_B from which the NBS wave function is defined. The choice of the operators can be regarded as the "scheme" to define the potential, since the potential itself is not a physical observable so that it can be scheme-dependent. If we calculate the physical observables, however, we obtain the unique result irrespective of the choice for the operators φ_A,φ_B as long as $U(\boldsymbol{x};\boldsymbol{y})$ is evaluated exactly. This is quite analogous to the running coupling, which is of course scheme-dependent. Physical matrix elements do not depend on the scheme of the running coupling, as long as they are evaluated exactly.

(2) Does the potential depend on the total energy at which the NBS wave function is defined ?

By construction, $U(\boldsymbol{x};\boldsymbol{y})$ is non-local but energy-independent, while the definition

$$V_{\boldsymbol{k}}(\boldsymbol{x}) \equiv E_k^{AB} - \frac{H_0^{AB}\psi_{AB}^W(\boldsymbol{x})}{\psi_{AB}^W(\boldsymbol{x})} \tag{2·13}$$

gives a local but energy(momentum)-dependent potential. It is easy to see that $V_{\boldsymbol{k}}(\boldsymbol{x})$ is equivalent to $U(\boldsymbol{x},\boldsymbol{y})$ since the number of degrees of freedom of $\boldsymbol{k}$ is equal to that of $\boldsymbol{y}$ in the finite volume.[3)] From the $\boldsymbol{k}$-dependence of the $V_{\boldsymbol{k}}(\boldsymbol{x})$, we therefore can determine the higher order terms of the derivative expansion $V(\boldsymbol{x},\nabla)$. It turns out, however, that the $\boldsymbol{k}$-dependence of $V_{\boldsymbol{k}}(\boldsymbol{x})$ for the nucleon potential is very small in quenched QCD between $k \simeq 0$ MeV($E_k^{NN} \simeq 0$ MeV) and $k \simeq 240$ MeV($E_k^{NN} \simeq 45$ MeV) for our scheme,[13),14),15),16)] where the local composite field of three quarks is used for nucleon operator.

§3. Hadron interactions above inelastic threshold

3.1. *NBS wave function in inelastic scattering*

We now consider the scatterings $A+B \to A+B$ and $A+B \to C+D$. We assume that $m_A + m_B < m_C + m_D < W$, where $W = E_k^A + E_k^B$ is the total energy of the system with $E_k^X = \sqrt{m_X^2 + \boldsymbol{k}^2}$. In this situation, the QCD eigenstate with the quantum numbers of the AB state and center of mass energy W is expressed in general as

$$|W\rangle = c_{AB}|AB,W\rangle + c_{CD}|CD,W\rangle + \cdots \tag{3·1}$$

$$|AB,W\rangle = |A,\boldsymbol{k}\rangle_{\rm in} \otimes |B,-\boldsymbol{k}\rangle_{\rm in}, \quad |CD,W\rangle = |C,\boldsymbol{q}\rangle_{\rm in} \otimes |D,-\boldsymbol{q}\rangle_{\rm in}, \tag{3·2}$$

where $W = E_k^A + E_k^B = E_q^C + E_q^D$. We define the following NBS wave functions,

$$\psi_{AB}(\boldsymbol{r},\boldsymbol{k}) = \lim_{\delta\to 0^+} \langle 0|T\{\varphi_A(\boldsymbol{x}+\boldsymbol{r},\delta)\varphi_B(\boldsymbol{x},0)\}|W\rangle, \tag{3·3}$$

$$\psi_{CD}(\boldsymbol{r},\boldsymbol{q}) = \lim_{\delta\to 0^+} \langle 0|T\{\varphi_C(\boldsymbol{x}+\boldsymbol{r},\delta)\varphi_D(\boldsymbol{x},0)\}|W\rangle, \tag{3·4}$$

which can be expressed as

$$\begin{aligned}\psi_{AB}(\boldsymbol{r},\boldsymbol{k}) = \sqrt{Z_A Z_B}\Bigg[c_{AB}\left\{e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \int \frac{d^3p}{(2\pi)^3}\frac{e^{i\boldsymbol{p}\cdot\boldsymbol{r}}}{\boldsymbol{p}^2 - \boldsymbol{k}^2 - i\epsilon}\frac{E_p^A + E_k^A}{4WE_p^A}T^{AB,AB}(p_A,p_B,k_A,k_B)\right\} \\ + c_{CD}\int \frac{d^3p}{(2\pi)^3}\frac{e^{i\boldsymbol{p}\cdot\boldsymbol{r}}}{\boldsymbol{p}^2 - \boldsymbol{k}^2 - i\epsilon}\frac{E_p^A + E_k^A}{4WE_p^A}T^{AB,CD}(p_A,p_B,q_C,q_D)\Bigg]\end{aligned} \tag{3·5}$$

