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Construction of energy-independent potentials above inelastic thresholds in quantum field theories

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Abstract

We construct energy independent but non-local potentials above inelastic thresholds, in terms of Nambu-Bethe-Salpeter wave functions defined in quantum field theories such as QCD. As an explicit example, we consider $NN \to NN + n\pi$ scattering processes for $n = 0, 1, 2, \cdots$. We show an existence of energy-independent coupled channel potentials with a non-relativistic approximation, where momenta of all particles are small compared with their own masses. In the case of two-body inelastic scatterings such as $\Lambda\Lambda \to \Lambda\Lambda, N\Xi, \Sigma\Sigma$, on the other hand, we show that energy-independent potentials can be constructed without relying on non-relativistic approximations. We also propose a method to extract these potentials using time-dependence of general correlation functions.

I. INTRODUCTION

It is important to understand hadronic interactions such as nuclear forces from the point of view of their constituents, quarks and gluons, whose dynamics is described by Quantum Chromodynamics (QCD). Since the running coupling constant in QCD becomes large at hadronic scale, however, non-perturbative methods such as the lattice QCD combined with numerical simulations must be employed to investigate this problem systematically. Conventionally the finite size method[1] has been employed to extract the scattering phase shift, but the method is applicable only below the inelastic (particle production) threshold. See Refs.[2, 3] for an extension of this method to multi-channel systems.

Recently an alternative method was proposed to investigate hadronic interactions and it has been successfully employed to extract the potential between nucleons below inelastic thresholds[4–6]. Since then, this method has been applied to other more general hadronic interactions such as baryon-baryon interactions[7–11], meson-baryon interactions[12, 13] and three nucleon forces[14, 15]. See Refs. [16, 17] for reviews of recent activities.

In the method, called the HALQCD method, a potential between composite particles is defined in quantum field theories such as QCD. There are two important properties to be proven in quantum field theories, in order to define the potential, which is a quantum mechanical object. Let us explain the HALQCD method and these two important properties, by considering the NN potential as an example. We first introduce the equal-time Nambu-Bethe-Salpeter (NBS) wave function[18] in the center of mass system defined by

$$\varphi_{W,c_0}(\boldsymbol{x}) \;=\; \langle 0|T\left\{N(\boldsymbol{r},0)N(\boldsymbol{r}+\boldsymbol{x},0)\right]\}\,|NN,W,c_0\rangle_{\rm in} \tag{1}$$

where $\langle 0| = {}_{\rm out}\langle 0| = {}_{\rm in}\langle 0|$ is the QCD vacuum (bra-)state, $|NN,W,c_0\rangle_{\rm in}$ is the two-nucleon asymptotic in state at the total energy $W = 2\sqrt{\boldsymbol{k}^2+m_N^2}$ with the nucleon mass m_N and the relative momentum $\boldsymbol{k}$, c_0 represent quantum numbers other than W such as helicity of nucleons and the direction of $\boldsymbol{k}$, T represents the time-ordered product, and $N(x)$ with $x=(\boldsymbol{x},t)$ is the nucleon operator defined by $N(x) = \varepsilon_{abc}(u_a(x)^T C\gamma_5 d_b(x))q_c(x)$ with the charge conjugation matrix C and $q(x)=(u(x),d(x))^T$. Note that a different choice for $N(x)$ is possible as long as $N(x)$ can annihilate the 1-particle nucleon state and the difference leads to a difference in NBS wave functions defined from them. Note also that $N(x)$ and $\varphi(\boldsymbol{x})$ implicitly have spinor and flavor indices.

An important property of the NBS wave function for the definition of the potential is that, as the distance between two nucleon operators, $x = |\boldsymbol{x}|$, becomes large, the NBS wave function satisfies the free Schrödinger(or equivalently the free Klein-Gordon) equation,

$$(E_W - H_0)\,\varphi_{W,c_0}(\boldsymbol{x}) \;\simeq\; 0, \qquad E_W = \frac{\boldsymbol{k}^2}{2\mu}, \quad H_0 = \frac{-\nabla^2}{2\mu} \tag{2}$$

where $\mu = m_N/2$ is the reduced mass. In addition, the asymptotic behavior of the NBS wave function is described in terms of the phase δ determined by the unitarity of the S-matrix, $S = e^{2i\delta}$, in QCD (or the corresponding quantum field theory). This has been shown originally for the elastic $\pi\pi$ scattering [19, 20], where the partial wave of NBS wave function for the orbital angular momentum L becomes

$$\varphi_W^L \;\simeq\; A_L \frac{\sin(kx - L\pi/2 + \delta_L(W))}{kx} \tag{3}$$

as $x \to \infty$ at $W < W_{\rm th} = 4m_\pi$ (the lowest inelastic threshold). The asymptotic behavior of the NBS wave function for the elastic NN scattering has been derived in Ref. [21]. The asymptotic behavior of the NBS wave function such as eq. (3) is the first important property that motivates the definition of the potential in QCD.

The (non-local) potential between two nucleons below the inelastic threshold is defined by the equation that

$$(E_W - H_0)\,\varphi_{W,c_0}(\boldsymbol{x}) \;=\; \int d^3y\, U(\boldsymbol{x},\boldsymbol{y})\;\varphi_{W,c_0}(\boldsymbol{y}) \tag{4}$$

at $W < W_{\rm th} = 2m_N + m_\pi$. In general, the non-local potential $U(\boldsymbol{x},\boldsymbol{y})$ could depend on the energy W[1]. As we will show, however, an energy-independent potential $U(\boldsymbol{x},\boldsymbol{y})$ such that eq. (4) is satisfied for all $W < W_{\rm th}$ can be constructed. Therefore, if we solve the Schrödinger equation with this potential in the infinite volume, its solutions automatically provide correct phase shifts in QCD at all $W < W_{\rm th}$ by construction. An existence of the W-independent potential U is the second important property to define the potential in the HAL-QCD method.

Using the inner product $(f,g) = \int d^3x\, \overline{f(\boldsymbol{x})} g(\boldsymbol{x})$ where $\overline{f}$ is the complex conjugate of f, we introduce a norm kernel defined by $\mathcal{N}_{W_1 c_0, W_2 d_0} = (\varphi_{W_1,c_0}, \varphi_{W_2,d_0})$. Since NBS wave functions at $W < W_{\rm th}$ are in general linearly independent[1], an inverse $\mathcal{N}^{-1}$ exists and it

[1] This holds at least for $(W_1, c_0) \neq (W_2, d_0)$ in the sufficiently large volume. Even if some wave functions accidentally become linearly-dependent in small volume, we can remove them, so that our construction of the energy-independent potential remains the same.

satisfies for $W_1, W_2 < W_{\rm th}$ [2]

$$\sum_{W<W_{\rm th},c_0} \mathcal{N}^{-1}_{W_1 d_0, W c_0}\, \mathcal{N}_{W c_0, W_2 e_0} \;=\; \sum_{W<W_{\rm th},c_0} \mathcal{N}_{W_1 d_0, W c_0}\, \mathcal{N}^{-1}_{W c_0, W_2 e_0} = \delta_{W_1,W_2}\delta_{d_0,e_0}. \tag{5}$$

