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Asymptotic behavior of Nambu-Bethe-Salpeter wave functions for multiparticles in quantum field theories

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We derive asymptotic behaviors of the Nambu-Bethe-Salpeter (NBS) wave function at large space separations for systems with more than two particles in quantum field theories. To deal with n particles in the center-of-mass frame coherently, we introduce the Jacobi coordinates of n particles and then combine their $3(n-1)$ coordinates into the one spherical coordinate in $D = 3(n-1)$ dimensions. We parametrize the on-shell T matrix for n scalar particles at low energy using the unitarity constraint of the S matrix. We then express asymptotic behaviors of the NBS wave function for n particles at low energy in terms of parameters of the T matrix and show that the NBS wave function carries information of the T matrix such as phase shifts and mixing angles of the n-particle system in its own asymptotic behavior, so that the NBS wave function can be considered as the scattering wave of n particles in quantum mechanics. This property is one of the essential ingredients of the HAL QCD scheme to define "potential" from the NBS wave function in quantum field theories such as QCD. Our results, together with an extension to systems with spin 1/2 particles, justify the HAL QCD's definition of potentials for three or more nucleons (or baryons) in terms of the NBS wave functions.

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I. INTRODUCTION

To understand hadronic interactions such as nuclear forces from the fundamental theory, quantum chromodynamics (QCD), nonperturbative methods such as the lattice QCD combined with numerical simulations are required, since the running coupling constant in QCD becomes large at hadronic scale. Conventionally, the finite size method [1] has been employed to extract the scattering phase shift in lattice QCD, but the method is so far limited to two-particle systems below the inelastic threshold, except for a few extensions [2–5].

Recently an alternative method has been proposed and employed to extract the potential between nucleons below inelastic thresholds [6–8]. This method has been extended in order to investigate more general hadronic interactions such as baryon-baryon interactions [9–13] and meson-baryon interactions [14–16]. See Refs. [17,18] for reviews of recent activities.

In the method called the HAL QCD method, a potential between hadrons is defined in quantum field theories such as QCD, through an equal-time Nambu-Bethe-Salpeter (NBS) wave function [19] in the center-of-mass system, which is defined for two nucleons as

$$\Psi_W(\boldsymbol{x}) = \langle 0|T\{N(\boldsymbol{r},0)N(\boldsymbol{r}+\boldsymbol{x},0)\}|NN,W\rangle_{\rm in}, \quad (1)$$

where $\langle 0| = {}_{\rm out}\langle 0| = {}_{\rm in}\langle 0|$ is the QCD vacuum (bra-)state, $|NN,W\rangle_{\rm in}$ is a 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 a relative momentum $\boldsymbol{k}$, T represents the time-ordered product, and $N(x)$ with $x = (\boldsymbol{x}, t)$ is a nucleon operator. As the distance between two nucleon operators $x = |\boldsymbol{x}|$ becomes large, the NBS wave function satisfies the free Schrödinger equation,

$$(E_W - H_0)\Psi_W(\boldsymbol{x}) \simeq 0, \qquad E_W = \frac{\boldsymbol{k}^2}{2\mu}, \qquad H_0 = \frac{-\nabla^2}{2\mu}, \quad (2)$$

where $\mu = m_N/2$ is the reduced mass. In addition, an 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 for the elastic $\pi\pi$ scattering [20,21], where the partial wave of the NBS wave function for the orbital angular momentum L becomes

$$\Psi_W^L \simeq A_L \frac{\sin(kx - L\pi/2 + \delta_L(W))}{kx}, \qquad k = |\boldsymbol{k}| \quad (3)$$

as $x \to \infty$ at $W \le W_{\rm th} = 4m_\pi$ (the lowest inelastic threshold). The asymptotic behavior of the NBS wave function for the elastic NN scattering has been derived in Ref. [22].

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The HAL QCD method has been applied also to investigate three nucleon forces (3NF) [23,24], even though asymptotic behaviors of the NBS wave function for three nucleons have not been derived yet. The 3NF is necessary to explain experimental binding energies of light nuclei [25,26] and high precision deuteron-proton elastic scattering data at intermediate energies [27]. It may also play an important role for various phenomena in nuclear physics and astrophysics [28–31].

The purpose of this paper is to derive asymptotic behaviors of the NBS wave functions for n particles with $n \geq 3$ at large distances where separations among n operators become large. To avoid complications due to nonzero spins of particles, we consider scalar fields in this paper. The results of this paper, together with an extension to spin $1/2$ particles, fills the logical gap in the derivation of 3NF by the HAL QCD method [23,24].

In Sec. II, we explain our notations and definitions such as the modified Jacobi coordinate, the Lippmann-Schwinger equation, and the NBS wave function for n scalar particles. In Sec. III, we parametrize the on-shell T matrix for n particles by solving the unitarity constraint of the S matrix. For the n-particle system, we introduce spherical coordinates in $D = 3(n-1)$ dimensions, which is equal to a number of degrees of freedom for n particles in three dimensions in the center-of-mass frame, together with the nonrelativistic approximation. In Sec. IV, using results obtained in Sec. III, we derive asymptotic behaviors of NBS wave functions for n particles, in terms of phase shifts and mixing angles of the n-particle scattering. Conclusions and discussions are given in Sec. V. Some technical details are collected in three appendixes.

II. SOME DEFINITIONS AND NOTATIONS

In this paper, to avoid complications arising from nucleon spins, we consider a system with n scalar particles which have the same mass m in the center-of-mass frame, whose coordinates and momenta are denoted by $\boldsymbol{x}_i$ and $\boldsymbol{p}_i$ ($i = 1, 2, \ldots, n$) with $\sum_{i=1}^n \boldsymbol{p}_i = 0$. We introduce modified Jacobi coordinates and corresponding momenta as

$$\boldsymbol{r}_k = \sqrt{\frac{k}{k+1}} \times \boldsymbol{r}_k^J, \qquad \boldsymbol{q}_k = \sqrt{\frac{k+1}{k}} \times \boldsymbol{q}_k^J, \tag{4}$$

where the standard Jacobi coordinates and momenta are given by

$$\boldsymbol{r}_k^J = \frac{1}{k}\sum_{i=1}^k \boldsymbol{x}_i - \boldsymbol{x}_{k+1}, \qquad \boldsymbol{q}_k^J = \frac{k}{k+1}\left(\frac{1}{k}\sum_{i=1}^k \boldsymbol{p}_i - \boldsymbol{p}_{k+1}\right), \tag{5}$$

for $k = 1, 2, \ldots, n-1$. It is easy to see

$$\sum_{i=1}^n \boldsymbol{p}_i \cdot \boldsymbol{x}_i = \sum_{i=1}^{n-1} \boldsymbol{q}_i \cdot \boldsymbol{r}_i, \qquad E = \frac{1}{2m}\sum_{i=1}^n \boldsymbol{p}_i^2 = \frac{1}{2m}\sum_{i=1}^{n-1} \boldsymbol{q}_i^2. \tag{6}$$

An integration measure for modified Jacobi momenta is given by

$$\prod_{i=1}^n d^3 p_i \delta^{(3)}\left(\sum_{i=1}^n \boldsymbol{p}_i\right) = \frac{1}{n^{3/2}} \prod_{i=1}^{n-1} d^3 q_i. \tag{7}$$

A. Lippmann-Schwinger equation

As mentioned in the Introduction, the asymptotic behavior of the NBS wave function for a two-particle system has already been derived in Refs. [8,20–22]. It is not straightforward, however, to extend their derivations to multiparticle systems. Instead, we utilize the Lippmann-Schwinger equation [32],

$$|\alpha\rangle_{\rm in} = |\alpha\rangle_0 + \int d\beta \frac{|\beta\rangle_0 T_{\beta\alpha}}{E_\alpha - E_\beta + i\varepsilon}, \qquad T_{\beta\alpha} = {}_0\langle\beta|V|\alpha\rangle_{\rm in}, \tag{8}$$

which is found to be a powerful tool to study multiparticle systems. For simplicity, we assume in this paper that no bound state appears in two or more particle systems. An extension of the present analysis to systems including bound states, however, will be considered in the future publications, since one of our ultimate goals in the HAL QCD Collaboration is to investigate bound states using potentials obtained in lattice QCD.