$$\begin{aligned}\Psi_{CD}(\boldsymbol{r},\boldsymbol{q}) = \sqrt{Z_C Z_D}\Bigg[c_{CD}\left\{e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + \int \frac{d^3p}{(2\pi)^3}\frac{e^{i\boldsymbol{p}\cdot\boldsymbol{r}}}{\boldsymbol{p}^2 - \boldsymbol{q}^2 - i\epsilon}\frac{E_p^C + E_q^C}{4WE_p^C}T^{CD,CD}(p_C,p_D,q_C,q_D)\right\} \\ + c_{AB}\int \frac{d^3p}{(2\pi)^3}\frac{e^{i\boldsymbol{p}\cdot\boldsymbol{r}}}{\boldsymbol{p}^2 - \boldsymbol{q}^2 - i\epsilon}\frac{E_p^C + E_q^C}{4WE_p^C}T^{CD,AB}(p_C,p_D,k_A,k_B)\Bigg]\end{aligned} \tag{3·6}$$

where $p_A = (E_p^A, \boldsymbol{p})$, $p_B = (W - E_p^A, -\boldsymbol{p})$, $p_C = (E_p^C, \boldsymbol{p})$, $p_D = (W - E_p^C, -\boldsymbol{p})$, $k_A = (E_k^A, \boldsymbol{k})$, $k_B = (E_k^B, -\boldsymbol{k})$, $q_C = (E_q^C, \boldsymbol{q})$ and $q_D = (E_q^D, -\boldsymbol{q})$.

Introducing

$$H^{AB,AB(CD)}(\boldsymbol{p}, \boldsymbol{k}(\boldsymbol{q})) = \frac{E_p^A + E_k^A}{4WE_p^A} T^{AB,AB(CD)}(p_A, p_B, k_A, k_B(q_C, q_D)) \quad (3\cdot7)$$

$$H^{CD,AB(CD)}(\boldsymbol{p}, \boldsymbol{k}(\boldsymbol{q})) = \frac{E_p^C + E_q^D}{4WE_p^C} T^{CD,AB(CD)}(p_C, p_D, k_A, k_B(q_C, q_D)) \quad (3\cdot8)$$

and using the partial wave decomposition such that*),

$$\psi_{XY}(\boldsymbol{r}, \boldsymbol{k}) = 4\pi \sum_{l,m} i^l \psi_{XY}^l(r,k) Y_{lm}(\Omega_{\boldsymbol{r}}) \overline{Y_{lm}(\Omega_{\boldsymbol{k}})} \quad (3\cdot9)$$

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = 4\pi \sum_{l,m} i^l j_l(kr) Y_{lm}(\Omega_{\boldsymbol{r}}) \overline{Y_{lm}(\Omega_{\boldsymbol{k}})} \quad (3\cdot10)$$

$$H^{XY,VZ}(\boldsymbol{p}, \boldsymbol{k}) = 4\pi \sum_{l,m} H_l^{XY,VZ}(p,k) Y_{lm}(\Omega_{\boldsymbol{p}}) \overline{Y_{lm}(\Omega_{\boldsymbol{k}})} \quad (3\cdot11)$$

with $XY, VZ = AB$ or CD, we have

$$\psi_{AB}^l(r,k) = \sqrt{Z_A Z_B}\left[c_{AB}\left\{j_l(kr) + \int \frac{p^2 dp}{2\pi^2} \frac{1}{p^2 - k^2 - i\epsilon} H_l^{AB,AB}(p,k) j_l(pr)\right\} + c_{CD} \int \frac{p^2 dp}{2\pi^2} \frac{1}{p^2 - k^2 - i\epsilon} H_l^{AB,CD}(p,q) j_l(pr)\right] \quad (3\cdot12)$$

$$\psi_{CD}^l(r,q) = \sqrt{Z_C Z_D}\left[c_{CD}\left\{j_l(qr) + \int \frac{p^2 dp}{2\pi^2} \frac{1}{p^2 - q^2 - i\epsilon} H_l^{CD,CD}(p,q) j_l(pr)\right\} + c_{AB} \int \frac{p^2 dp}{2\pi^2} \frac{1}{p^2 - q^2 - i\epsilon} H_l^{CD,AB}(p,k) j_l(pr)\right]. \quad (3\cdot13)$$