Using the inverse norm kernel, we define a ket vector $|\varphi_{W,c_0}\rangle$ as $\langle \boldsymbol{x}|\varphi_{W,c_0}\rangle \equiv \varphi_{W,c_0}(\boldsymbol{x})$ and its conjugate bra vector $\langle\psi_{W,c_0}|$ as

$$\langle\psi_{W,c_0}|\boldsymbol{x}\rangle \;\equiv \sum_{W_1<W_{\rm th},d_0} \mathcal{N}^{-1}_{W c_0, W_1 d_0}\overline{\varphi_{W_1,d_0}(\boldsymbol{x})}, \quad \langle\psi_{W_1,c_0}|\varphi_{W_2,d_0}\rangle = \delta_{W_1,W_2}\delta_{c_0,d_0}, \tag{6}$$

so that the non-local potential can be constructed as[6]

$$U \;=\; \sum_{W<W_{\rm th},c_0} (E_W - H_0)\,|\varphi_{W,c_0}\rangle\langle\psi_{W,c_0}|, \tag{7}$$

since it is easy to see that it satisfies the Schrödinger equation (4) as

$$U|\varphi_{W,c_0}\rangle \;=\; \sum_{W_1<W_{\rm th},d_0} (E_{W_1} - H_0)\,|\varphi_{W_1,d_0}\rangle\langle\psi_{W_1,d_0}|\varphi_{W,c_0}\rangle = (E_W - H_0)\,|\varphi_{W,c_0}\rangle \tag{8}$$

as long as $W < W_{\rm th}$. It should be noted that the non-local potential which satisfies eq. (4) at $W < W_{\rm th}$ is not unique. For example, we may add an arbitrary term proportional to $(1-P)$ to the non-local potential U without affecting eq. (4), where the projection is defined by $P = \sum_{W<W_{\rm th},c_0} |\varphi_{W.c_0}\rangle\langle\psi_{W,c_0}|$.

The purpose of this paper is to construct an energy independent (non-local) potential which satisfies an appropriate Schrödinger equation at low energy but above inelastic thresholds in quantum field theories. To make our argument more concrete, we mainly consider the NN scattering in this paper.

In Sec. II, we demonstrate that energy-independent potentials can be constructed above inelastic thresholds if the total energy is small enough such that the non-relativistic approximation is applicable. In Sec. II A we consider $NN \to NN, NN\pi$ scattering as a simplest case, where the total energy W is above $2m_N + m_\pi$ but below $2m_N + 2m_\pi$. In Sec. II B, we generalize our construction to larger value of W where the $NN \to NN + n\pi$ scattering for higher integer n can occur. In this case, momenta of all particles must be still non-relativistic. In Sec. II C we treat a special case of inelastic scattering such as $AB \to AB, CD$, where non-relativistic approximation is not required to construct energy independent coupled channel

[2] We first consider the finite volume, so that W_1, W_2 take discrete values. We then take the infinite volume limit, so that δ_{W_1,W_2} and $\sum_W$ should be replaced by $\delta(W_1 - W_2)$ and $\int dW$, respectively.

potentials. In Sec. III, using results obtained in the previous section, we generalize the time dependent method for the extraction of the potential[23] to the case at $W \geq W_{\rm th}$, in order to treat inelastic processes. Conclusions and discussions are given in Sec. IV. In Appendix A, we compare the construction of the energy-independent potential above inelastic threshold given in the main text with other possible variations.

II. CONSTRUCTION OF ENERGY-INDEPENDENT POTENTIALS ABOVE INELASTIC THRESHOLDS

We here construct energy-independent (non-local) potentials even above inelastic thresholds for the NN scattering in the center of mass system. In this report we only consider pion productions whose n-th threshold energy is given by $W_{\rm th}^n = 2m_N + n \times m_\pi$ with m_π being the pion mass. Extensions to other particle productions such as $N\bar{N}$ or $K\bar{K}$, etc. are straightforward.

We introduce energy intervals defined by $\Delta_n = [W_{\rm th}^n, W_{\rm th}^{n+1})$ for $n = 0, 1, 2, \cdots$. Given the total energy W, the kinetic energy of the $NN + n\pi$ system is denoted by E_W^n, which is given by

$$E_W^n \;=\; \frac{\boldsymbol{p}_1^2}{2m_N} + \frac{\boldsymbol{p}_2^2}{2m_N} + \sum_{i=1}^{n} \frac{\boldsymbol{k}_i^2}{2m_\pi}, \quad W = \sqrt{m_N^2 + \boldsymbol{p}_1^2} + \sqrt{m_N^2 + \boldsymbol{p}_2^2} + \sum_{i=1}^{n} \sqrt{m_\pi^2 + \boldsymbol{k}_i^2}, \quad (9)$$

where $\boldsymbol{p}_1 + \boldsymbol{p}_2 + \sum_{i=1}^n \boldsymbol{k}_i = 0$. The corresponding free hamiltonian is denoted by H_0^n. Note that E_W^n cannot be determined from the total energy W alone, except for the elastic scattering at $n = 0$, where E_W^0 is uniquely determined from a given value of W. Since the determination of E_W^n from W is important to construct potentials from the Schrödinger equation and E_W^n for $n \geq 1$ cannot be determined from W in general, we restrict our considerations in this paper to cases where all momenta $\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{k}_1, \boldsymbol{k}_2, \cdots, \boldsymbol{k}_n$ are non-relativistic, so that we can write $W \simeq W_{\rm th}^k + E_W^k$ for $k = 1, 2, \cdots, n$ at $W \in \Delta_n$. (We can exclude $k = 0$ case since E_W^0 can always be determined from W without non-relativistic approximation.) This condition is explicitly written as $\boldsymbol{p}_i^2 < m_N^2$ for $i = 1, 2$ and $\boldsymbol{k}_i^2 < m_\pi^2$ for $i = 1, 2, \cdots, n$. Unless otherwise stated, we assume this condition in this paper. We roughly estimate how many pions can be treated within this approximation. If the total energy of two nucleons with one pion at rest is equal to the minimum energy of n-pion production such that $2\sqrt{m_N^2 + \boldsymbol{p}^2} + m_\pi = 2m_N + nm_\pi$, the non-relativistic condition, say $\boldsymbol{p}^2 \simeq 0.9 \times m_N^2$, leads to $n - 1 \leq \frac{m_N}{m_\pi}(\sqrt{7.6} - 2) \simeq 5$.

Therefore we may consider up to $NN + 6\pi$ with roughly 5% relativistic corrections. Note that some configurations of momenta may become relativistic for a given value of W. We exclude such configurations in our consideration of this paper.

A. Simplest case

To illustrate our strategy to construct energy-independent potentials, let us consider the simplest case at $W < W_{\rm th}^2 = 2m_N + 2m_\pi$ in this subsection. If $W \in \Delta_1$ ($2m_N + m_\pi \le W < 2m_N + 2m_\pi$), the inelastic scattering with one pion production ($NN \to NN + \pi$) becomes possible. We can define in this case a set of 4-independent equal time NBS wave function as

$$Z_N \varphi^{00}_{W,c_0}(\boldsymbol{x}_0) = \langle 0|T\{N(\boldsymbol{x},0)N(\boldsymbol{x}+\boldsymbol{x}_0,0)\}|NN,W,c_0\rangle_{\rm in}, \tag{10}$$

$$Z_N Z_\pi^{1/2} \varphi^{10}_{W,c_0}(\boldsymbol{x}_0,\boldsymbol{x}_1) = \langle 0|T\{N(\boldsymbol{x},0)N(\boldsymbol{x}+\boldsymbol{x}_0,0)\pi(\boldsymbol{x}+\boldsymbol{x}_1,0)\}|NN,W,c_0\rangle_{\rm in}, \tag{11}$$

$$Z_N \varphi^{01}_{W,c_1}(\boldsymbol{x}_0) = \langle 0|T\{N(\boldsymbol{x},0)N(\boldsymbol{x}+\boldsymbol{x}_0,0)\}|NN+\pi,W,c_1\rangle_{\rm in}, \tag{12}$$

$$Z_N Z_\pi^{1/2} \varphi^{11}_{W,c_1}(\boldsymbol{x}_0,\boldsymbol{x}_1) = \langle 0|T\{N(\boldsymbol{x},0)N(\boldsymbol{x}+\boldsymbol{x}_0,0)\pi(\boldsymbol{x}+\boldsymbol{x}_1,0)\}|NN+\pi,W,c_1\rangle_{\rm in}, \tag{13}$$