Here the asymptotic in-state $|\alpha\rangle_{\rm in}$ satisfies

$$(H_0 + V)|\alpha\rangle_{\rm in} = E_\alpha |\alpha\rangle_{\rm in}, \tag{9}$$

whereas the noninteracting state $|\alpha\rangle_0$ satisfies

$$H_0|\alpha\rangle_0 = E_\alpha|\alpha\rangle_0. \tag{10}$$

The off-shell T-matrix element or the "potential" $T_{\beta\alpha} = {}_0\langle\beta|V|\alpha\rangle_{\rm in}$ is related to the on-shell S-matrix element as

$$S_{\beta\alpha} \equiv {}_{\rm out}\langle\beta|\alpha\rangle_{\rm in} \equiv {}_0\langle\beta|S|\alpha\rangle_0 = \delta(\beta - \alpha) - 2\pi i \delta(E_\alpha - E_\beta) T_{\beta\alpha}. \tag{11}$$

If we define $S = 1 - iT$, we obtain

$${}_0\langle\beta|T|\alpha\rangle_0 = 2\pi\delta(E_\alpha - E_\beta) T_{\beta\alpha}. \tag{12}$$

B. NBS wave functions

An equal-time NBS wave function for n scalar particles is defined by

$$\Psi_\alpha^n([\boldsymbol{x}]) = {}_{\rm in}\langle 0|\varphi^n([\boldsymbol{x}], 0)|\alpha\rangle_{\rm in}, \tag{13}$$

where

$$\varphi^n([\boldsymbol{x}], t) = T\left\{\prod_{i=1}^n \varphi_i(\boldsymbol{x}_i, t)\right\}, \tag{14}$$

with the time-ordered product T, $[\boldsymbol{x}] = \boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$, and i represents a "flavor" of a scalar field. For simplicity, we regard all n scalar particles as different but have the same mass m.

From the Lippmann-Schwinger Eq. (8), the vacuum in-state is expressed as

$$|0\rangle_{\rm in} = |0\rangle_0 + \int d\gamma \frac{|\gamma\rangle_0 T_{\gamma 0}}{E_0 - E_\gamma + i\varepsilon}. \tag{15}$$

As shown in Appendix A, at large distances we have

$$_{\rm in}\langle 0|\varphi^n([\boldsymbol{x}], 0)|\alpha\rangle_0 \simeq \frac{1}{Z_\alpha}\,{}_0\langle 0|\varphi^n([\boldsymbol{x}], 0)|\alpha\rangle_0, \tag{16}$$

where Z_α is the normalization factor whose deviation from the unity comes from the off-shell T matrix $T_{\gamma 0}$ in the second term of Eq. (15). Using this and the Lippmann-Schwinger Eq. (8), the NBS wave function can be written as

$$\Psi^n_\alpha([\boldsymbol{x}]) = \frac{1}{Z_\alpha}\,{}_0\langle 0|\varphi^n([\boldsymbol{x}], 0)|\alpha\rangle_0 + \int d\beta \frac{1}{Z_\beta} \frac{{}_0\langle 0|\varphi^n([\boldsymbol{x}], 0)|\beta\rangle_0 T_{\beta\alpha}}{E_\alpha - E_\beta + i\varepsilon}. \tag{17}$$

To evaluate the above expression explicitly, we quantize all complex scalar fields in the Heisenberg representation at $t = 0$ as

$$\varphi_i(\boldsymbol{x}, 0) = \int \frac{d^3k}{\sqrt{(2\pi)^3 2E_{k_i}}}\{a_i(\boldsymbol{k})e^{i\boldsymbol{k}\cdot\boldsymbol{x}} + b_i^\dagger(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\}, \tag{18}$$

$$|\alpha\rangle_0 \equiv |[\boldsymbol{k}]_n\rangle_0 = \prod_{i=1}^n a_i^\dagger(\boldsymbol{k}_i)|0\rangle_0, \quad E_{k_i} = \sqrt{\mathbf{k}_i^2 + m^2}, \tag{19}$$

where $[\boldsymbol{k}]_n = \boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_n$ with $\sum_{i=1}^n \boldsymbol{k}_i = 0$, and the time evolution is given by $\varphi^n([\boldsymbol{x}],t)=e^{iHt}\varphi^n([\boldsymbol{x}],0)e^{-iHt}$. Our state normalization is given by

$$_0\langle\beta_m|\alpha_n\rangle_0 = \delta(\beta_m - \alpha_n). \tag{20}$$

Using the above for the n-particle system in the center-of-mass frame, we have

$$\begin{aligned} {}_0\langle 0|\varphi^n([\boldsymbol{x}], 0)|[\boldsymbol{k}]_n\rangle_0 &= \left(\frac{1}{\sqrt{(2\pi)^3}}\right)^n \prod_{i=1}^n \frac{1}{\sqrt{2E_{k_i}}} e^{i\boldsymbol{k}_i\cdot\boldsymbol{x}_i} \\ &= \left(\frac{1}{\sqrt{(2\pi)^3}}\right)^n \left(\prod_{i=1}^n \frac{1}{\sqrt{2E_{k_i}}}\right) \\ &\quad \times \exp\left[i\sum_{j=1}^{n-1} \boldsymbol{q}_j\cdot\boldsymbol{r}_j\right], \end{aligned} \tag{21}$$

where $\boldsymbol{r}_j$ and $\boldsymbol{q}_j$ are modified Jacobi coordinates and momenta, respectively.

III. UNITARITY OF THE S MATRIX AND PARAMETRIZATION OF THE T MATRIX

The unitarity of the S matrix implies

$$T^\dagger - T = iT^\dagger T. \tag{22}$$

Defining

$$\begin{aligned} {}_0\langle[\boldsymbol{p}^A]_n|T|[\boldsymbol{p}^B]_n\rangle_0 &\equiv \delta(E^A - E^B)\delta^{(3)}(\boldsymbol{P}^A - \boldsymbol{P}^B) \\ &\quad \times T([\boldsymbol{q}^A]_n, [\boldsymbol{q}^B]_n), \end{aligned} \tag{23}$$

where $[\boldsymbol{p}^X]_n = \boldsymbol{p}_1^X, \boldsymbol{p}_2^X, \ldots, \boldsymbol{p}_n^X$, $[\boldsymbol{q}^X]_n = \boldsymbol{q}_1^X, \boldsymbol{q}_2^X, \ldots, \boldsymbol{q}_{n-1}^X$ with $X = A, B$, and

$$\begin{aligned} E^A &\equiv \sum_{i=1}^n E_{p_i^A}, & E^B &\equiv \sum_{i=1}^n E_{p_i^B}, \\ \boldsymbol{P}^A &\equiv \sum_{i=1}^n \boldsymbol{p}^A{}_i, & \boldsymbol{P}^B &\equiv \sum_{i=1}^n \boldsymbol{p}^B{}_i. \end{aligned} \tag{24}$$

Here we parametrize the T-matrix element in terms of modified Jacobi momenta $[\boldsymbol{q}^A]$ and $[\boldsymbol{q}^B]$, where $T_{\beta\alpha}$ in the Lippmann-Schwinger equation is expressed as

$$T_{\beta\alpha} = \frac{1}{2\pi}\delta^{(3)}(\boldsymbol{P}^A - \boldsymbol{P}^B)T([\boldsymbol{q}^A]_n, [\boldsymbol{q}^B]_n). \tag{25}$$

Using the above expression, the unitarity constraint to the T matrix can be written as

$$\begin{aligned} &T^\dagger([\boldsymbol{q}^A]_n, [\boldsymbol{q}^B]_n) - T([\boldsymbol{q}^A]_n, [\boldsymbol{q}^B]_n) \\ &\quad = \frac{i}{n^{3/2}} \int \prod_{i=1}^{n-1} d^3q_i^C \delta(E^A - E^C)T^\dagger([\boldsymbol{q}^A]_n, [\boldsymbol{q}^C]_n) \\ &\qquad \times T([\boldsymbol{q}^C]_n, [\boldsymbol{q}^B]_n). \end{aligned} \tag{26}$$

Our task is to solve this constraint.