Here the spherical harmonic function Y_{lm} is normalized as

$$\int d\Omega_{\boldsymbol{r}}\ \overline{Y_{lm}(\Omega_{\boldsymbol{r}})} Y_{l'm'}(\Omega_{\boldsymbol{r}}) = \delta_{ll'}\delta_{mm'} \quad (3\cdot14)$$

with the solid angle $\Omega_{\boldsymbol{r}}$ of the vector $\boldsymbol{r}$, and the spherical Bessel function $j_l(x)$ is given by

$$j_l(x) = (-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \left(\frac{\sin x}{x}\right) \simeq \frac{\sin(x - l\pi/2)}{x}, \quad x \to \infty. \quad (3\cdot15)$$

The p integral gives[8),9),10)]

$$\psi_{AB}^l(r,k) = \sqrt{Z_A Z_B}\left[c_{AB}\left\{j_l(kr) + \frac{k}{4\pi} H_l^{AB,AB}(k,k)\left\{n_l(kr) + i j_l(kr)\right\}\right\}\right.$$

*) Here we ignore spins for simplicity.

$$+ c_{CD}\frac{k}{4\pi}H_l^{AB,CD}(k,q)\left\{n_l(kr)+ij_l(kr)\right\}\Big] + \mathcal{I}^l_{AB}(r) \tag{3·16}$$

$$\psi^l_{CD}(r,q) = \sqrt{Z_C Z_D}\Big[c_{CD}\Big\{j_l(qr) + \frac{q}{4\pi}H_l^{CD,CD}(q,q)\left\{n_l(qr)+ij_l(qr)\right\}\Big\}$$

$$+ c_{AB}\frac{q}{4\pi}H_l^{CD,AB}(q,k)\left\{n_l(qr)+ij_l(qr)\right\}\Big] + \mathcal{I}^l_{CD}(r) \tag{3·17}$$

where $\mathcal{I}^l_{XY}(r)$, which represents all contributions except those from the pole at $p = k$ or $p = q$, is exponentially suppressed for large r, and another spherical Bessel function $n_l(x)$ is given by

$$n_l(x) = (-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\left(\frac{\cos x}{x}\right) \simeq \frac{\cos(x - l\pi/2)}{x}, \quad x\to\infty. \tag{3·18}$$

The unitarity relation

$$T - T^\dagger = iT^\dagger T \tag{3·19}$$

for the on-shell T-matrix T of the 2 channel scattering gives

$$T_l^{I,J}(W) = \frac{8\pi W}{p_I}\left[O(W)\begin{pmatrix} e^{i\delta_l^1(W)}\sin\delta_l^1(W) & 0 \\ 0 & e^{i\delta_l^2(W)}\sin\delta_l^2(W)\end{pmatrix}O^{-1}(W)\right]^{I,J} \tag{3·20}$$

$$O(W) = \begin{pmatrix}\cos\theta(W) & -\sin\theta(W) \\ \sin\theta(W) & \cos\theta(W)\end{pmatrix}, \qquad I = 1,2 \quad J = 1,2 \tag{3·21}$$

where $\delta_l^i(W)$ is the scattering phase shift , whereas $\theta(W)$ is the mixing angle between 1 and 2. Here index 1 represents AB while 2 represents CD. With this notation $p_1 = k$ and $p_2 = q$. We therefore obtain

$$\frac{p_I}{4\pi}H_l^{I,J}(p_I,p_J) = \left[O(W)\begin{pmatrix} e^{i\delta_l^1(W)}\sin\delta_l^1(W) & 0 \\ 0 & e^{i\delta_l^2(W)}\sin\delta_l^2(W)\end{pmatrix}O^{-1}(W)\right]^{I,J} \tag{3·22}$$

Using these results, the NBS wave functions of the 2 channel system behave for large r as

$$\begin{pmatrix}\hat\psi^l_{AB}(r,k) \\ \hat\psi^l_{CD}(r,q)\end{pmatrix} \simeq \begin{pmatrix} j_l(kr) & 0 \\ 0 & j_l(qr)\end{pmatrix}\begin{pmatrix} c_{AB} \\ c_{CD}\end{pmatrix} + \begin{pmatrix} n_l(kr)+ij_l(kr) & 0 \\ 0 & n_l(qr)+ij_l(qr)\end{pmatrix}$$

$$\times\, O(W)\begin{pmatrix} e^{i\delta_l^1(W)}\sin\delta_l^1(W) & 0 \\ 0 & e^{i\delta_l^2(W)}\sin\delta_l^2(W)\end{pmatrix}O^{-1}(W)\begin{pmatrix} c_{AB} \\ c_{CD}\end{pmatrix} \tag{3·23}$$

where $\hat\psi^l_{XY} = \psi^l_{XY}/\sqrt{Z_X Z_Y}$. This expression shows that the NBS wave function for large r agree with scattering waves described by two scattering phases $\delta_l^i(W)$ $(i = 1,2)$ and one mixing angle $\theta(W)$.