where Z_N and Z_π are renormalization factors for nucleon and pion fields, such that $N(x) = Z_N^{1/2} N^r(x)$ and $\pi(x) = Z_\pi^{1/2}\pi^r(x)$, where $N^r(x)$ and $\pi^r(x)$ are renormalized nucleon and pion fields, respectively. We here consider two asymptotic in states $|NN,W,c_0\rangle_{\rm in}$ and $|NN+\pi,W,c_1\rangle_{\rm in}$ corresponding to two nucleons and two nucleons plus one pion, where c_0 and c_1 represent quantum numbers other than the total energy W. In the present case, (W,c_0) and (W,c_1) are equivalent to $(s_1,s_2,\boldsymbol{p}_1)$ and $(s_1,s_2,\boldsymbol{p}_1,\boldsymbol{k}_1)$ where s_i is the helicity of the i-th nucleon and $\boldsymbol{p}_2$ is not independent due to the momentum conservation. As mentioned before, $W \simeq W_0 + E_W^0 \simeq W_1 + E_W^1$. If distances between all operators become large ($|\boldsymbol{x}_0|, |\boldsymbol{x}_1|, |\boldsymbol{x}_1 - \boldsymbol{x}_0| \to \infty$), we expect (and will indeed show in the separated paper[22]) that all NBS wave functions given above satisfy free Schrödinger equations such that

$$\left(E_W^0 - H_0^0\right)\varphi^{0i}_{W,c_0} \simeq 0, \quad \left(E_W^1 - H_0^1\right)\varphi^{1i}_{W,c_0} \simeq 0, \quad i = 0,1. \tag{14}$$

We consider the coupled channel Schrödinger equations for NN and $NN+\pi$, which is given by

$$(E_W^k - H_0^k)\varphi^{ki}_{W,c_i} = \sum_{l=0,1}\int \prod_{n=0}^{l} d^3y_n\, U^{kl}([\boldsymbol{x}]_k,[\boldsymbol{y}]_l)\varphi^{li}_{W,c_i}([\boldsymbol{y}]_l), \quad k,i \in (0,1), \tag{15}$$

where $[\boldsymbol{x}]_0 = \boldsymbol{x}_0$ and $[\boldsymbol{x}]_1 = \boldsymbol{x}_0, \boldsymbol{x}_1$. Note that $E^1_W \simeq W - W^1_{\rm th} < 0$ if $W \in \Delta_0$. Our task is to show that a W-independent 2×2 potential matrix U^{kl} exists.

For this purpose, we define vectors from these NBS wave functions at $W \in \Delta_1$ as

$$\varphi^i_{W,c_i} \equiv \left(\varphi^{0i}_{W,c_i}([\boldsymbol{x}]_0), \varphi^{1i}_{W,c_i}([\boldsymbol{x}]_1)\right)^T, \quad i = 0, 1, \tag{16}$$

while at $W \in \Delta_0$ we take only φ^0_{W,c_0} as

$$\varphi^0_{W,c_0} \equiv \left(\varphi^{00}_{W,c_0}([\boldsymbol{x}]_0), \varphi^{10}_{W,c_0}([\boldsymbol{x}]_1)\right)^T, \tag{17}$$

where the second component $\varphi^{10}_{W,c_1}([\boldsymbol{x}]_1)$ vanishes as distances between all operators go to infinity. (No asymptotic $NN + \pi$ state exists at $W < 2m_N + m_\pi$.) Note that, instead of eq. (17), we may define

$$\varphi^0_{W,c_0} \equiv \left(\varphi^{00}_{W,c_0}([\boldsymbol{x}]_0), 0\right)^T, \tag{18}$$

at $W \in \Delta_0$. Since the definition of φ^0_{W,c_0} at $W \in \Delta_0$ in eq. (17) will be required in Sec. III for the time-dependent method, we use it in the main text of this paper, and the construction with eq. (18) and other variations will be discussed in Appendix A.

As in the elastic case, we introduce the norm kernel in the space spanned by φ^i_{W,c_i} as

$$\mathcal{N}^{ij}_{W_1 c_i, W_2 d_j} = \left(\varphi^i_{W_1,c_i}, \varphi^j_{W_2,d_j}\right) \equiv \sum_{k=0,1} \int \prod_{l=0}^{k} d^3x_l \, \overline{\varphi^{ki}_{W_1,c_i}([\boldsymbol{x}]_k)} \varphi^{kj}_{W_2,d_j}([\boldsymbol{x}]_k). \tag{19}$$

Here indices i, j run over different ranges depending on values of W_1, W_2 such that $i \in I(W_1)$ and $j \in I(W_2)$, where $I(W) = \{0\}$ for $W \in \Delta_0$ and $I(W) = \{0, 1\}$ for $W \in \Delta_1$. Otherwise stated, we assume this in this subsection.

As long as φ^i_{W,c_i} are linearly independent, the Hermitian operator $\mathcal{N}$ has an inverse as

$$\sum_{W \in \Delta_0 + \Delta_1} \sum_{h \in I(W),\, e_h} (\mathcal{N}^{-1})^{ih}_{W_1 c_i, W e_h} \mathcal{N}^{hj}_{W e_h, W_2 d_j} = \delta^{ij} \delta_{W_1,W_2} \delta_{c_i,d_j}. \tag{20}$$

Schematically $\mathcal{N}$ has a following structure:

$$\mathcal{N} = \begin{pmatrix} \mathcal{N}^{00}(\Delta_0, \Delta_0), & \mathcal{N}^{00}(\Delta_0, \Delta_1), & \mathcal{N}^{01}(\Delta_0, \Delta_1) \\ \mathcal{N}^{00}(\Delta_1, \Delta_0), & \mathcal{N}^{00}(\Delta_1, \Delta_1), & \mathcal{N}^{01}(\Delta_1, \Delta_1) \\ \mathcal{N}^{10}(\Delta_1, \Delta_0), & \mathcal{N}^{10}(\Delta_1, \Delta_1), & \mathcal{N}^{11}(\Delta_1, \Delta_1) \end{pmatrix} \tag{21}$$

where $\mathcal{N}^{ab}(\Delta_i, \Delta_j)$ represent a sub-matrix whose components are given by $\mathcal{N}^{ab}_{W_i c_a, W_j d_b}$ with $W_i \in \Delta_i$ and $W_j \in \Delta_j$ for $i, j, a, b = 0$ or 1. The corresponding inverse $\mathcal{N}^{-1}$ has of course the same structure.

Using this inverse, we define the ket vector $|\varphi^i_{W,c_i}\rangle$ and the corresponding bra vector $\langle\psi^i_{W,c_i}|$, whose k-th components are given by

$$\langle[\boldsymbol{x}]_k|\varphi^i_{W,c_i}\rangle \;=\; \varphi^{ki}_{W,c_i}([\boldsymbol{x}]_k), \tag{22}$$

$$\langle\psi^i_{W,c_i}|[\boldsymbol{x}]_k\rangle \;=\; \sum_{W_1\in\Delta_0\cup\Delta_1}\sum_{j\in I(W_1),d_j}(\mathcal{N}^{-1})^{ij}_{Wc_i,W_1d_j}\overline{\varphi^{kj}_{W_1,d_j}([\boldsymbol{x}]_k)} \tag{23}$$

for $k=0,1$, where d_j runs over states which satisfies non-relativistic condition. It is then easy to see that

$$\begin{aligned}\langle\psi^i_{W_1,c_i}|\varphi^j_{W_2,d_j}\rangle \;&=\; \sum_{k=0,1}\int\prod_{l=0}^{k}d^3x_l\,\langle\psi^i_{W_1,c_i}|[\boldsymbol{x}]_k\rangle\langle[\boldsymbol{x}]_k|\varphi^j_{W_2,d_j}\rangle = (\mathcal{N}^{-1}\cdot\mathcal{N})^{ij}_{W_1c_i,W_2d_j}\\ &=\; \delta^{ij}\delta_{W_1,W_2}\delta_{c_i,d_j}.\end{aligned} \tag{24}$$