A. $n = 2$

Let us consider the simplest case, $n = 2$. In this case, we can parametrize the T matrix in terms of spherical harmonic functions Y_{lm} as

$$T(\boldsymbol{q}^A, \boldsymbol{q}^B) = \sum_{l,m} T_l(q^A, q^B)Y_{lm}(\Omega_{\boldsymbol{q}^A})\overline{Y_{lm}(\Omega_{\boldsymbol{q}^B})}, \tag{27}$$

where $q^{A,B} = |\boldsymbol{q}^{A,B}|$ and $\Omega_{\boldsymbol{q}}$ is a solid angle of a vector $\boldsymbol{q}$. Using the orthogonal property of Y_{lm}, the constraint becomes

$$\begin{aligned} \bar{T}_l(q, q) - T_l(q, q) &= \frac{i}{2^{3/2}} \int (q^C)^2 dq^C \delta(E - E_C) \\ &\quad \times \bar{T}_l(q, q^C)T_l(q^C, q), \end{aligned} \tag{28}$$

where $q = q^A = q^B$, $E = E^A = E^B = 2\sqrt{m^2 + q^2/2}$, and $E^C = 2\sqrt{m^2 + (q^C)^2/2}$. After the q^C integral, the constraint now becomes

$$\bar{T}_l(q,q) - T_l(q,q) = i\frac{qE}{2\times 2^{3/2}}\bar{T}_l(q,q)T_l(q,q), \quad (29)$$

which can be solved as [33]

$$T_l(q) \equiv T_l(q,q) = -\frac{4\times 2^{3/2}}{qE}e^{i\delta_l(E)}\sin\delta_l(E), \quad (30)$$

where $\delta_l(q)$ is the phase shift for the partial wave with the angular momentum l at the energy of $E = 2\sqrt{m^2 + q^2/2}$.

B. General *n*

In the case of general n, we introduce the nonrelativistic approximation for the energy in the delta function as

$$E^A - E^C \simeq \frac{(p^A)^2 - (p^C)^2}{2m} = \frac{(q^A)^2 - (q^C)^2}{2m}, \quad (31)$$

where $(q^{A,C})^2 = \sum_{i=1}^{n-1}(\boldsymbol{q}_i^{A,C})^2$ for modified Jacobi momenta $[\boldsymbol{q}^{A,C}]_n$. To perform the three-dimensional momentum integral $(n-1)$ times, we consider a $D = 3(n-1)$-dimensional space. Denoting that $s = |\boldsymbol{s}|$ is a D-dimensional hyper-radius and Ω_s are angular variables for the vector $\boldsymbol{s}$ in D dimensions, the Laplacian operator is decomposed as

$$\nabla^2 = \frac{\partial^2}{\partial s^2} + \frac{D-1}{s}\frac{\partial}{\partial s} - \frac{\hat{L}^2}{s^2}, \quad (32)$$

where $\hat{L}^2$ is angular momentum in D dimensions. A hyperspherical harmonic function [34], an extension of spherical harmonic function in three dimensions to general D dimensions satisfies

$$\hat{L}^2 Y_{[L]}(\Omega_s) = L(L+D-2)Y_{[L]}(\Omega_s) \quad (33)$$

with a set of "quantum" numbers of $[L] = L, M_1, M_2, \ldots$. The hyperspherical harmonic function is orthogonal such that

$$\int d\Omega_s \overline{Y_{[L]}(\Omega_s)}Y_{[L']}(\Omega_s) = \delta_{[L][L']}, \quad (34)$$

and is complete as

$$\sum_{[L]}\overline{Y_{[L]}(\Omega_s)}\,Y_{[L]}(\Omega_t)\delta(s-t) = s^{D-1}\delta^{(D)}(\boldsymbol{s}-\boldsymbol{t}), \quad (35)$$

so that an arbitrary function $f(\mathbf{s})$ of $\mathbf{s}\in R^D$ can be expanded as

$$f(\boldsymbol{s}) = \sum_{[L]} f_{[L]}(s)Y_{[L]}(\Omega_s). \quad (36)$$

Using the hyperspherical function, we expand the T matrix as

$$T([\boldsymbol{q}^A]_n, [\boldsymbol{q}^B]_n) \equiv T(\boldsymbol{Q}_A, \boldsymbol{Q}_B) = \sum_{[L],[K]} T_{[L][K]}(Q_A, Q_B)Y_{[L]}(\Omega_{\boldsymbol{Q}_A})\overline{Y_{[K]}(\Omega_{\boldsymbol{Q}_B})}, \quad (37)$$

where $\boldsymbol{Q}_X = (\boldsymbol{q}^X{}_1, \boldsymbol{q}^X{}_2, \ldots, \boldsymbol{q}^X{}_{n-1})$ for $X = A,\ B$ is a momentum vector in $D = 3(n-1)$ dimensions.[1]

With the nonrelativistic approximation and the orthogonal property, the unitarity relation in Eq. (26) after Ω_{Q_C} integration leads to

$$\begin{aligned} T^\dagger_{[L][K]}(Q_A, Q_A) - T_{[L][K]}(Q_A, Q_A) &= \frac{i}{n^{3/2}}\int Q^{D-1}dQ\,\delta(E_A - E) \times \sum_{[N]} T^\dagger_{[L][N]}(Q_A, Q)T_{[N][K]}(Q, Q_A) \\ &= i\frac{m(Q_A)^{D-2}}{n^{3/2}}\sum_{[N]} T^\dagger_{[L][N]}(Q_A, Q_A)T_{[N][K]}(Q_A, Q_A), \end{aligned} \quad (38)$$

where $Q_A = Q_B$ is used. By diagonalizing T with a unitary matrix U as

$$T_{[L][K]}(Q,Q) = \sum_{[N]} U_{[L][N]}(Q)T_{[N]}(Q)U^\dagger_{[N][K]}(Q), \quad (39)$$

the above constraint can be solved as

$$T_{[L]}(Q) = -\frac{2n^{3/2}}{mQ^{3n-5}}e^{i\delta_{[L]}(Q)}\sin\delta_{[L]}(Q), \quad (40)$$

where $\delta_{[L]}(Q)$ are real phases which depend on Q and $[L]$ in $D = 3(n-1)$ dimensions. This is a main result of this section. Unfortunately, a relation of the phase shifts in the hyperspherical coordinates with physical observables for n particles in the standard Jacobi coordinates is not transparent. Therefore, it will be an important task in the future to make the relation between them clear. Note also that the result at $n = 3$ is already given in Ref. [38].

At $n = 2$, we have

$$T_{[L]}(Q) = -\frac{2\times 2^{3/2}}{mQ}e^{i\delta_{[L]}(Q)}\sin\delta_{[L]}(Q), \quad (41)$$

which agrees with Eq. (30) under the nonrelativistic approximation that $E \simeq 2m$, together with the replacement that $Q \to q$ and $[L] \to l$ and $U \to 1$.

[1]For $n \geq 3$, the T matrix can have singularities at particular on-shell values of external momenta [35–37], which are expressed in terms of delta functions and principles values with the $i\varepsilon$ prescription for propagators. Even for such cases, however, our expansion of the T matrix in Eq. (37) is still valid in a sense of distributions, and these singularities originate from a sum over infinite terms [38]. We would like to thank Prof. S. R. Sharpe and Dr. M. T. Hansen for pointing out this problem and relevant references.