3.2. *Coupled channel potentials*

Let us now consider QCD in the finite volume V. In the finite volume, $|AB, W\rangle$ and $|CD, W\rangle$ are no longer eigenstates of the hamiltonian. True eigenvalues are shifted from W to $W_i = W + O(V^{-1})$ $(i = 1, 2)$. By diagonalization method in lattice QCD simulations, it is relatively easy to determine W_1 and W_2. With these values Lüscher's finite volume formula gives two conditions, which, however, are insufficient to determine three observables, δ_l^1, δ_l^2 and θ. (See 17), 18), 19) for recent proposals to overcome this difficulty.) We here propose alternative approach to extract three observables, δ_l^1, δ_l^2 and θ, in lattice QCD through the above NBS wave functions. We consider the (normalized) NBS wave functions at two different values of energy, W_1 and W_2, in the finite volume:

$$\psi_{AB}(\boldsymbol{r}, \boldsymbol{k}_i) = \frac{1}{\sqrt{Z_A Z_B}} \lim_{\delta\to 0^+} \langle 0| T\{\varphi_A(\boldsymbol{x}+\boldsymbol{r}, \delta)\varphi_B(\boldsymbol{x}, 0)\}|W_i\rangle \quad (3\cdot 24)$$

$$\psi_{CD}(\boldsymbol{r}, \boldsymbol{q}_i) = \frac{1}{\sqrt{Z_C Z_D}} \lim_{\delta\to 0^+} \langle 0| T\{\varphi_C(\boldsymbol{x}+\boldsymbol{r}, \delta)\varphi_D(\boldsymbol{x}, 0)\}|W_i\rangle, \quad i = 1, 2. \quad (3\cdot 25)$$

(We here omit ˜ on ψ.) We then define the coupled channel non-local potentials from the coupled channel Schrödinger equation as

$$\left[E_{k_i}^{AB} - H_0^{AB}\right] \psi_{AB}(\boldsymbol{x}, \boldsymbol{k}_i) = \int d^3y\ U_{AB,AB}(\boldsymbol{x}; \boldsymbol{y})\ \psi_{AB}(\boldsymbol{y}, \boldsymbol{k}_i) + \int d^3y\ U_{AB,CD}(\boldsymbol{x}; \boldsymbol{y})\ \psi_{CD}(\boldsymbol{y}, \boldsymbol{q}_i) \quad (3\cdot 26)$$

$$\left[E_{q_i}^{CD} - H_0^{CD}\right] \psi_{CD}(\boldsymbol{x}, \boldsymbol{k}_i) = \int d^3y\ U_{CD,AB}(\boldsymbol{x}; \boldsymbol{y})\ \psi_{AB}(\boldsymbol{y}, \boldsymbol{k}_i) + \int d^3y\ U_{CD,CD}(\boldsymbol{x}; \boldsymbol{y})\ \psi_{CD}(\boldsymbol{y}, \boldsymbol{q}_i) \quad (3\cdot 27)$$

for $i = 1, 2$. As before we introduce the derivative expansion as

$$U_{XY,VZ}(\boldsymbol{x}; \boldsymbol{y}) = V_{XY,VZ}(\boldsymbol{x}, \nabla)\delta^3(\boldsymbol{x}-\boldsymbol{y}) = \left[V_{XY,VZ}(\boldsymbol{x}) + O(\nabla)\right]\delta^3(\boldsymbol{x}-\boldsymbol{y}) \quad (3\cdot 28)$$

and at the leading order of the expansion, we have

$$K_{AB}(\boldsymbol{x}, \boldsymbol{k}_i) \equiv \left[E_{k_i}^{AB} - H_0^{AB}\right] \psi_{AB}(\boldsymbol{x}, \boldsymbol{k}_i) = V_{AB,AB}(\boldsymbol{x})\ \psi_{AB}(\boldsymbol{x}, \boldsymbol{k}_i) + V_{AB,CD}(\boldsymbol{x})\ \psi_{CD}(\boldsymbol{x}, \boldsymbol{q}_i) \quad (3\cdot 29)$$

$$K_{CD}(\boldsymbol{x}, \boldsymbol{q}_i) \equiv \left[E_{q_i}^{CD} - H_0^{CD}\right] \psi_{CD}(\boldsymbol{x}, \boldsymbol{k}_i) = V_{CD,AB}(\boldsymbol{x})\ \psi_{AB}(\boldsymbol{x}, \boldsymbol{k}_i) + U_{CD,CD}(\boldsymbol{x})\ \psi_{CD}(\boldsymbol{x}, \boldsymbol{q}_i). \quad (3\cdot 30)$$