Introducing operators E_W, H_0 and U such that

$$\langle[\boldsymbol{x}]_k|(E_W-H_0)|[\boldsymbol{y}]_l\rangle \;\equiv\; \delta_{kl}(E^k_W-H^k_0)\prod_{n=0}^{k}\delta^{(3)}(\boldsymbol{x}_n-\boldsymbol{y}_n) \tag{25}$$

$$\langle[\boldsymbol{x}]_k|U|[\boldsymbol{y}]_l\rangle \;\equiv\; U^{kl}([\boldsymbol{x}]_k,[\boldsymbol{y}]_l), \tag{26}$$

the coupled channel Schrödinger equation (15) can be compactly written as[3]

$$(E_W-H_0)|\varphi^i_{W,c_i}\rangle \;=\; U|\varphi^i_{W,c_i}\rangle. \tag{27}$$

Now it is easy to construct U which satisfies the above equation as

$$U \;=\; \sum_{W\in\Delta_0\cup\Delta_1}\sum_{i\in I(W)}\sum_{c_i}(E_W-H_0)|\varphi^i_{W,c_i}\rangle\langle\psi^i_{W,c_i}|, \tag{28}$$

since

$$U|\varphi^i_{W,c_i}\rangle \;=\; \sum_{W_1\in\Delta_0\cup\Delta_1}\sum_{j\in I(W_1)}\sum_{d_j}(E_W-H_0)|\varphi^j_{W_1,d_j}\rangle\langle\psi^j_{W_1,d_j}|\varphi^i_{W,c_i}\rangle = (E_W-H_0)|\varphi^i_{W,c_i}\rangle \tag{29}$$

An energy-independent potential matrix U indeed exists. Note that U is not unique since, for example, one can use eq. (18) instead of eq. (17) for φ^i_{W,c_i}, so that the resulting potential from eq. (28) differs from the one with eq. (17).

Finally let us consider the Hermiticity of U. A matrix element of U is evaluated as

$$U^{ij}_{W_1c_i,W_2d_j} \;\equiv\; \langle\varphi^i_{W_1,c_i}|U|\varphi^j_{W_2,d_j}\rangle = \langle\varphi^i_{W_1,c_i}|(E_{W_2}-H_0)|\varphi^j_{W_2,d_j}\rangle, \tag{30}$$

[3] Here and hereafter the sum over c_i with $i\neq 0$ is always restricted to non-relativistic states if the number of particles is more than 2.

while

$$(U^\dagger)^{ij}_{W_1c_i,W_2d_j} \;=\; \overline{\langle\varphi^j_{W_2,d_j}|(E_{W_1}-H_0)|\varphi^i_{W_1,c_i}\rangle} = \langle\varphi^i_{W_1,c_i}|(E_{W_1}-H_0)|\varphi^j_{W_2,d_j}\rangle. \qquad (31)$$

Therefore potential U is not Hermite in general. However it is effectively Hermite since in practice we solve the Schrödinger equation under the condition that $E_{W_1} = E_{W_2}$, which is equivalent to $W_1 = W_2$ in our non-relativistic approximation.

B. General cases

It is not so difficult to extend the argument in the previous subsection to more general cases, where the total energy satisfies $W < W^{n_{\max}+1}$. As discussed before, the validity of the non-relativistic approximation requires $n_{\max} = 5$ at most.

Let us consider $W \in \Delta_0 \cup \Delta_1 \cup \cdots \cup \Delta_{n_{\max}}$. At $W \in \Delta_s$ with $s \le n_{\max}$, we define a set of the equal time NBS wave functions as

$$\begin{aligned} Z_N Z_\pi^{k/2}\varphi^{ki}_{W,c_i}([\boldsymbol{x}]_k) \;&=\; \langle 0|T\{N(\boldsymbol{x},0)N(\boldsymbol{x}+\boldsymbol{x}_0,0)\prod_{l=1}^{k}\pi(\boldsymbol{x}+\boldsymbol{x}_l,0)\}|NN+i\pi,W,c_i\rangle_{\rm in},\ i\le s, \\ &=\; 0, \qquad i>s, \end{aligned} \qquad (32)$$

where indices k, i run from 0 to $n_{\max}$, but $\varphi^{ki}_{W,c_i}([\boldsymbol{x}]_k)$ with $k > s$ vanishes, as distances among all operators (two nucleons and k pions) becomes large, $[\boldsymbol{x}]_k = \boldsymbol{x}_0, \boldsymbol{x}_1, \cdots, \boldsymbol{x}_k$ and c_i represents quantum number other than the total energy W of the in state. In the present case, (W, c_i) are equivalent to $s_1, s_2, \boldsymbol{p}_1, \boldsymbol{k}_1, \boldsymbol{k}_2, \cdots, \boldsymbol{k}_i$ where s_l is a helicity of the l-th nucleon.

The coupled channel Schrödinger equation for this system at $W \in \Delta_s$ ($s \le n_{\max}$) is given by

$$(E^k_W - H^k_0)\varphi^{ki}_{W,c_i}([\boldsymbol{x}]_k) \;=\; \sum_{l=0}^{n_{\max}}\int d[\boldsymbol{y}]_l\, U^{kl}([\boldsymbol{x}]_k,[\boldsymbol{y}]_l)\varphi^{li}_{W,c_i}([\boldsymbol{y}]_l), \quad i\in I(W) \qquad (33)$$

where $d[\boldsymbol{y}]_l = \prod_{m=0}^{l} d^3y_m$, $I(W) = \{0,1,\cdots,s\}$ for $W \in \Delta_s$, and $k = 0,1,\cdots,n$. Note that $E^k_W \simeq W - W^k_{\rm th} < 0$ if $k \notin I(W)$. It is now clear that the non-relativistic condition is necessary here to determine E^k_W from W, c_i if $k \ne i$. Our task is to show that a W-independent $(n_{\max}+1)\times(n_{\max}+1)$ potential matrix U exists.

As in the previous subsection, we define vectors of NBS wave functions with $(n_{\max}+1)$ components at $W \in \Delta_s$ as

$$\varphi^i_{W,c_i} \equiv \left(\varphi^{0i}_{W,c_i}([\boldsymbol{x}]_0), \varphi^{1i}_{W,c_i}([\boldsymbol{x}]_1), \cdots, \varphi^{n_{\max} i}_{W,c_i}([\boldsymbol{x}]_{n_{\max}})\right)^T, \tag{34}$$

where i runs over $I(W)$.

The norm kernel is defined by

$$\mathcal{N}^{ij}_{W_1 c_i, W_2 d_j} \equiv \left(\varphi^i_{W_1,c_i}, \varphi^j_{W_2,d_j}\right) = \sum_{k=0}^{n_{\max}} \int d[\boldsymbol{x}]_k \overline{\varphi^{ki}_{W_1,c_i}([\boldsymbol{x}]_k)}\, \varphi^{kj}_{W_2,d_j}([\boldsymbol{x}]_k), \tag{35}$$

whose inverse is denoted by $\mathcal{N}^{-1}$, where $i \in I(W_1)$ and $j \in I(W_2)$. The bra and ket vectors, defined by

$$\langle [\boldsymbol{x}]_k | \varphi^i_{W,c_i} \rangle = \varphi^{ki}_{W,c_i}([\boldsymbol{x}]_k), \tag{36}$$

$$\langle \psi^i_{W,c_i} | [\boldsymbol{x}]_k \rangle = \sum_{W_1} \sum_{j \in I(W_1)} \sum_{d_j} (\mathcal{N}^{-1})^{ij}_{W c_i, W_1 d_j} \overline{\varphi^{kj}_{W_1,d_j}([\boldsymbol{x}]_k)}, \tag{37}$$

satisfy

$$\langle \psi^i_{W_1,c_i} | \varphi^j_{W_2,d_j} \rangle = \sum_{k=0}^{n_{\max}} \int d[\boldsymbol{x}]_k \langle \psi^i_{W_1,c_i} | [\boldsymbol{x}]_k \rangle \langle [\boldsymbol{x}]_k | \varphi^j_{W_2,d_j} \rangle = \delta^{ij} \delta_{W_1,W_2} \delta_{c_i,d_j}. \tag{38}$$