IV. ASYMPTOTIC BEHAVIORS OF NBS WAVE FUNCTIONS FOR *n* PARTICLES

In this section, we derive asymptotic behaviors of NBS wave functions for multiparticle systems using expressions (17)

$$\Psi^n_\alpha([\boldsymbol{x}]) = \frac{1}{Z_\alpha}{}_0\langle 0|\varphi^n([\boldsymbol{x}],0)|\alpha\rangle_0 + \int d\beta \frac{1}{Z_\beta}\frac{{}_0\langle 0|\varphi^n([\boldsymbol{x}],0)|\beta\rangle_0 T_{\beta\alpha}}{E_\alpha - E_\beta + i\varepsilon} \quad (42)$$

and (21)

$${}_0\langle 0|\varphi^n([\boldsymbol{x}],0)|[\boldsymbol{k}]_n\rangle_0 = \left(\frac{1}{\sqrt{(2\pi)^3}}\right)^n\left(\prod_{i=1}^n \frac{1}{\sqrt{2E_{k_i}}}\right) \times \exp\left[i\sum_{j=1}^{n-1}\boldsymbol{q}_j\cdot\boldsymbol{r}_j\right]. \quad (43)$$

A. *n* = 2

As an exercise, let us first consider the $n=2$ case, whose result is already known. Using $\boldsymbol{r} = (\boldsymbol{x}_2 - \boldsymbol{x}_1)/\sqrt{2}$, $\boldsymbol{p}_1 = -\boldsymbol{p}_2 = \boldsymbol{q}/\sqrt{2}$, and $E_q = \sqrt{m^2 + q^2/2}$, the NBS wave function at $n=2$ is given by

$$\Psi^2_{\boldsymbol{q}}(\boldsymbol{r}) = \frac{1}{2E_q Z_q}\left[\frac{e^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{(2\pi)^3} + \int \frac{d^3k}{2^{3/2}(2\pi)^3}\frac{Z_q E_q}{Z_k E_k} \times \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}T(\boldsymbol{k},\boldsymbol{q})}{4\pi(E_q - E_k + i\varepsilon)}\right], \quad (44)$$

where $\boldsymbol{k}$ is also the modified Jacobi momentum. Using expansions that

$$e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = 4\pi\sum_{lm} i^l j_l(qr) Y_{lm}(\Omega_{\boldsymbol{r}})\overline{Y_{lm}(\Omega_{\boldsymbol{q}})}, \quad (45)$$

$$\Psi^2_{\boldsymbol{q}}(\boldsymbol{r}) = \sum_{lm} i^l \Psi^2_l(r,q) Y_{lm}(\Omega_{\boldsymbol{r}})\overline{Y_{lm}(\Omega_{\boldsymbol{q}})}, \quad (46)$$

where $j_l(x)$ is the spherical Bessel function of the first kind, together with Eq. (27), and integrating over $\Omega_{\boldsymbol{k}}$, we obtain

$$\Psi^2_l(r,q) = \frac{4\pi}{(2\pi)^3 2E_q Z_q}\left[j_l(qr) + \int_0^\infty \frac{k^2 dk}{2\pi 2^{3/2}}\frac{Z_q E_q}{Z_k E_k} \times \frac{j_l(kr)T_l(k,q)}{2(E_q - E_k + i\varepsilon)}\right]. \quad (47)$$

Since E_q is below inelastic thresholds, we assume that $T_l(q,k)$ does not have any poles in the positive real axis. In this case, the k integral can be performed for $r \gg 1$ as [8,21]

$$\int_0^\infty k^2 dk \frac{j_l(kr)}{q^2 - k^2 + i\varepsilon}F_l(k) \simeq -\frac{\pi q}{2}F_l(q)[n_l(qr) + i j_l(qr)], \quad (48)$$

where $n_l(x)$ is the spherical Bessel function of the second kind. Here $F_l(k)$ does not have any poles in the positive real axis and satisfies $\int k^{-l} j_0(kr) F_l(k) k^2 dk \simeq 0$ for large r. In Eq. (47), the second property follows from $(\nabla^2 + q^2)\Psi^2_{\boldsymbol{q}}(\boldsymbol{r}) \simeq 0$ for large r [8]. After the k integral using this formula, the second term in Eq. (47) becomes

$$-[n_l(qr) + i j_l(qr)]\frac{qE_q}{2\times 2^{3/2}}T_l(q,q) = [n_l(qr) + i j_l(qr)]e^{i\delta_l(q)}\sin\delta_l(q), \quad (49)$$

where the unitarity constraint (30) for $T_l(q,q)$ is used to obtain the last equality. We then have

$$\Psi^2_l(r,q) = \frac{4\pi}{(2\pi)^3 2E_q Z_q}e^{i\delta_l(q)}[j_l(qr)\cos\delta_l(q) + n_l(qr)\sin\delta_l(q)] \quad (50)$$

$$\simeq \frac{4\pi}{(2\pi)^3 2E_q Z_q}\frac{e^{i\delta_l(q)}}{qr}\sin(qr - l\pi/2 + \delta_l(q)) \quad (51)$$

for $r \gg 1$, where asymptotic behaviors that $j_l(x) \simeq \sin(x - l\pi/2)/x$ and $n_l(x) \simeq \cos(x - l\pi/2)/x$ are employed. The phase of the S matrix $\delta_l(q)$ can be interpreted as the scattering phase shift of the NBS wave function for the $n=2$ case.

B. General *n*

The NBS wave function in the case of general n is expressed as

$$\Psi^n(\boldsymbol{R},\boldsymbol{Q}_A) = C(\boldsymbol{Q}_A)\left[e^{i\boldsymbol{Q}_A\cdot\boldsymbol{R}} + \frac{n^{-3/2}}{2\pi}\int d^D Q \frac{C(\boldsymbol{Q})}{C(\boldsymbol{Q}_A)} \times \frac{e^{i\boldsymbol{Q}\cdot\boldsymbol{R}}}{E_{Q_A} - E_Q + i\varepsilon}T(\boldsymbol{Q},\boldsymbol{Q}_A)\right], \quad (52)$$

where $\boldsymbol{R} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_{n-1})$ and $\boldsymbol{Q}^{(A)} = (\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_{n-1})^{(A)}$ are modified Jacobi coordinates and momenta in $D = 3(n-1)$ dimensions,

$$C(\boldsymbol{Q}_A) = \frac{1}{Z(\boldsymbol{Q}_A)}\prod_{j=1}^n \frac{1}{\sqrt{(2\pi)^3 2E_{p_j^A}}}, \quad (53)$$

with $\boldsymbol{p}_j^{(A)}$ as the momentum of the jth particle. In the nonrelativistic limit that

$$C(\boldsymbol{Q}_A) \to C(Q_A) = \frac{1 + c\frac{Q_A^2}{m}}{((2\pi)^3 2m)^{n/2}}, \qquad \frac{C(\boldsymbol{Q})}{C(\boldsymbol{Q}_A)} \to \frac{C(Q)}{C(Q_A)}, \qquad (E_{Q_A} - E_Q) \to \frac{Q_A^2 - Q^2}{2m} \quad (54)$$

with some constant c, we obtain

$$\Psi^n(\boldsymbol{R}, \boldsymbol{Q}_A) = C(Q_A)\Big[e^{i\boldsymbol{Q}_A\cdot\boldsymbol{R}} + \frac{2m}{2\pi n^{3/2}}\int d^D Q \frac{C(Q)}{C(Q_A)} \times \frac{e^{i\boldsymbol{Q}\cdot\boldsymbol{R}}}{Q_A^2 - Q^2 + i\varepsilon} T(\boldsymbol{Q}, \boldsymbol{Q}_A)\Big]. \tag{55}$$

In D dimensions, we have [34]

$$e^{i\boldsymbol{Q}\cdot\boldsymbol{R}} = (D-2)!!\frac{2\pi^{D/2}}{\Gamma(D/2)}\sum_{[L]} i^L j_L^D(QR) Y_{[L]}(\Omega_{\boldsymbol{R}})\overline{Y_{[L]}(\Omega_{\boldsymbol{Q}})}, \tag{56}$$

which is a generalization of the $D = 3$ formula in Eq. (45), where j_L^D is the hyperspherical Bessel function of the first kind defined by

$$j_L^D(x) = \frac{\Gamma(\frac{D-2}{2})2^{\frac{D-4}{2}}}{(D-4)!!x^{\frac{D-2}{2}}} J_{L_D}(x), \tag{57}$$

with $L_D = L + \frac{D-2}{2}$ and the Bessel function of the first kind, $J_{L_D}(x)$.