These equations for $i = 1, 2$ can be solved as

$$\begin{pmatrix} V_{AB,AB}(\boldsymbol{x}) & V_{AB,CD}(\boldsymbol{x}) \\ V_{CD,AB}(\boldsymbol{x}) & V_{CD,CD}(\boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} K_{AB}(\boldsymbol{x}, \boldsymbol{k}_1) & K_{AB}(\boldsymbol{x}, \boldsymbol{k}_2) \\ K_{CD}(\boldsymbol{x}, \boldsymbol{q}_1) & K_{CD}(\boldsymbol{x}, \boldsymbol{q}_2) \end{pmatrix} \times \begin{pmatrix} \psi_{AB}(\boldsymbol{x}, \boldsymbol{k}_1) & \psi_{AB}(\boldsymbol{x}, \boldsymbol{k}_2) \\ \psi_{CD}(\boldsymbol{x}, \boldsymbol{q}_1) & \psi_{CD}(\boldsymbol{x}, \boldsymbol{q}_2) \end{pmatrix}^{-1}. \quad (3\cdot 31)$$

Once we obtain the coupled channel local potentials $V_{XY,VZ}(\boldsymbol{x})$, we solve the coupled channel Scrödinger equation in *infinite* volume with some appropriate boundary condition such that the incoming wave has a definite l and consists of the AB state only , in order to extract three observables for each l, $\delta_l^1(W)$, $\delta_l^2(W)$ and $\theta(W)$, at all values of W. Of course, since $V_{XY,VZ}$ is the leading order approximation in the velocity expansion of $U_{XY,VZ}(\boldsymbol{x};\boldsymbol{y})$, results for three observables $\delta_l^1(W)$, $\delta_l^2(W)$ and $\theta(W)$ at $W \neq W_1, W_2$ are also approximate ones and might be different from the exact values. By performing an additional extraction of $V_{XY,VZ}(\boldsymbol{x})$ at $(W_3, W_4) \neq (W_1, W_2)$, we can test how good the leading order approximation is, as in the case of the elastic scattering.[13)]

The above result can be easily extended to the coupled channel among n states $A_I B_I$ $(I = 1, 2, \cdots, n)$. Local potentials at the LO in the velocity expansion are given by

$$V_{I,J}(\boldsymbol{r}) = \sum_{M=1}^{n} K_I(\boldsymbol{r}, \boldsymbol{k}_M^I) X^{-1}(\boldsymbol{r})_{MJ} \tag{3·32}$$

$$K_I(\boldsymbol{r}, \boldsymbol{k}_M^I) \equiv \left[E_M^I - H_0^I\right] \psi_I(\boldsymbol{r}, \boldsymbol{k}_M^I) \tag{3·33}$$

where $X^{-1}(\boldsymbol{r})$ is the inverse of the $n \times n$ NBS wave function matrix

$$X(\boldsymbol{r})_{IJ} \equiv \psi_I(\boldsymbol{r}, \boldsymbol{k}_J^I) = \frac{1}{\sqrt{Z_{A_I} Z_{B_I}}} \lim_{\delta \to 0^+} \langle 0 | T\{\varphi_{A_I}(\boldsymbol{x}+\boldsymbol{r}, \delta) \varphi_{B_I}(\boldsymbol{x}, 0)\} | W_J \rangle \tag{3·34}$$

the momentum $\boldsymbol{k}_J^I$ satisfies the relation that $W_J = \sqrt{(\boldsymbol{k}_J^I)^2 + m_{A_I}^2} + \sqrt{(\boldsymbol{k}_J^I)^2 + m_{B_I}^2}$ for $J = 1, 2, \cdots, n$, $E_J^I = (\boldsymbol{k}_J^I)^2/(2\mu_{A_I B_I})$ and $H_0^I = -\nabla^2/(2\mu_{A_I B_I})$.

3.3. *Inelasticity and non-locality*

We now consider the 2-channel problem again. Let us assume that the leading order approximation for the coupled channel potential works reasonably well. Instead of considering the coupled channel potential, the effective potential for the AB channel is given by

$$U_{AB,AB}^{\mathrm{eff}}(\boldsymbol{x}, \boldsymbol{y}) = V_{AB,AB}(\boldsymbol{x}) \delta^{(3)}(\boldsymbol{x} - \boldsymbol{y}) + V_{AB,CD}(\boldsymbol{x}) \frac{1}{E_q^{CD} - H_0^{CD} - V_{CD.CD}}(\boldsymbol{x}, \boldsymbol{y}) V_{CD,AB}(\boldsymbol{y}), \tag{3·35}$$

where the non-locality becomes manifest in the second term. The magnitude of momentum $\boldsymbol{q}$ for the CD channel is expressed as

$$4W^2 \boldsymbol{q}^2 = (W^2 - (m_C + m_D)^2)(W^2 - (m_C - m_D)^2). \tag{3·36}$$