Introducing operators E_W, H_0 and U, defined as in eqs. (25) and (26), we can construct

$$U = \sum_W \sum_{i \in I(W)} \sum_{c_i} (E_W - H_0) |\varphi^i_{W,c_i}\rangle \langle \psi^i_{W,c_i}|, \tag{39}$$

which satisfies the coupled channel equation

$$(E_W - H_0)|\varphi^i_{W,c_i}\rangle = U|\varphi^i_{W,c_i}\rangle. \tag{40}$$

It is also easy to see the effective Hermiticity of U: $U^{ij}_{W_1 c_i, W_2 d_j} = (U^\dagger)^{ij}_{W_1 c_i, W_2 d_j}$ at $W_1 = W_2$ (with non-relativistic approximation).

C. Special case without non-relativistic approximation

In this subsection, we discuss a special case of inelastic scatterings where non-relativistic approximation is not required to construct energy independent potentials. Here, coupled two-particle scattering channels such as $A_i B_i \to A_j B_j$ with $i, j = 1, 2, \cdots, n_{\max}$ are considered. For example, in the baryon scattering in the strangeness $S = -2$ and isospin $I = 0$

channel, $\Lambda\Lambda, N\Xi$ and $\Sigma\Sigma$ appear as asymptotic states if the total energy W in the center of mass system is $2m_\Sigma \le W < 2m_\Sigma + m_\pi$. The method to extract coupled channel potentials in this kind of situation has already been proposed in Ref. [24], under an assumption that energy independent coupled channel potentials exist. In this subsection we prove this assumption.

Given the total energy W, the relative momentum $\boldsymbol{p}_i$(squared) and the kinetic energy E_W^i, together with the free Hamiltonian H_0, for A_iB_i are given by

$$W = \sqrt{\boldsymbol{p}_i^2 + m_{A_i}^2} + \sqrt{\boldsymbol{p}_i^2 + m_{B_i}^2}, \qquad E_W^i = \frac{\boldsymbol{p}_i^2}{2m_r^i},\ H_0 = \frac{-\nabla^2}{2m_r^i}, \quad m_r^i = \frac{m_{A_i} m_{B_i}}{m_{A_i} + m_{B_i}}, \tag{41}$$

where m_{A_i} and m_{B_i} are masses of A_i and B_i, and m_r^i is their reduced mass. We here assume $m_{A_i} + m_{B_i} < m_{A_j} + m_{B_j}$ for $i < j$. Note that if $W < W_{\rm th}^i \equiv m_{A_i} + m_{B_i}$, $\boldsymbol{p}_i^2$ and E_W^i become negative.

We defined NBS wave function for A_kB_k as

$$(Z_{A_k} Z_{B_k})^{1/2} \varphi_{W,c_i}^{ki}(\boldsymbol{x}) \ = \ \langle 0 | T\{A_k(\boldsymbol{r}, 0) B_k(\boldsymbol{r} + \boldsymbol{x}, 0)\} | A_i B_i, W, c_i \rangle_{\rm in}, \tag{42}$$

where Z_{A_k}, Z_{B_k} are renormalization factors defined by $A_k(x) = Z_{A_k}^{1/2} A_k^r(x)$ and $B_k(x) = Z_{B_k}^{1/2} B_k^r(x)$ with bare fields A_k, B_k and renormalized fields A_k^r, B_k^r, and c_i represents quantum number of the asymptotic in state $|A_iB_i, W, c_i\rangle_{\rm in}$ other than W. The index k always runs from 1 to $n_{\rm max}$, while the index i runs over $I(W) = 1, 2, \cdots, s-1$ if $W_{\rm th}^{s-1} \le W < W_{\rm th}^s$. We can show that

$$\lim_{|\boldsymbol{x}| \to \infty} (E_W^k - H_0) \varphi_{W,c_i}^{ki}(\boldsymbol{x}) = 0, \tag{43}$$

and $\varphi_{W,c_i}^{ki}(\boldsymbol{x})$ carries the information of scattering phase shifts [24].

We define vectors $|\varphi_{W,c_i}^i\rangle$ and the corresponding norm kernel as

$$\langle \boldsymbol{x}, k | \varphi_{W,c_i}^i \rangle \ = \ \varphi_{W,c_i}^{ki}(\boldsymbol{x}), \tag{44}$$

$$\mathcal{N}_{W_1 c_i, W_2 c_j}^{ij} \ = \ (\varphi_{W_1,c_i}^i, \varphi_{W_2,c_j}^j) \equiv \sum_{k=1}^{n_{\rm max}} \int d^3x\, \overline{\varphi_{W_1,c_i}^{ki}(\boldsymbol{x})}\ \varphi_{W_2,c_j}^{kj}(\boldsymbol{x}), \tag{45}$$

where $i \in I(W_1)$ and $j \in I(W_2)$. Using the inverse $\mathcal{N}^{-1}$ of $\mathcal{N}$, we construct dual vectors

$$\langle \psi_{W,c_i}^i | \boldsymbol{x}, k \rangle = \sum_{W_1, j \in I(W_1), c_j} \left(\mathcal{N}^{-1}\right)_{W c_i, W_1 c_j}^{ij} \overline{\langle \boldsymbol{x}, k | \varphi_{W_1,c_j}^j \rangle}, \tag{46}$$

which satisfies

$$\sum_{k=1}^{n_{\rm max}} \int d^3x\, \langle \psi_{W_1,c_i}^i | \boldsymbol{x}, k \rangle \cdot \langle \boldsymbol{x}, k | \varphi_{W_2,d_j}^j \rangle \ = \ \delta^{ij} \delta_{W_1,W_2} \delta_{c_i,d_j}. \tag{47}$$

An energy independent $n_{\max} \times n_{\max}$ potential matrix which satisfies the coupled channel equation that

$$(E_W^k - H_0)\varphi_{W,c_i}^{ki}(\boldsymbol{x}) \;=\; \sum_{l=1}^{n_{\max}} \int d^3y\, U^{kl}(\boldsymbol{x},\boldsymbol{y})\varphi_{W,c_i}^{li}(\boldsymbol{y}), \tag{48}$$

can be constructed as

$$U^{kl}(\boldsymbol{x},\boldsymbol{y}) \;=\; \sum_{W,i\in I(W),c_i} (E_W^k - H_0)\langle \boldsymbol{x},k|\varphi_{W,c_i}^i\rangle\langle\psi_{W,c_i}^i|\boldsymbol{y},l\rangle, \tag{49}$$

which is manifestly energy (W) independent, and is Hermite at fixed W.

III. TIME DEPENDENT METHOD

In Ref. [23], a method to extract hadronic potentials below inelastic thresholds from time dependence of correlation functions has been proposed, in order to overcome difficulties in the conventional method where NBS wave functions with definite energies are extracted from asymptotic behaviors of correlation functions in time. In this section, we extend the method so that it can be applicable to the case above inelastic thresholds.