Using an expansion that

$$\Psi^n(\boldsymbol{R}, \boldsymbol{Q}_A) = \sum_{[L],[K]} \Psi^n_{[L],[K]}(R, Q_A) Y_{[L]}(\Omega_{\boldsymbol{R}})\overline{Y_{[K]}(\Omega_{\boldsymbol{Q}_A})}, \tag{58}$$

together with Eqs. (37) and (56), and performing $d\Omega_{\boldsymbol{Q}}$ integral, we obtain

$$\Psi^n_{[L],[K]}(R, Q_A) = C(Q_A)\frac{i^L(2\pi)^{D/2}}{(Q_A R)^{\frac{D-2}{2}}}\Big[J_{L_D}(Q_A R)\delta_{LK} + \int dQ \frac{J_{L_D}(QR)}{Q_A^2 - Q^2 + i\varepsilon} H_{[L],[K]}(Q, Q_A)\Big], \tag{59}$$

where

$$H_{[L],[K]}(Q, Q_A) = \frac{m}{\pi n^{3/2}}\frac{C(Q)}{C(Q_A)} Q^{D/2} Q_A^{D/2-1} T_{[L],[K]}(Q, Q_A). \tag{60}$$

We now perform the Q integral, assuming that $T_{[L],[K]}(Q, Q_A)$ does not have any poles on the positive real axis at Q_A below inelastic thresholds. We consider the $n = 2k$ and $n = 2k + 1$ cases separately.

1. *n* = 2*k* case

In this case,

$$J_{L_D}(x) = j_{L_k}(x)\sqrt{\frac{2}{\pi}}x^{1/2}, \tag{61}$$

where $L_k = L + 3(k-1)$ and j_{L_k} is the spherical Bessel function of the first kind. Using Eq. (48), the second term in Eq. (59) can be evaluated as [8,21]

$$\begin{aligned}\int dQ \frac{j_{L_k}(QR)}{Q_A^2 - Q^2 + i\varepsilon}&\sqrt{\frac{2}{\pi}}(QR)^{1/2} H_{[L],[K]}(Q, Q_A) \\ &\simeq -[n_{L_k}(Q_A R) + i j_{L_k}(Q_A R)]\frac{\pi}{2Q_A} \times \sqrt{\frac{2}{\pi}}(Q_A R)^{1/2} H_{[L],[K]}(Q_A, Q_A) \\ &= [N_{L_D}(Q_A R) + i J_{L_D}(Q_A R)] \times \sum_{[N]} U_{[L][N]}(Q_A) e^{i\delta_{[N]}(Q_A)} \sin\delta_{[N]}(Q_A) U^\dagger_{[N][K]}(Q_A)\end{aligned} \tag{62}$$

for $R \gg 1$, where the unitarity constraint to T in Eq. (40) is used to obtain the last equation, and J_{L_D} and N_{L_D} are Bessel functions of the first and second kinds, respectively.

2. *n* = 2*k* + 1 case

In this case, $L_D = L + 3k - 1$ is an integer, and for large R, $J_{L_D}(x)$ becomes

$$\begin{aligned} J_{L_D}(x) &\simeq \sqrt{\frac{2}{\pi x}}\sin(x - \Delta_L), \\ N_{L_D}(x) &\simeq \sqrt{\frac{2}{\pi x}}\cos(x - \Delta_L), \\ \Delta_L &= \frac{2L_D - 1}{4}\pi. \end{aligned} \tag{63}$$

Using this asymptotic behavior, the Q integral in Eq. (59) can be performed, and we obtain for $R \gg 1$

$$\begin{aligned} I &\equiv \int dQ \frac{J_{L_D}(QR)}{Q_A^2 - Q^2 + i\varepsilon} H_{[L],[K]}(Q, Q_A) \\ &\simeq -\sqrt{\frac{2}{\pi Q_A R}}\Big[\frac{\pi e^{i(Q_A R - \Delta_L)}}{2Q_A} H_{[L],[K]}(Q_A, Q_A) + O(R^{(3-D)/2})\Big] \end{aligned} \tag{64}$$

$$\simeq [N_{L_D}(Q_A R) + i J_{L_D}(Q_A R)] \times \sum_{[N]} U_{[L][N]}(Q_A) e^{i\delta_{[N]}(Q_A)} \sin\delta_{[N]}(Q_A) U^\dagger_{[N][K]}(Q_A), \tag{65}$$

where in the last equation, the $O(1/R)$ contribution is neglected for large R, the unitarity condition for T in Eq. (40) is used, and $e^{i(Q_A R - \Delta_D)}$ is replaced by asymptotic behaviors of J_n and H_n. The detailed calculation of the Q integral is given in Appendix B.

C. Asymptotic behavior

For both $n = 2k$ and $n = 2k + 1$, we finally obtain

$$\Psi^n_{[L],[K]}(R, Q_A) \simeq Ci^L \frac{(2\pi)^{D/2}}{(Q_A R)^{\frac{D-2}{2}}} \sum_{[N]} U_{[L][N]}(Q_A) e^{i\delta_{[N]}(Q_A)} \times U^\dagger_{[N][K]}(Q_A)[J_{L_D}(Q_A R)\cos\delta_{[N]}(Q_A) + N_{L_D}(Q_A R)\sin\delta_{[N]}(Q_A)] \tag{66}$$

$$\simeq Ci^L \frac{(2\pi)^{D/2}}{(Q_A R)^{\frac{D-1}{2}}} \sum_{[N]} U_{[L][N]}(Q_A) e^{i\delta_{[N]}(Q_A)} \times U^\dagger_{[N][K]}(Q_A)\sqrt{\frac{2}{\pi}}\sin(Q_A R - \Delta_L + \delta_{[N]}(Q_A)) \tag{67}$$

for $R \gg 1$, which agrees with Eq. (51) at $n = 2$. Equation (67) is the main result of this paper, which shows that the NBS wave function of n particles for large R can be considered as the generalized scattering wave of n particles, whose generalized scattering phase shift $\delta_{[N]}(Q_A)$ is nothing but the phase of the S matrix in QCD determined in Eq. (40) by the unitarity.

V. CONCLUSION AND DISCUSSION

In this paper, we have investigated asymptotic behaviors of NBS wave functions at large separations for n complex scalar fields. We have first solved the unitarity constraint of the S matrix for $n \geq 3$ using the $D = 3(n-1)$ coordinate space and employing the hyperspherical harmonic function, together with the nonrelativistic approximation for the energy. The results are summarized in Eqs. (39) and (40). We then have calculated asymptotic behaviors of NBS wave functions at large separations for $n \geq 3$ using again the hyperspherical harmonic function, which is found to be quite useful for this purpose. We have finally obtained Eq. (67), which is the main result in this paper. In Appendix C, we generalize our results to the coupled channels, where the particle mixing occurs during the scattering.

Using results in this paper, we can generalize the HAL QCD method to hadron interactions for n-particle systems with $n \geq 3$. This gives a firm theoretical foundation to extract interactions among many hadrons by the HAL QCD method, in particular, the three nucleon forces [23,24], together with an extension to systems with spin 1/2 particles, which is a straightforward but much more complicated task in the future. Moreover, combining them with the results in our previous paper [39], which shows that nonlocal but energy-independent potentials can be constructed from NBS wave functions above the inelastic threshold, the HAL QCD method can be extended to hadronic interactions above the inelastic threshold energy, where particle productions such as $NN \to NN\pi$ can occur.