To estimate the magnitude of non-locality in eq.(3·35), we here ignore the $V_{CD,CD}$ term in the denominator. In this case, if the total energy W is below the inelastic threshold $m_C + m_D$ such that $\boldsymbol{q}^2 = -M^2 < 0$, we have

$$\frac{1}{H_0^{CD} - E_q^{CD}}(\boldsymbol{x}, \boldsymbol{y}) = \frac{2\mu_{CD}}{4\pi |\boldsymbol{x} - \boldsymbol{y}|} e^{-M|\boldsymbol{x} - \boldsymbol{y}|} \tag{3·37}$$

Therefore, non-locality of the potential $U_{AB,AB}^{\mathrm{eff}}(\boldsymbol{x}, \boldsymbol{y})$ is exponentially suppressed as long as M is large enough. As W approaches $m_C + m_D$, however, non-locality of the potential becomes larger and manifest. In this simple example, this non-locality of the single channel potential can be completely removed by introducing the CD state and *coupled channel* potentials between AB and CD. Therefore, in practice, the non-locality caused by inelastic final states whose thresholds are closed to the total energy W is expected to become milder for the coupled channel potentials including these states.

§4. Extension: Inelastic scattering with particle production

The method considered in the previous section can be generalized to inelastic scattering where a number of particles is not conserved. For illustration, we consider a case that the scatterings $A + B \to A + B$ and $A + B \to A + B + C$ occur and the total energy W satisfies $m_A + m_B + m_C < W < m_A + m_B + 2m_C$.

We consider the following NBS wave functions in the center of mass system:

$$\psi^W_{AB}(\boldsymbol{x}) = \frac{1}{\sqrt{Z_A Z_B}} \lim_{\delta\to 0^+} \langle 0|\varphi_A(\boldsymbol{r}+\boldsymbol{x},\delta)\varphi_B(\boldsymbol{r},0)|W\rangle \tag{4·1}$$

$$\psi^W_{ABC}(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{\sqrt{Z_A Z_B Z_C}} \lim_{\delta\to 0^+} \langle 0|\varphi_A(\boldsymbol{r}+\boldsymbol{x}+\frac{\boldsymbol{y}\,\mu_{BC}}{m_C},\delta)\varphi_B(\boldsymbol{r}+\boldsymbol{y},0)\varphi_C(\boldsymbol{r},-\delta)|W\rangle \tag{4·2}$$

where

$$|W\rangle = c_1\ |\boldsymbol{k}\rangle_{\rm in}\otimes|-\boldsymbol{k}\rangle_{\rm in} + c_2\ |\boldsymbol{q}_x\rangle_{\rm in}\otimes|\boldsymbol{q}_y-\boldsymbol{q}_x\frac{\mu_{BC}}{m_C}\rangle_{\rm in}\otimes|-\boldsymbol{q}_y-\boldsymbol{q}_x\frac{\mu_{BC}}{m_B}\rangle_{\rm in} \tag{4·3}$$

with

$$\begin{aligned} W &= \sqrt{\boldsymbol{k}^2+m_A^2}+\sqrt{\boldsymbol{k}^2+m_B^2} \\ &= \sqrt{\boldsymbol{q}_x^2+m_A^2}+\sqrt{(\boldsymbol{q}_y-\boldsymbol{q}_x\frac{\mu_{BC}}{m_C})^2+m_B^2}+\sqrt{(\boldsymbol{q}_y+\boldsymbol{q}_x\frac{mu_{BC}}{m_B})^2+m_C^2} \end{aligned} \tag{4·4}$$

and $1/\mu_{BC} = 1/m_B + 1/m_C$. Here $\boldsymbol{y} = \boldsymbol{r}_B - \boldsymbol{r}_C$ is a relative coordinate between B and C with the reduced mass μ_{BC}, while $\boldsymbol{x} = \boldsymbol{r}_A - \mathbf{R}_{BC}$ is the one between A and the center of mass of B and C with $\mathbf{R}_{BC} = (m_B\boldsymbol{r}_B + m_C\boldsymbol{r}_C)/(m_B+m_C)$. We here assume the property that ψ^W_{ABC} has asymptotic behavior of the scattering wave of $A+B+C$ as $|\boldsymbol{x}|,|\boldsymbol{y}|\to\infty$, as shown for ψ^W_{AB} in the previous section. Although this property has not been shown so far, it is reasonable to assume this. We leave the proof for this important property to the future investigation.

