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Asymptotic behavior of Nambu–Bethe–Salpeter wave functions for scalar systems with a bound state

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We study the asymptotic behaviors of the Nambu–Bethe–Salpeter (NBS) wave functions, which are important for the HAL QCD potential method to extract hadron interactions, in the case that a bound state exists in the system. We consider the complex scalar particles, two of which lead to the formation of a bound state. In the case of the two-body system, we show that the NBS wave functions for the bound state, as well as scattering states in the asymptotic region, behave like the wave functions in quantum mechanics, which carry the information of the binding energy as well as the scattering phase shift. This analysis theoretically establishes under some conditions that the HAL QCD potential can correctly reproduce not only the scattering phase shift but also the binding energy. As an extension of the analysis, we also study the asymptotic behaviors of all possible NBS wave functions in the case of three-body systems, two of which can form a bound states.

Subject Index B64, C00, D00, D20, D34

1. Introduction

Lattice quantum chromodynamics (QCD) is a successful non-perturbative method to study hadron physics from the underlying degrees of freedom, i.e. quarks and gluons. Masses of the single stable hadrons obtained from lattice QCD show good agreement with the experimental results, and even hadron interactions have recently been explored in lattice QCD. Using the Nambu–Bethe–Salpeter (NBS) wave function, linked to the S-matrix in QCD [1–9], the hadron interactions have been investigated mainly by two methods: the finite volume method [1] and the HAL QCD potential method [5–7]. Theoretically, the two methods in principle give the same results for the scattering phase shift between two hadrons, while in practice they sometimes show different numerical results for two baryon systems, whose origin has been clarified recently in Refs. [10,11].

The first method relies on Lüscher's finite volume formula [1] that relates the energies of two hadrons on a finite volume to the phase shifts in infinite volume by utilizing the NBS wave function in the asymptotic region. In practice, the energies of the two-hadron system are extracted from the temporal correlation of the NBS wave function summed over spatial coordinates and are transformed into the corresponding phase shifts via the finite volume formula. The second method utilizes the NBS wave function in the non-asymptotic (interacting) region, and extracts the non-local but energy-independent potentials from the space and time dependences of the NBS wave function. Physical observables such as phase shifts and binding energies are then calculated by solving the Schrödinger equation in infinite volume using the obtained potentials, since the asymptotic behavior of the NBS

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wave function is related to the T-matrix element and thus to the phase shifts [9]. In practice, the non-local potential is given by the form of the derivative expansion, which is truncated by the first few orders [12]. This method has been successfully applied to a wide range of two (or three) hadron systems at heavy pion masses [13–28], as well as at nearly physical mass [29–35].

While a relation of the asymptotic behaviors of the NBS wave functions to the scattering phase shift (or more generally the S-matrix) is important for both methods, and in particular for the HAL QCD potential method, the theoretical arguments for the relation are rather limited: Two-body relativistic systems without bound states have been discussed in several different ways [2–4,36], while n-body non-relativistic systems without bound states have been considered in Ref. [9], using the Lippmann–Schwinger equation.

In these systems, its Hilbert space is of course expanded only by scattering states, so that the asymptotic states are also composed of only the scattering states. If the system contains bound states, on the other hand, the Hilbert space is expanded by bound states as well as the scattering states. This situation has never been considered in previous works and will be discussed in this paper.

The aim of this paper is to relate the asymptotic behaviors of NBS wave functions in scalar systems to their phase shifts and binding energy in the presence of one bound state. We apply the Lippmann–Schwinger approach in Ref. [9] to two- and three-body systems with a bound state. In this approach, we split the Hamiltonian into a free part, which reproduces all the energy spectrum, and an interacting part. The free part includes not only scattering states but also a bound state, since both appear as asymptotic states and thus there is no reason to exclude the latter. We first consider the Lippman–Schwinger equations for the two-body scalar system with a bound state in Sect. 2, and then derive the asymptotic behaviors of the corresponding NBS wave functions in Sect. 3. We then generalize our analysis to the three-body scalar system with a bound state: We consider the three-body Lippmann–Schwinger equations in Sect. 4, and derive the asymptotic behaviors of the corresponding NBS wave functions in Sect. 5.