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APPENDIX A: CONTRIBUTION FROM VACUUM

In this appendix, we derive Eq. (16). Assuming each flavor is conserved, ${}_0\langle\gamma|$ which contributes in Eq. (16) is a sum of the following form:

$${}_0\langle I_k| = {}_0\langle 0|\prod_{i\in I_k} a_i(\boldsymbol{k}_i^A) b_i(\boldsymbol{k}_i^B) \tag{A1}$$

with $\sum_{i\in I_k}(\boldsymbol{k}_i^A + \boldsymbol{k}_i^B) = 0$, where $k \leq n$ and $I_k = \{i_1, i_2, \ldots, i_k\}$ with $1 \leq i_1 < i_2 < \cdots < i_k \leq n$. Note that the operator $a_i b_i$ creates a particle-antiparticle pair with flavor i. Using this notation, we have

$${}_{\rm in}\langle 0|\varphi^n([\boldsymbol{x}], 0)|[\boldsymbol{k}]_n\rangle_0 = {}_0\langle 0|\varphi^n([\boldsymbol{x}], 0)|[\boldsymbol{k}]_n\rangle_0 + \sum_{k=1}^n \sum_{I_k}\prod_{i\in I_k}\int d^3k_i^A d^3k_i^B \delta^{(3)} \times\left(\sum_{i\in I_k}(\boldsymbol{k}_i^A + \boldsymbol{k}_i^B)\right)\frac{T^\dagger_{0I_k}}{E_0 - E_{I_k} + i\varepsilon} \times {}_0\langle I_k|\varphi^n([\boldsymbol{x}], 0)|[\boldsymbol{k}]_n\rangle_0, \tag{A2}$$

where $E_0 = 0$ for the vacuum.

Using

$$(2\pi)^{3n/2}{}_0\langle I_k|\varphi^n([\boldsymbol{x}], 0)|[\boldsymbol{k}]_n\rangle_0 = \prod_{i\in I_k}\frac{e^{-i\boldsymbol{k}^B_i\boldsymbol{x}_i}}{\sqrt{2E_{k_i^B}}}\delta^{(3)}(\boldsymbol{k}_i - \boldsymbol{k}_i^A)\prod_{j\in \bar{I}_k}\frac{e^{i\boldsymbol{k}_j\boldsymbol{x}_j}}{\sqrt{2E_{k_j}}}, \tag{A3}$$

where $\bar{I}_k \cup I_k = \{1, 2, 3, \ldots, n\}$ and $\bar{I}_k \cap I_k = \phi$, the second term in Eq. (A2) becomes

$$C_n \sum_{k=1}^n \sum_{I_k}\prod_{i\in I_k}\int \frac{d^3k_i^B}{\sqrt{2E_{k_i^B}}} e^{-i\boldsymbol{k}_i^B\boldsymbol{x}_i} \times \delta^{(3)}\left(\sum_{i\in I_k}(\boldsymbol{k}_i + \boldsymbol{k}_i^B)\right)\prod_{j\in\bar{I}_k}\frac{e^{i\boldsymbol{k}_j\boldsymbol{x}_j}}{\sqrt{2E_{k_j}}} \times \frac{T^\dagger_{0;I_k}(0;[\boldsymbol{k}, \boldsymbol{k}^B])}{E_0 - E_{[\boldsymbol{k},\boldsymbol{k}^B]}}, \tag{A4}$$

where $C_n = (2\pi)^{-\frac{3n}{2}}$, $E_{[\boldsymbol{k},\boldsymbol{k}^B]} = \sum_{i\in I_k}(\sqrt{\boldsymbol{k}_i^2 + m^2} + \sqrt{(\boldsymbol{k}_i^B)^2 + m^2})$, $T^\dagger_{0;I_k}(0;[\boldsymbol{k}, \boldsymbol{k}^B])$ is the off-shell T matrix from the vacuum to $2k$ particles, and $[\boldsymbol{k}, \boldsymbol{k}^B] = \{\boldsymbol{k}_{i_1}, \boldsymbol{k}^B_{i_1}, \boldsymbol{k}_{i_2}, \boldsymbol{k}^B_{i_2}, \ldots, \boldsymbol{k}_{i_k}, \boldsymbol{k}^B_{i_k}\}$.

We first show that terms at $k \geq 2$ in Eq. (A4) do not contribute at large distances. After the $\boldsymbol{k}^B_{i_k}$ integral, the factor in the first exponential is written as $-i\sum_{i\in I_{k-1}} \boldsymbol{k}^B_i(\boldsymbol{x}_i - \boldsymbol{x}_{i_k}) + i\sum_{i\in I_k} \boldsymbol{k}_i \boldsymbol{x}_{i_k}$, where $I_{k-1} = \{i_1, i_2, \ldots, i_{k-1}\}$. Since $I_{k-1} \neq \phi$ for $k \geq 2$, we perform the $\boldsymbol{k}^B_{i_1}$ integral in Eq. (A4). Using the same method which leads to Eq. (48) from Eq. (44) and noticing the fact that there is no real pole for the $\boldsymbol{k}^B_{i_1}$ integral in Eq. (A4), it is clear that the contribution is suppressed exponentially in large $|\boldsymbol{x}_{i_1} - \boldsymbol{x}_{i_k}|$. This means that terms at $k = 1$ only contribute in Eq. (A4) and other terms at $k \geq 2$ are suppressed asymptotically at large distances.

The term at $k = 1$ is easily evaluated as

$$C_n \prod_{j=1}^{n} \frac{e^{i\boldsymbol{k}_j \boldsymbol{x}_j}}{\sqrt{2E_{k_j}}} \sum_{i=1}^{n} \frac{T^\dagger_{0;i-i}(0; \boldsymbol{k}_i, -\boldsymbol{k}_i)}{-2\sqrt{\boldsymbol{k}_i^2 + m^2}}, \tag{A5}$$

where $T_{0;i,-i}$ is the off-shell T matrix from the vacuum to a pair of particle-antiparticle with the flavor i.

We finally obtain

$${}_{\text{in}}\langle 0|\varphi^n([\boldsymbol{x}], 0)|[\boldsymbol{k}]_n\rangle_0 \simeq \frac{1}{Z([\boldsymbol{k}]_n)} {}_0\langle 0|\varphi^n([\boldsymbol{x}], 0)|[\boldsymbol{k}]_n\rangle_0 \tag{A6}$$

with

$$\frac{1}{Z([\boldsymbol{k}]_n)} = 1 + \sum_{i=1}^{n} \frac{T^\dagger_{0;i-i}(0; \boldsymbol{k}_i, -\boldsymbol{k}_i)}{-2\sqrt{\boldsymbol{k}_i^2 + m^2}}, \tag{A7}$$

which proves Eq. (16) with $Z_\alpha = Z([\boldsymbol{k}]_n)$.