We define the non-local potential from the coupled channel equations as

$$\begin{aligned} K^W_{AB}(\boldsymbol{x}) &\equiv \left[E^{AB}_k - H^{AB}_{0,x}\right]\psi^W_{AB}(\boldsymbol{x}) = \int d^3 z\ U_{AB,AB}(\boldsymbol{x};\boldsymbol{z})\,\psi^W_{AB}(\boldsymbol{z}) \\ &\quad + \int d^3 z\ d^3 w\ U_{AB,ABC}(\boldsymbol{x};\boldsymbol{z},\boldsymbol{w})\,\psi^W_{ABC}(\boldsymbol{z},\boldsymbol{w}) \end{aligned} \tag{4·5}$$

$$\begin{aligned} K^W_{ABC}(\boldsymbol{x},\boldsymbol{y}) &\equiv \left[E^{A,BC}_{q_x} + E^{BC}_{q_y} - H^{A,BC}_{0,x} - H^{BC}_{0,y}\right]\psi^W_{ABC}(\boldsymbol{x},\boldsymbol{y}) = \int d^3 z\ U_{ABC,AB}(\boldsymbol{x},\boldsymbol{y};\boldsymbol{z}) \\ &\quad \times\psi^W_{AB}(\boldsymbol{z}) + \int d^3 z\ d^3 w\ U_{ABC,ABC}(\boldsymbol{x},\boldsymbol{y};\boldsymbol{z},\boldsymbol{w})\,\psi^W_{ABC}(\boldsymbol{z},\boldsymbol{w}) \end{aligned}$$

where

$$H_{0,x}^{AB} = \frac{-\nabla_{\boldsymbol{x}}^2}{2\mu_{AB}}, \quad H_{0,x}^{A,BC} = \frac{-\nabla_{\boldsymbol{x}}^2}{2\mu_{A,BC}}, \quad H_{0,y}^{BC} = \frac{-\nabla_{\boldsymbol{y}}^2}{2\mu_{BC}}, \tag{4·6}$$

$$E_k^{AB} = \frac{\boldsymbol{k}^2}{2\mu_{AB}}, \quad E_{q_x}^{A,BC} = \frac{\boldsymbol{q}_x^2}{2\mu_{A,BC}}, \quad E_{q_y}^{BC} = \frac{\boldsymbol{q}_y^2}{2\mu_{BC}} \tag{4·7}$$

with another reduced mass defined by $1/\mu_{A,BC} = 1/m_A + 1/(m_B + m_C)$.

We consider the following velocity expansions

$$U_{AB,AB}(\boldsymbol{x};\boldsymbol{z}) = [V_{AB,AB}(\boldsymbol{x}) + O(\nabla_x)]\, \delta^3(\boldsymbol{x}-\boldsymbol{z}) \tag{4·8}$$

$$U_{AB,ABC}(\boldsymbol{x};\boldsymbol{z},\boldsymbol{w}) = [V_{AB,ABC}(\boldsymbol{x},\boldsymbol{w}) + O(\nabla_x)]\, \delta^3(\boldsymbol{x}-\boldsymbol{z}) \tag{4·9}$$

$$U_{ABC,AB}(\boldsymbol{x},\boldsymbol{y};\boldsymbol{z}) = [V_{ABC,AB}(\boldsymbol{x},\boldsymbol{y}) + O(\nabla_x)]\, \delta^3(\boldsymbol{x}-\boldsymbol{z}) \tag{4·10}$$

$$U_{ABC,ABC}(\boldsymbol{x},\boldsymbol{y};\boldsymbol{z},\boldsymbol{w}) = [V_{ABC,ABC}(\boldsymbol{x},\boldsymbol{y}) + O(\nabla_x,\nabla_y)]\, \delta^3(\boldsymbol{x}-\boldsymbol{z})\delta^3(\boldsymbol{y}-\boldsymbol{w}) \tag{4·11}$$

where the hermiticity of the non-local potentials gives $V_{AB,ABC}(\boldsymbol{x},\boldsymbol{y}) = V_{ABC,AB}(\boldsymbol{x},\boldsymbol{y})$.