2. Lippmann–Schwinger equation for two scalar fields

Let us first consider a Hamiltonian H composed of two complex scalar fields with the same (physical) mass $m_a = m_b = m$ (denoted by ϕ_a and ϕ_b) whose interaction leads to an S-wave bound state with the (physical) mass $m_B(< 2m)$. In this section, we derive the Lippmann–Schwinger equation in the two-body system, following the definition and notation in Refs. [9] and [37]. The Hamiltonian is divided into two terms, a free Hamiltonian H_0 and an interaction V,

$$H = H_0 + V, \tag{1}$$

where a free eigenstate $|\alpha\rangle_0$ and an asymptotic in-state $|\alpha\rangle_{\rm in}$ satisfy

$$H_0\,|\alpha\rangle_0 = E_\alpha\,|\alpha\rangle_0\,, \qquad H\,|\alpha\rangle_{\rm in} = E_\alpha\,|\alpha\rangle_{\rm in} \tag{2}$$

for the same energy E_α. In order to deal with the bound state in this description, we include the scalar field ϕ_B corresponding to the bound state composed of ϕ_a and ϕ_b in the Hamiltonian as

$$H_0 = \int d^3x \left[\sum_{i=a,b} \frac{1}{2}\left(\pi_i^2 + |\phi_i|^2 + m^2|\phi_i|^2\right) + \frac{1}{2}\left(\pi_B^2 + |\phi_B|^2 + m_B^2|\phi|^2\right)\right], \tag{3}$$

with π_i $(i = a, b)$ and π_B conjugate momenta for ϕ_i $(i = a, b)$ and ϕ_B, respectively. The Heisenberg operator for the scalar fields at $t = 0$ can be expressed in terms of the creation operator of the free anti-particle and annihilation operator of the free particle as

$$\phi_i(\mathbf{x}_i, 0) = \int \frac{d^3k_i}{\sqrt{(2\pi)^3 2E_{\mathbf{k}_i}}} \left[a_i(\mathbf{k}_i) e^{i\mathbf{k}_i\cdot\mathbf{x}_i} + b_i^\dagger(\mathbf{k}_i) e^{-i\mathbf{k}_i\cdot\mathbf{x}_i} \right], \quad i = a, b, B, \tag{4}$$

with $E_{\mathbf{k}_i} = \sqrt{m_i^2 + (\mathbf{k}_i)^2}$. Note that this form fixed at $t = 0$ does not hold generally at $t \neq 0$ if $V \neq 0$.

In general, eigenstates $|\alpha\rangle_{0,\text{in}}$ contain n_a $(n_{\bar{a}})$ ϕ_a-particles (anti-particles), n_b $(n_{\bar{b}})$ ϕ_b-particles (anti-particles), and n_B $(n_{\bar{B}})$ ϕ_B-bound states (anti-bound states). In this section, to consider two-body scattering, we focus on states with $n_a = n_b = 1$ and $n_B = 1$, denoted as

$$|\mathbf{k}^a, \mathbf{k}^b\rangle_{0,\text{in}}, \qquad |\mathbf{k}^B\rangle_{0,\text{in}}, \tag{5}$$

whose eigenenergies are given by

$$E_{\mathbf{k}^a,\mathbf{k}^b} = \sqrt{(k^a)^2 + m^2} + \sqrt{(k^b)^2 + m^2}, \qquad E_{\mathbf{k}^B} = \sqrt{(k^B)^2 + m_B^2}, \tag{6}$$

with $k^i = |\mathbf{k}^i|$ $(i = a, b, B)$. Explicitly, we can write

$$|\mathbf{k}^a, \mathbf{k}^b\rangle_0 = a_a^\dagger(\mathbf{k}^a) a_b^\dagger(\mathbf{k}^b)|0\rangle_0, \qquad |\mathbf{k}^B\rangle_0 = a_B^\dagger(\mathbf{k}^B)|0\rangle_0. \tag{7}$$