The normalized correlation function is defined by

$$Z_N Z_\pi^{k/2} R^k([\boldsymbol{x}]_k,t) \;=\; \frac{1}{e^{-W_{\rm th}^k t}}\langle 0|T\{N(\boldsymbol{x},t)N(\boldsymbol{x}+\boldsymbol{x}_0,t)\prod_{l=1}^{k}\pi(\boldsymbol{x}+\boldsymbol{x}_l,t)\mathcal{J}_{NN}(0)\}|0\rangle \tag{50}$$

for $k = 0,1,2,\cdots,n_{\max}$, where $\mathcal{J}_{NN}$ is some source operator which couples to NN states. Inserting the complete set for the NN system that

$$\mathbf{1} \;=\; \sum_W \sum_{i\in I(W)} \sum_{c_i} |NN+i\pi,W,c_i\rangle_{\rm in\ in}\langle NN+i\pi,W,c_i| + \cdots, \tag{51}$$

where the ellipsis represents states with $W > W_{\rm th}^{n_{\max}}$ and are neglected hereafter, into the above correlation function, we obtain

$$R^k([\boldsymbol{x}]_k,t) \;=\; \sum_W \sum_{i\in I(W)} \sum_{c_i} e^{-\Delta^k W\, t}\varphi_{W,c_i}^{ki}([\boldsymbol{x}]_k)A_{W,c_i}^i, \tag{52}$$

where

$$A_{W,c_i}^i \;=\; {}_{\rm in}\langle NN+i\pi,W,c_i|\mathcal{J}_{NN}(0)|0\rangle, \quad \Delta^k W \equiv W - W_{\rm th}^k \simeq E_W^k. \tag{53}$$

Note that R^k automatically contains a sum over $W, i\in I(W), c_i$, which is necessary to define the non-local potentials in the previous section but is difficult in practice to perform one by

one. Note however that states with relativistic momenta may appear in the sum. We here assume that contributions from such states can be suppressed by an appropriate choice of $\mathcal{J}_{NN}$. Using the non-relativistic approximation, we can derive

$$\begin{aligned}\left\{-H_0^k - \frac{\partial}{\partial t}\right\} \cdot R^k([\boldsymbol{x}]_k, t) &= \sum_{W,i\in I(W),c_i} e^{-\Delta^k W t} \sum_{l=0}^{n_{\max}} \int d[\boldsymbol{y}]_l \, U^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l) \varphi^{li}_{W,c_i}([\boldsymbol{y}]_l) A^i_{W,c_i} \\ &= \sum_{l=0}^{n_{\max}} e^{-(l-k)m_\pi t} \int d[\boldsymbol{y}]_l U^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l) \sum_{W,i\in I(W),c_i} e^{-\Delta^l W t} \varphi^{li}([\boldsymbol{y}]_l) A^i_{W,c_i} \\ &= \sum_{l=0}^{n_{\max}} e^{-(l-k)m_\pi t} \int d[\boldsymbol{y}]_l U^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l) R^l([\boldsymbol{y}]_l, t). \end{aligned} \tag{54}$$

We then finally obtain

$$\left\{-H_0^k - \frac{\partial}{\partial t}\right\} \cdot R^k([\boldsymbol{x}]_k, t) = e^{k m_\pi t} \sum_{l=0}^{n_{\max}} e^{-l m_\pi t} \int d[\boldsymbol{y}]_l U^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l) R^l([\boldsymbol{y}]_l, t), \tag{55}$$

which can be used to obtain U^{kl}, combined with the derivative expansion [23].

We here propose a method to extract U^{kl} directly. For this purpose, we consider a set of more complicated correlation functions defined by

$$\begin{aligned} R^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l, t) &= \frac{1}{e^{-W^k_{\rm th} t}} \langle 0 | T\{ N(\boldsymbol{x}, t) N(\boldsymbol{x} + \boldsymbol{x}_0, t) \prod_{m=1}^{k} \pi(\boldsymbol{x} + \boldsymbol{x}_m, t) \\ &\times \int d^3 y \, \bar{N}(\boldsymbol{y}, 0) \bar{N}(\boldsymbol{y} + \boldsymbol{y}_0, 0) \prod_{s=1}^{l} \pi^\dagger(\boldsymbol{y} + \boldsymbol{y}_s, 0) \} | 0 \rangle, \end{aligned} \tag{56}$$

which satisfies

$$\left\{-H_0^k - \frac{\partial}{\partial t}\right\} \cdot R^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l, t) = \sum_{s=0}^{n_{\max}} e^{-(s-k)m_\pi t} \int d[\boldsymbol{z}]_s U^{ks}([\boldsymbol{x}]_k, [\boldsymbol{z}]_s) R^{sl}([\boldsymbol{z}]_s, [\boldsymbol{y}]_l, t) \tag{57}$$

Using real eigenvalues λ_m of the Hermitian operator R and their eigenvectors v_m whose k-th component is given by $v^k_m([\boldsymbol{x}]_k, t)$ with $m = 0, 1, \cdots, n_{\max}$, we can construct the inverse of R as

$$(R^{-1})^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l, t) = \sum_{m=n_0}^{n_{\max}} \frac{1}{\lambda_m} v^k_m([\boldsymbol{x}]_k, t) \{ v^l_m([\boldsymbol{y}]_l, t) \}^\dagger. \tag{58}$$

Note that we remove zero modes with $\lambda_m = 0$ from R and R^{-1}, so that the dimension of R and R^{-1} are effectively reduced from $(n_{\max}+1)\times(n_{\max}+1)$ to $(n_{\max}+1-n_0)\times(n_{\max}+1-n_0)$ where n_0 is the number of zero modes.

Using the inverse R^{-1}, we can extract U as

$$U^{kl}([\boldsymbol{x}]_k, [\boldsymbol{y}]_l) = e^{-k m_\pi t} \sum_{s=0}^{n_{\max}} \int d[\boldsymbol{z}]_s \left\{-H_0^k - \frac{\partial}{\partial t}\right\} \cdot R^{ks}([\boldsymbol{x}]_k, [\boldsymbol{z}]_s, t) (R^{-1})^{sl}([\boldsymbol{z}]_s, [\boldsymbol{y}]_l, t) e^{l m_\pi t}. \tag{59}$$

IV. CONCLUSION AND DISCUSSION

In this paper, we have shown that energy independent and non-local potentials can be constructed from a particular set of NBS wave functions even above inelastic thresholds as long as momenta of all particles involved are non-relativistic (Sec. II A and Sec. II B) or a number of particles is always two (Sec. II C). We have also derived a formula to extract non-local potentials with non-relativistic approximations using the time dependent method proposed in Ref. [23].

By the same method in Sec. II A and Sec. II B, we can construct an energy independent non-local potential for three-nucleon systems[14, 15] and even for systems with more than 3 nucleons. In the case of inelastic scattering such as $\Lambda\Lambda \to \Lambda\Lambda, N\Xi, \Sigma\Sigma$ [25], the result in Sec. II C has completed the HALQCD method proposed in Ref. [24], where non-relativistic approximation is not required.

An existence of energy independent potentials, which is one of the important properties necessary for the HALQCD method to investigate hadronic interactions, is now established in rather general situations. A remaining important property to be proven is an asymptotic behavior of NBS wave functions for more than 2 particles and its relation to S-matrix of the corresponding quantum field theory. Results on this issue will be published elsewhere[22].

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Appendix A: Comparisons among different constructions

The energy-independent $(n_{\rm max}+1)\times(n_{\rm max}+1)$ potential matrix in the main text is given in the coordinate space by

$$U^{kl} \;=\; \sum_{W}\sum_{i\in I(W)}\sum_{c_i}(E_W^k - H_0^k)|\varphi^{ki}_{W,c_i}\rangle\langle\psi^{li}_{W,c_i}| \tag{A1}$$

for $0 \le k,l \le n_{\rm max}$, where $\langle[\boldsymbol{x}]_k|\varphi^{ki}_{W,c_i}\rangle = \varphi^{ki}_{W,c_i}([\boldsymbol{x}]_k)$ and $\sum_{k=0}^{n_{\rm max}}\langle\psi^{ki}_{W_1,c_i}|\varphi^{kj}_{W_2,d_j}\rangle = \delta^{ij}\delta_{W_1,W_2}\delta_{c_i,d_j}$. The corresponding coupled channel Schrödinger equation is given by

$$(E_W - H_0)|\varphi^{ki}_{W,c_i}\rangle \;=\; \sum_{l=0}^{n_{\rm max}} U^{kl}|\varphi^{li}_{W,c_i}\rangle \tag{A2}$$

for $0 \le k \le n_{\rm max}$ and $i \in I(W)$.