At the leading order of the velocity expansions, the coupled channel equations become

$$K_{AB}^{W}(\boldsymbol{x}) = V_{AB,AB}(\boldsymbol{x})\psi_{AB}^{W}(\boldsymbol{x}) + \int d^3 w\; V_{AB,ABC}(\boldsymbol{x},\boldsymbol{w})\psi_{ABC}^{W}(\boldsymbol{x},\boldsymbol{w}) \tag{4·12}$$

$$K_{ABC}(\boldsymbol{x},\boldsymbol{y}) = V_{ABC,AB}(\boldsymbol{x},\boldsymbol{y})\psi_{AB}^{W}(\boldsymbol{x}) + V_{ABC,ABC}(\boldsymbol{x},\boldsymbol{y})\psi_{ABC}^{W}(\boldsymbol{x},\boldsymbol{y}). \tag{4·13}$$

By considering two values of energy such that $W = W_1, W_2$, we can determine $V_{ABC,AB}$ and $V_{ABC,ABC}$ from the second equation as

$$\begin{aligned}\begin{pmatrix} V_{ABC,AB}(\boldsymbol{x},\boldsymbol{y}) & V_{ABC,ABC}(\boldsymbol{x},\boldsymbol{y}) \end{pmatrix} &= \begin{pmatrix} K_{ABC}^{W_1}(\boldsymbol{x},\boldsymbol{y}) & K_{ABC}^{W_2}(\boldsymbol{x},\boldsymbol{y}) \end{pmatrix} \\ &\quad \times \begin{pmatrix} \psi_{AB}^{W_1}(\boldsymbol{x}) & \psi_{AB}^{W_2}(\boldsymbol{x}) \\ \psi_{ABC}^{W_1}(\boldsymbol{x},\boldsymbol{y}) & \psi_{ABC}^{W_2}(\boldsymbol{x},\boldsymbol{y}) \end{pmatrix}^{-1}\end{aligned} \tag{4·14}$$

Using the hermiticity $V_{AB,ABC}(\boldsymbol{x},\boldsymbol{y}) = V_{ABC,AB}(\boldsymbol{x},\boldsymbol{y})$, we can extract $V_{AB,AB}$ from the first equation as

$$V_{AB,AB}(\boldsymbol{x}) = \frac{1}{\psi_{AB}^{W}(\boldsymbol{x})}\left[K_{AB}^{W}(\boldsymbol{x}) - \int d^3 w\; V_{ABC,AB}(\boldsymbol{x},\boldsymbol{w})\psi_{ABC}^{W}(\boldsymbol{x},\boldsymbol{w})\right] \tag{4·15}$$

for $W = W_1, W_2$. A difference of $V_{AB,AB}(\boldsymbol{x})$ between two estimates at W_1 and W_2 gives an estimate for higher order contributions in the velocity expansions.

Once we obtain $V_{AB,AB}$, $V_{AB,ABC} = V_{ABC,AB}$ and $V_{ABC,ABC}$, we can solve the coupled channel Schrödinger equations in the *infinite* volume, in order to extract physical observables. As W increases and becomes larger than $m_A + m_B + nm_C$, the inelastic scattering $A + B \to A + B + nC$ becomes possible. As in the case of $A + B \to A + B + C$ in the above, we can define the coupled channel potentials including this channel, though calculations of the NBS wave functions for multi-hadron operators become more and more difficult in practice.

§5. Summary

In this paper, we propose extensions of the method of extracting potentials through NBS wave functions to the case where inelastic scatterings becomes important. We first consider the case that $A + B \to C + D$ scattering occurs and present an explicit formula to extract the coupled channel potentials between AB and CD. The general formula for the scattering among n states is also given. An extension to the case where the particle production occurs during the scattering such as $A+B \to A+B+C$ is also considered. This can also be extended to more general cases such as $A + B \to A + B + nC$ ($n = 1, 2, 3, \cdots .$).

Recently the potential method has been used to extract potentials for the flavor SU(3) limit in lattice QCD where up, down and strange quark masses are all equal.[20] In this limit there exist 6-independent potentials corresponding to the irreducible representations of the flavor SU(3), and among these, the flavor singlet potential is strong attractive, suggesting an existence of a bound state in this channel. This expectation has been confirmed by more detailed study in lattice QCD and a bound state of two up quarks, two down quarks and two strange quarks, called the H dibaryon, indeed exists in the flavor SU(3) limit.[21] To study the property of the H dibaryon in the real world where the strange quark is much heavier than up and down quarks so that the flavor SU(3) symmetry is broken, the extension presented in this paper for the coupled channels is indeed necessary: The SU(3) breaking in nature appears in the octet baryon mass as $m_N = 939$ MeV, $m_\Lambda = 1116$MeV, $m_\Sigma = 1193$ MeV and $m_\Xi = 1318$ MeV. Therefore thresholds of two baryon systems with strangeness $S = -2$ and ispspin $I = 0$, to which the H dibaryon belongs, are given by

$$W_{\Lambda\Lambda} = 2232\,\text{MeV} < W_{N\Xi} = 2257\,\text{MeV} < W_{\Sigma\Sigma} = 2386\,\text{MeV}. \tag{5·1}$$

A study for coupled channel potentials in this case has started using the 2+1 flavor lattice QCD and a preliminary result has already been presented.[22] More details results for this study will be published soon.

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