APPENDIX B: Q INTEGRALS

In this appendix, we evaluate the Q integral in the following form:

$$I = \int_0^\infty dQ \frac{J_{L_D}(QR)}{Q_A^2 - Q^2 + i\varepsilon} H_{[L],[K]}(Q, Q_A) \tag{B1}$$

for large R, assuming that $H_{[L],[K]}(Q, Q_A)$ have no poles in the real axis at $Q \geq 0$. Using the asymptotic form of $J_{L_D}(x)$ at large R given in Eq. (63), we write

$$I \simeq \sqrt{\frac{2}{\pi R}} \frac{1}{2i}(I_+ - I_-), \qquad R \to \infty, \tag{B2}$$

where

$$I_\pm = \int_0^\infty \frac{e^{\pm i(QR - \Delta_L)}}{Q_A^2 - Q^2 + i\varepsilon} f(Q), \qquad f(Q) \equiv \sqrt{\frac{1}{Q}} H_{[L],[K]}(Q, Q_A). \tag{B3}$$

We evaluate I_+ and I_- separately. For I_+, we consider an integration in the complex Q plane on a closed path $C = [0, \infty] \oplus C_\theta \oplus i[\infty, 0]$ in Fig. 1, which leads to

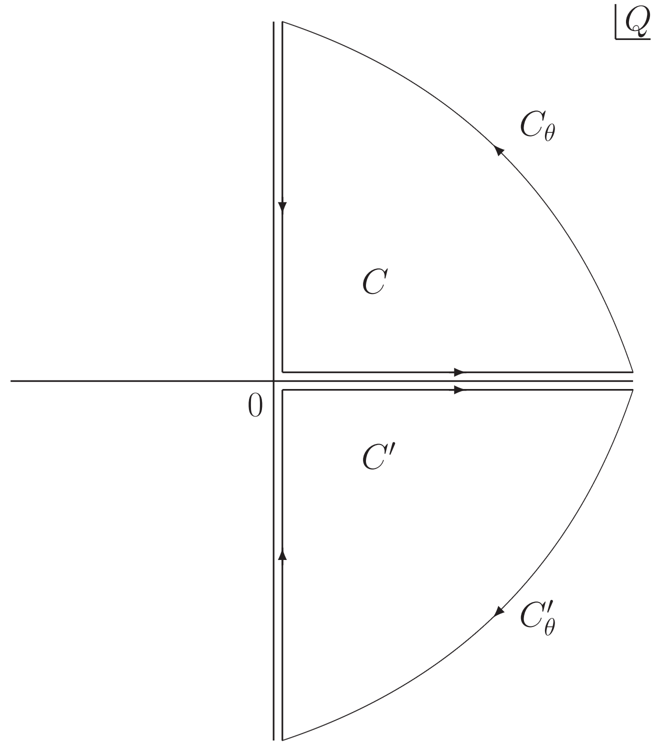

FIG. 1. Closed paths C and C' in the complex Q plane.

$$I_+ + I_1 + I_2 = \int_C \frac{e^{i(QR - \Delta_L)}}{Q_A^2 - Q^2 + i\varepsilon} f(Q) = -\frac{\pi i}{Q_A} e^{i(Q_A R - \Delta_L)} f(Q_A) + O(e^{-cR}), \tag{B4}$$

where

$$I_1 \equiv \lim_{q\to\infty} \int_0^{\pi/2} q e^{i\theta} i d\theta \frac{e^{i(QR - \Delta_L)}}{Q_A^2 - Q^2 + i\varepsilon} f(Q)|_{Q = qe^{i\theta}}, \tag{B5}$$

$$I_2 \equiv \int_{i\infty}^{i0} dQ \frac{e^{i(QR - \Delta_L)}}{Q_A^2 - Q^2 + i\varepsilon} f(Q) = -\int_0^\infty idq \frac{e^{-qR - i\Delta_L}}{Q_A^2 + q^2 + i\varepsilon} f(iq), \tag{B6}$$

and the term $O(e^{-cR})$ with $c > 0$ represents the contributions from complex poles inside C. It is easy to show that I_1 vanishes as

$$\begin{aligned} |I_1| &\leq \lim_{q\to\infty} \underbrace{\frac{q}{(q^2 - Q_A^2)} \max_{0\leq\theta\leq\pi/2} |f(qe^{i\theta})|}_{\equiv F(q)} \int_0^{\pi/2} d\theta e^{-qR\sin\theta} \\ &\leq \lim_{q\to\infty} F(q) \int_0^{\pi/2} d\theta e^{-2qR\theta/\pi} \\ &= \lim_{q\to\infty} F(q) \frac{\pi}{2qR}(1 - e^{-qR}) \to 0, \end{aligned} \tag{B7}$$

where we assume that $\max_{0\leq\theta\leq\pi/2} |f(qe^{i\theta})|$ does not grow as fast as q^2 in the large q^2 limit. Similarly, we estimate

$$|I_2| \le \int_0^\infty dq \frac{e^{-qR}}{Q_A^2 + q^2} |f(iq)| \le \frac{1}{Q_A^2} \max_{0<q} |f(iq)| \int_0^\infty dq e^{-qR} = \frac{1}{Q_A^2} \max_{0<q} |f(iq)| \frac{1}{R} \tag{B8}$$

for $Q_A \neq 0$, which vanishes as $1/R$ for large R as long as $\max_{0<q} |f(iq)| < \infty$. If some poles happen to exist on the positive imaginary axis, we can modify the path a little to avoid poles, so that the above estimate still holds. We indeed have a stronger bound of $|I_2|$ for all Q_A including $Q_A = 0$ as shown below at $n \ge 3$. (At $n = 2$, we can evaluate I by the different method.) Since we can write $f(Q) = Q^{(D-1)/2} g(Q)$ with $|g(0)| < \infty$ from Eqs. (60) and (B3), we have

$$|I_2| \le \max_{0<q} |g(iq)| \int_0^\infty dq q^{(D-5)/2} e^{-qR} = \max_{0<q} |g(iq)| R^{(3-D)/2} \int_0^\infty dt t^{(D-5)/2} e^{-t}, \tag{B9}$$

which vanishes as $R^{(3-D)/2}$ for large R at $n \ge 3$ ($D \ge 6$), as long as $\max_{0<q} |g(iq)| < \infty$. (Again we can modify the path if poles exit on the positive imaginary axis.) Altogether we obtain

$$I_+ \simeq -\frac{\pi i}{Q_A} e^{i(Q_A R - \Delta_L)} f(Q_A) + O(R^{(3-D)/2}). \tag{B10}$$

For I_-, we take another closed path $C' = [0, \infty] \oplus C'_\theta \oplus i[-\infty, 0]$ in Fig. 1. Since poles at $Q = \pm(Q_A + i\varepsilon)$ are not contained in this closed path, we have

$$I_+ + I'_1 + I'_2 = \int_{C'} \frac{e^{-i(QR-\Delta_L)}}{Q_A^2 - Q^2 + i\varepsilon} f(Q) = O(e^{-c'R}) \tag{B11}$$

with $c' > 0$, where

$$I'_1 \equiv \lim_{q\to\infty} \int_0^{-\pi/2} q e^{i\theta} i d\theta \frac{e^{-i(QR-\Delta_L)}}{Q_A^2 - Q^2 + i\varepsilon} f(Q)|_{Q=qe^{i\theta}}, \tag{B12}$$

$$I'_2 \equiv \int_{-i\infty}^{-i0} dQ \frac{e^{-i(QR-\Delta_L)}}{Q_A^2 - Q^2 + i\varepsilon} f(Q) = \int_0^\infty i dq \frac{e^{-qR + i\Delta_L}}{Q_A^2 + q^2 + i\varepsilon} f(-iq). \tag{B13}$$

As in the case before, it is easy to show that

$$|I'_1| = 0, \qquad |I'_2| = O(R^{(3-D)/2}), \tag{B14}$$

which leads to $I_- = O(R^{(3-D)/2})$.

Combining these, we finally obtain

$$I = -\sqrt{\frac{2}{\pi Q_A R}} \left[\frac{\pi e^{i(Q_A R - \Delta_L)}}{2 Q_A} H_{[L],[K]}(Q_A, Q_A) + O(R^{(3-D)/2}) \right], \tag{B15}$$

which proves Eq. (64).

APPENDIX C: COUPLED-CHANNEL CASES

In this appendix, we extend our investigation to the case where $l \to n$ scatterings with $l \neq n$ can occur.