In this appendix we consider some other constructions of energy-independent potentials in terms of NBS wave functions and compare them with eq. (A1).

1. Modified wave function vectors

As already mentioned in the main text, we can define the vectors of NBS wave functions using eq. (18) instead of eq. (17). The corresponding modification to eq. (32) becomes

$$\begin{aligned} Z_N Z_\pi^{k/2}\varphi^{ki}_{W,c_i}([\boldsymbol{x}]_k) \;&=\; \langle 0|T\{N(\boldsymbol{x},0)N(\boldsymbol{x}+\boldsymbol{x}_0,0)\prod_{l=1}^{k}\pi(\boldsymbol{x}+\boldsymbol{x}_l,0)\}|NN+i\pi,W,c_i\rangle_{\rm in},\;\; k,i\le s,\\ &=\; 0, \qquad \text{otherwise.} \end{aligned} \tag{A3}$$

The energy-independent potential U_M^{kl} (where M represents "modified") is given by the same formula in eq. (A1) with modifications by (A3) to $|\varphi^i_{W,c_i}\rangle$ and $\langle\psi^i_{W,c_i}|$, while the corresponding Schrödinger equation reads

$$(E_W - H_0)|\varphi^{ki}_{W,c_i}\rangle \;=\; \sum_{l\in I(W)} U_M^{kl}|\varphi^{li}_{W,c_i}\rangle \tag{A4}$$

for $k,i \in I(W)$, where $I(W) = 0,1,2,\cdots,s$ at $W \in \Delta_s = [W^s_{\rm th}, W^{s+1}_{\rm th})$.

2. Recursive construction

We construct another energy-independent potential recursively starting from the potential for the elastics NN scattering.

We first define the U_R^{00} corresponding to $NN \to NN$ elastic scattering as

$$U_R^{00} \;=\; \sum_{W\in\Delta_0}\sum_{c_0}(E_W - H_0)|\varphi^{00}_{W,c_0}\rangle\langle\psi^{00}_{W,c_0}| \tag{A5}$$

where the dual wave function $\langle\psi^{00}_{W,c_0}|$ to $|\varphi^{00}_{W,c_0}\rangle$ satisfies $\langle\psi^{00}_{W_1,c_0}|\varphi^{00}_{W_2,d_0}\rangle = \delta_{W_1,W_2}\delta_{c_0,d_0}$ at $W_1, W_2 \in \Delta_0$. This U_R^{00} is identical to the elastic potential given in eq. (7) and satisfies

$$(E_W - H_0)|\varphi^{00}_{W,c_0}\rangle \;=\; U_R^{00}|\varphi^{00}_{W,c_0}\rangle \tag{A6}$$

at $W \in \Delta_0$.

We then increase the energy so that $W \in \Delta_1$. A condition that φ^{ki}_{W,c_i} for $0 \le k, i \le 1$ satisfy the corresponding Schrödinger equation leads to

$$U_R^{01} \;=\; \sum_{W\in\Delta_1}\sum_{i=0,1}\sum_{c_i}\left[(E_W - H_0)|\varphi^{0i}_{W,c_i}\rangle - U_R^{00}|\varphi^{0i}_{W,c_i}\rangle\right]\langle\psi^{1i}_{W,c_i}|, \tag{A7}$$

where $\langle\psi^{1i}_{W,c_i}|$ for $i = 0, 1$ satisfy $\langle\psi^{1i}_{W_1,c_i}|\varphi^{1j}_{W_2,d_j}\rangle = \delta^{ij}\delta_{W_1,W_2}\delta_{c_i,d_j}$ at $W_1, W_2 \in \Delta_1$. Note that U_R^{00} used here is determined in eq. (A6) at the elastic region. We define U_R^{10} by imposing hermiticity for the potential, i.e. $U_R^{10} = (U_R^{01})^\dagger$, from which we can finally determine

$$U_R^{11} \;=\; \sum_{W\in\Delta_1}\sum_{i=0,1}\sum_{c_i}\left[(E_W - H_0)|\varphi^{1i}_{W,c_i}\rangle - U_R^{10}|\varphi^{0i}_{W,c_i}\rangle\right]\langle\psi^{1i}_{W,c_i}|. \tag{A8}$$

We now have U_R^{00} at $W \in \Delta_0$ and U_R^{ij} for $0 \le i, j \le 1$ at $W \in \Delta_1$.

It is not so difficult to extend the above construction to larger W recessively. We assume that the $s \times s$ potential matrix U_R^{ij} is already determined at $W \in \Delta_{s-1}$ for $s \le n_{\max}$. At $W \in \Delta_s$, U_{ks} for $k < s$ can be obtained by

$$U_R^{ks} \;=\; \sum_{W\in\Delta_s}\sum_{i\in I(W)}\sum_{c_i}\left[(E_W - H_0)|\varphi^{ki}_{W,c_i}\rangle - \sum_{l=0}^{s-1}U_R^{kl}|\varphi^{li}_{W,c_i}\rangle\right]\langle\psi^{si}_{W,c_i}|, \tag{A9}$$

where $\langle\psi^{sj}_{W,c_i}|$ for $i = 0, 1, \cdots, s$ satisfy $\langle\psi^{si}_{W_1,c_i}|\varphi^{sj}_{W_2,d_j}\rangle = \delta^{ij}\delta_{W_1,W_2}\delta_{c_i,d_j}$ at $W_1, W_2 \in \Delta_s$. Using the Hermiticity relation that $U_R^{sk} = (U_R^{ks})^\dagger$ for $k = 0, 1, \cdots, s-1$, we obtain U_R^{ss} as

$$U_R^{ss} \;=\; \sum_{W\in\Delta_s}\sum_{i\in I(W)}\sum_{c_i}\left[(E_W - H_0)|\varphi^{si}_{W,c_i}\rangle - \sum_{l=0}^{s-1}U_R^{sl}|\varphi^{li}_{W,c_i}\rangle\right]\langle\psi^{si}_{W,c_i}|. \tag{A10}$$

The $(s+1) \times (s+1)$ potential matrix U_R^{kl} for $0 \le k, l \le s$ is constructed. We can continue this recursive construction until $s = n_{\max}$.

The corresponding Schrödinger equation at $W \in \Delta_s$ becomes

$$(E_W - H_0)|\varphi^{ki}_{W,c_i}\rangle \;=\; \sum_{l=0}^{s}U_R^{kl}|\varphi^{li}_{W,c_i}\rangle \tag{A11}$$

for $0 \le k, i \le s$, where off-diagonal elements U^{kl} for $k \ne l$ are Hermite by construction.

3. Construction at each energy interval

We finally give a construction of the potential matrix different at each energy interval. At $W \in \Delta_s$ for $0 \le s \le n_{\max}$, the $(s+1) \times (s+1)$ potential matrix can be constructed as

$$U_s^{kl} \;=\; \sum_{W \in \Delta_s} \sum_{i \in I(W)} \sum_{c_i} (E_W - H_0) |\varphi_{W,c_i}^{ki}\rangle \langle \psi_{W,c_i}^{li}| \tag{A12}$$

for $0 \le k, l \le s$, where $\langle \psi_{W,c_i}^{ki}|$ for $i = 0, 1, \cdots, s$ satisfy $\sum_{k=0}^{s} \langle \psi_{W_1,c_i}^{ki} | \varphi_{W_2,d_j}^{kj} \rangle = \delta^{ij} \delta_{W_1,W_2} \delta_{c_i,d_j}$ at $W_1, W_2 \in \Delta_s$. Note that U_0^{00} is identical to U^{00} given in eq. (7).

The corresponding Schrödinger equation at $W \in \Delta_s$ becomes

$$(E_W - H_0) |\varphi_{W,c_i}^{ki}\rangle \;=\; \sum_{l=0}^{s} U_s^{kl} |\varphi_{W,c_i}^{li}\rangle \tag{A13}$$

for $0 \le k, i \le s$.

4. Comparison

Properties of the original construction in the main text are as follows.

1. A size of the potential matrix U^{kl} is always $(n_{\max}+1)^2$ at all $W \in [W_{\rm th}^0, W_{\rm th}^{n_{\max}+1})$.
2. A form of the potential matrix given in eq. (A1) is also same at all energy.
3. We use $(n_{\max}+1)$-length vectors $\{|\varphi_{W,c_i}^{0i}\rangle, |\varphi_{W,c_i}^{1i}\rangle, \cdots, |\varphi_{W,c_i}^{n_{\max} i}\rangle\}$, which are taken to be linearly independent for different values of $W \in [W_{\rm th}^0, W_{\rm th}^{n_{\max}+1})$, $i \in I(W)$ and c_i.
4. The construction can be combined with the time dependent method in Sec. III.

In the case of the modified wave function vectors, we have

1. A size of the potential matrix U_M^{kl} is $(s+1)^2$ at $W \in \Delta_s$.
2. The form of U_M^{kl} is same at all energy where U_M^{kl} is defined.
3. We use vectors $\{|\varphi_{W,c_i}^{0i}\rangle, |\varphi_{W,c_i}^{1i}\rangle, \cdots, |\varphi_{W,c_i}^{si}\rangle, 0, \cdots, 0\}$, which are linearly independent for different values of $W \in [W_{\rm th}^0, W_{\rm th}^{n_{\max}+1})$, $i \in I(W)$ and c_i. The (effective) length of these vectors is $s+1$ at $W \in \Delta_s$.

For the recursive construction, we have

1. A size of the potential matrix U_R^{kl} is $(s+1)^2$ at $W \in \Delta_s$.

2. The form of U_R^{kl} is same at all energy where U_R^{kl} is defined.

3. We use $|\varphi_{W,c_i}^{si}\rangle$, which are inearly independent for different values of $W \in \Delta_s$, $i \in I(W)$ and c_i.

4. The potential matrix is recursively constructed: At $W \in \Delta_s$, U_R^{ks} for $k = 0, 1, 2, \cdots, s$ are determined from $\{U^{k's} \mid k' < k\}$, while U_R^{sk} can be obtained from U_R^{ks} using Hermiticity.

For the construction in Appendix A 3, we have

1. A size of the potential matrix U^{kl} is $(s+1)^2$ at $W \in \Delta_s$.

2. The form of U_s^{kl} is different for each s at $W \in \Delta_s$.

3. We use the $(s+1)$ length vectors $\{|\varphi_{W,c_i}^{0i}\rangle, |\varphi_{W,c_i}^{1i}\rangle, \cdots, |\varphi_{W,c_i}^{si}\rangle\}$, which are linearly independent for different values of $W \in \Delta_s$, $i \in I(W)$ and c_i.

4. U_s^{kl} can be determined at each energy interval Δ_s, without using information of other energy intervals.

We summarize the above properties in table I.

TABLE I: A comparison of different constructions

construction	original	modified(App. A 1)	recursive(App. A 2)	interval(App. A 3)
size of U at $W \in \Delta_s$	$(n_{\max}+1)^2$	$(s+1)^2$	$(s+1)^2$	$(s+1)^2$
Δ_s dependence of U	no	no	no	yes
vectors	$\{\|\varphi_{W,c_i}^{k,i}\rangle\}_{k \le n_{\max}}$	$\{\|\varphi_{W,c_i}^{k,i}\rangle\}_{k \le s}$	$\|\varphi_{W,c_i}^{s,i}\rangle$	$\{\|\varphi_{W,c_i}^{k,i}\rangle\}_{k \le s}$
feature	t-dependent method		recursive	each Δ_s

[1] M. Lüscher, *Nucl. Phys.* B 354 (1991) 531

[2] M. T. Hansen and S. R. Sharpe, arXiv:1211.0511 [hep-lat].

[3] R. A. Briceno and Z. Davoudi, arXiv:1204.1110 [hep-lat].

[4] N. Ishii, S. Aoki and T. Hatsuda, Phys. Rev. Lett. 99 (2007) 022001 [arXiv:nucl-th/0611096].

[5] S. Aoki, T. Hatsuda and N. Ishii, Comput. Sci. Dis. 1 (2008) 015009 [arXiv:0805.2462 [hep-ph]].

[6] S. Aoki, T. Hatsuda and N. Ishii, *Prog. Theor. Phys.* 123 (2010) 89 [arXiv:0909.5585 [hep-lat]].

[7] H. Nemura, N. Ishii, S. Aoki and T. Hatsuda, *Phys. Lett.* B 673 (2009) 136 [arXiv:0806.1094 [nucl-th]].

[8] H. Nemura, N. Ishii, S. Aoki and T. Hatsuda [PACS-CS Collaboration], PoS LATTICE2008 (2008) 156 [arXiv:0902.1251 [hep-lat]].

[9] T. Inoue *et al.* [HAL QCD collaboration], *Prog. Theor. Phys.* 124 (2010) 591 [arXiv:1007.3559 [hep-lat]].

[10] T. Inoue *et al.* [HAL QCD Collaboration], *Phys. Rev. Lett.* 106 (2011) 162002 [arXiv:1012.5928 [hep-lat]].

[11] T. Inoue *et al.* [HAL QCD Collaboration], Nucl. Phys. A **881**, 28 (2012) [arXiv:1112.5926 [hep-lat]].

[12] Y. Ikeda *et al.*, PoS LATTICE2010 (2010) 143 arXiv:1002.2309 [hep-lat].

[13] T. Kawanai and S. Sasaki, *Phys. Rev.* D 82 (2010) 091501 [arXiv:1009.3332 [hep-lat]].

[14] T. Doi for HAL QCD Collaboration, PoS LATTICE2010 (2010) 136 [arXiv:1011.0657 [hep-lat]].

[15] T. Doi *et al.* [HAL QCD Collaboration], Prog. Theor. Phys. **127**, 723 (2012) [arXiv:1106.2276 [hep-lat]].

[16] S. Aoki for HAL QCD Collaboration, Prog. Part. Nucl. Phys. **66**, 687 (2011) [arXiv:1107.1284 [hep-lat]].

[17] S. Aoki *et al.* [HAL QCD Collaboration], Prog. Theor. Exp. Phys. **2012**, 01A105 (2012) [arXiv:1206.5088 [hep-lat]].

[18] J. Balog, M. Niedermaier, F. Niedermayer, A. Patrascioiu, E. Seiler and P. Weisz, Nucl. Phys. B **618**, 315 (2001) [hep-lat/0106015].

[19] C. J. D. Lin, G. Martinelli, C. T. Sachrajda and M. Testa, Nucl. Phys. B **619**, 467 (2001).

[20] S. Aoki *et al.* [CP-PACS Collaboration], Phys. Rev. D **71**, 094504 (2005) [hep-lat/0503025].

[21] N. Ishizuka, *PoS* LAT2009 (2009) 119

[22] S. Aoki *et al.* [HAL QCD Collaboration], in preparation.

[23] N. Ishii *et al.* [HAL QCD Collaboration], Phys. Lett. B **712**, 437 (2012) [arXiv:1203.3642

[hep-lat]].

[24] S. Aoki *et al.* [HAL QCD Collaboration], Proc. Japan Acad. B **87**, 509 (2011) [arXiv:1106.2281 [hep-lat]].

[25] K. Sasaki for HAL QCD Collaboration, PoS LATTICE2010 (2010) 157 [arXiv:1012.5684 [nucl-th]].