1. Unitarity constraint to the T matrix

The unitarity relation to the T matrix in Eq. (26) can be generalized to

$$T^\dagger(\boldsymbol{Q}_n, \boldsymbol{Q}_l) - T(\boldsymbol{Q}_n, \boldsymbol{Q}_l) = \sum_k \frac{i}{k^{3/2}} \int d\boldsymbol{Q}_k \delta(E_{\boldsymbol{Q}_n} - E_{\boldsymbol{Q}_k}) T^\dagger(\boldsymbol{Q}_n, \boldsymbol{Q}_k) T(\boldsymbol{Q}_k, \boldsymbol{Q}_l) \tag{C1}$$

for general n and l, where the energy conservation that $E_{\boldsymbol{Q}_n} = E_{\boldsymbol{Q}_l}$ is always satisfied.

As in the case of the single channel, we expand T in terms of the hyperspherical harmonic function as

$$T(\boldsymbol{Q}_n, \boldsymbol{Q}_l) = \sum_{[N_n],[L_l]} T_{[N_n],[L_l]}(Q_n, Q_l) Y_{[N_n]}(\Omega_{\boldsymbol{Q}_n}) \overline{Y_{[L_l]}(\Omega_{\boldsymbol{Q}_l})}, \tag{C2}$$

where $Q_n^2 - Q_l^2 = 2m^2(l-n)$ in the nonrelativistic approximation. Putting this into Eq. (C1), we have

$$T^\dagger_{[N_n],[L_l]}(Q_n, Q_l) - T_{[N_n],[L_l]}(Q_n, Q_l) = \sum_{k,[K_k]} i \frac{m Q_k^{D_k - 2}}{k^{3/2}} T^\dagger_{[N_n],[K_k]}(Q_n, Q_k) T_{[K_k],[L_l]}(Q_k, Q_l), \tag{C3}$$

where $D_k = 3(k-1)$ and $Q_n^2 - Q_k^2 = 2m^2(k-n)$. Defining and diagonalizing $\hat{T}$ as

$$\hat{T}_{[N_n],[L_l]}(Q_n, Q_l) \equiv \frac{Q_n^{D_n/2-1}}{n^{3/4}} T_{[N_n],[L_l]}(Q_n, Q_l) \frac{Q_l^{D_l/2-1}}{l^{3/4}} = \sum_{k,[K_k]} U_{[N_n],[K_k]}(Q_k) \hat{T}_{[K_k]}(Q_k) U^\dagger_{[K_k],[L_l]}(Q_k), \tag{C4}$$

where $Q_n^2 - Q_k^2 = 2m^2(k-n)$, Eq. (C3) leads to

$$\hat{T}_{[K_k]}(Q_k) = -\frac{2}{m} e^{i\delta_{[K_k]}(Q_k)} \sin \delta_{[K_k]}(Q_k). \tag{C5}$$

This gives us the final result,

$$T_{[N_n],[L_l]}(Q_n, Q_l) = -\frac{2n^{3/4}l^{3/4}}{mQ_n^{D_n/2-1}Q_l^{D_l/2-1}}\sum_{k,[K_k]} U_{[N_n],[K_k]}(Q_k)e^{i\delta_{[K_k]}(Q_k)}\sin\delta_{[K_k]}(Q_k)U^\dagger_{[K_k],[L_l]}(Q_k), \tag{C6}$$

which reproduces Eq. (40) for the single channel at $n = l = k$.

2. Asymptotic behavior of the NBS wave function

For the coupled channel, the NBS wave function corresponding to Eq. (55) in the nonrelativistic approximation becomes

$$\Psi^{nl}(\boldsymbol{R}, \boldsymbol{Q}_l) = C_n\left[\delta_{nl}e^{i\boldsymbol{Q}_l\cdot\boldsymbol{R}_n} + \frac{2m}{2\pi n^{3/2}}\int d\boldsymbol{P}_n\frac{e^{i\boldsymbol{P}_n\cdot\boldsymbol{R}_n}T(\boldsymbol{P}_n,\boldsymbol{Q}_l)}{Q_l^2 - P_n^2 + 2m^2(l-n) + i\varepsilon}\right], \tag{C7}$$

where $C_n = ((2\pi)^3 2m)^{-n/2}$. (We here omit irrelevant $\frac{Q_n^2}{m}$ contributions.) Expanding the NBS wave function in terms of the hyperspherical function as

$$\Psi^{nl}(\boldsymbol{R}_n, \boldsymbol{Q}_l) = \sum_{[N_n],[L_l]}\Psi_{[N_n],[L_l]}(R_n, Q_l)Y_{[N_n]}(\Omega_{\boldsymbol{R}_n})\overline{Y_{[L_l]}(\Omega_{\boldsymbol{Q}_l})}, \tag{C8}$$

together with Eq. (56), we have

$$\Psi_{[N_n],[L_l]}(R_n, Q_l) = C_n i^{N_n}\frac{(2\pi)^{D_n/2}}{(Q_nR_n)^{D_n/2-1}}\left[J_{\tilde N_n}(Q_nR_n)\delta_{nl}\delta_{[N_n],[L_l]} + \int dP_n\frac{J_{\tilde N_n}(P_nR_n)}{Q_l^2 - P_n^2 + 2m^2(l-n) + i\varepsilon}H_{[N_n],[L_l]}(P_n, Q_l)\right], \tag{C9}$$

where $\tilde N_n = N_n + (3n-5)/2$ and

$$H_{[N_n],[L_l]}(P_n, Q_l) = \frac{m}{\pi n^{3/2}}P_n^{D_n/2}Q_n^{D_n/2-1}T_{[N_n],[L_l]}(P_n, Q_l). \tag{C10}$$

As before, after the P_n integral, the second term in Eq. (C9) for large R_n is given by

$$\simeq [H_{\tilde N_n}(Q_nR_n) + iJ_{\tilde N_n}(Q_nR_n)]\left(\frac{l}{n}\right)^{3/4}\frac{Q_n^{D_n/2-1}}{Q_l^{D_l/2-1}}\sum_{k,[K_k]}U_{[N_n],[K_k]}(Q_k)e^{i\delta_{[K_k]}(Q_k)}\sin\delta_{[K_k]}(Q_k)U^\dagger_{[K_k],[L_l]}(Q_k), \tag{C11}$$

where $Q_n^2 = Q_l^2 + 2m^2(l-n)$ and $Q_k^2 = Q_l^2 + 2m^2(l-k)$. We finally obtain

$$\begin{aligned}\Psi_{[N_n],[L_l]}(R_n, Q_l) &\simeq C_n i^{N_n}\frac{(2\pi)^{D_n/2}}{(Q_nR_n)^{D_n/2-1}}\left(\frac{l}{n}\right)^{3/4}\frac{Q_n^{D_n/2-1}}{Q_l^{D_l/2-1}}\sum_{k,[K_k]}U_{[N_n],[K_k]}(Q_k)e^{i\delta_{[K_k]}(Q_k)}\\ &\quad\times[J_{\tilde N_n}(Q_nR_n)\cos\delta_{[K_k]}(Q_k) + H_{\tilde N_n}(Q_nR_n)\sin\delta_{[K_k]}(Q_k)]U^\dagger_{[K_k],[L_l]}(Q_k)\\ &\simeq C_n i^{N_n}\frac{(2\pi)^{D_n/2}}{(Q_nR_n)^{D_n/2}}\left(\frac{l}{n}\right)^{3/4}\frac{Q_n^{D_n/2-1}}{Q_l^{D_l/2-1}}\sum_{k,[K_k]}U_{[N_n],[K_k]}(Q_k)e^{i\delta_{[K_k]}(Q_k)}\\ &\quad\times\sqrt{\frac{2}{\pi}}\sin(Q_nR_n - \Delta_{N_n} + \delta_{[K_k]}(Q_k))U^\dagger_{[K_k],[L_l]}(Q_k),\end{aligned} \tag{C12}$$

where $\Delta_{N_n} = (2\tilde N_n - 1)\pi/4$, which correctly reproduces Eq. (67) in the single-channel case at $n = l = k$.

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