The Lippmann–Schwinger equation formally relates the in-state $|\alpha\rangle_{\text{in}}$ to the free-particle state $|\alpha\rangle_0$ as

$$|\alpha\rangle_{\text{in}} = |\alpha\rangle_0 + (E_\alpha - H_0 + i\epsilon)^{-1}\, V\, |\alpha\rangle_{\text{in}}\,. \tag{8}$$

By inserting a complete set of free-particle states into the second term, the equation reduces to

$$|\alpha\rangle_{\text{in}} = |\alpha\rangle_0 + \frac{1}{2\pi}\int d\beta \frac{|\beta\rangle_0\, T_{\beta;\alpha}}{E_\alpha - E_\beta + i\epsilon}, \quad \frac{T_{\beta;\alpha}}{2\pi} \equiv {}_0\langle\beta|\, V\, |\alpha\rangle_{\text{in}}\,, \tag{9}$$

where $\int d\beta$ represents both summation over all bound states and integration over all scattering states. Note that, unlike the system without a bound state discussed in Ref. [9], the complete set of free particle states includes the bound states.

Let us consider the Lippmann–Schwinger equation for the two particle (scattering) state $\left|\mathbf{k}^a, \mathbf{k}^b\right\rangle_{\text{in}}$ as

$$\left|\mathbf{k}^a, \mathbf{k}^b\right\rangle_{\text{in}} = \left|\mathbf{k}^a, \mathbf{k}^b\right\rangle_0 + \frac{1}{2\pi}\int d^3q^a\, d^3q^b\, \frac{\left|\mathbf{q}^a, \mathbf{q}^b\right\rangle_0 T_{\mathbf{q}^a,\mathbf{q}^b;\mathbf{k}^a,\mathbf{k}^b}}{E_{\mathbf{k}^a,\mathbf{k}^b} - E_{\mathbf{q}^a,\mathbf{q}^b} + i\epsilon} + \frac{1}{2\pi}\int d^3q^B \frac{\left|\mathbf{q}^B\right\rangle_0 T_{\mathbf{q}^B;\mathbf{k}^a,\mathbf{k}^b}}{E_{\mathbf{k}^a,\mathbf{k}^b} - E_{\mathbf{q}^B} + i\epsilon}, \tag{10}$$

where the third term appears since the bound state has the same quantum number as the two-particle state with $n_a = n_b = 1$. We therefore need to consider the equation for the bound state as

$$\left|\mathbf{k}^B\right\rangle_{\text{in}} = \left|\mathbf{k}^B\right\rangle_0 + \frac{1}{2\pi}\int d^3q^a\, d^3q^b\, \frac{\left|\mathbf{q}^a, \mathbf{q}^b\right\rangle_0 T_{\mathbf{q}^a,\mathbf{q}^b;\mathbf{k}^B}}{E_{\mathbf{k}^B} - E_{\mathbf{q}^a,\mathbf{q}^b} + i\epsilon}, \tag{11}$$

where the LSZ reduction formula tells us that $T_{\mathbf{q}^B,\mathbf{k}^B}$ vanishes. Let us also remind readers that $T_{\mathbf{q}^a,\mathbf{q}^b;\mathbf{k}^a,\mathbf{k}^b}$ has a pole corresponding to the bound state at an imaginary momentum.

For simplicity we consider the center-of-mass frame, which implies $\mathbf{k} \equiv \mathbf{k}_a = -\mathbf{k}_b$ for the scattering state and $\mathbf{k}_B = \mathbf{0}$ for the bound state. By using the momentum conservation, the equations can be written as

$$|\mathbf{k}, -\mathbf{k}\rangle_{\rm in} = |\mathbf{k}, -\mathbf{k}\rangle_0 + \frac{1}{2\pi}\frac{|\mathbf{q}_B = \mathbf{0}\rangle_0\, T_{1-2}(\mathbf{0}; \mathbf{k})}{E_k - m_B} + \frac{1}{2\pi}\int d^3q \frac{|\mathbf{q}, -\mathbf{q}\rangle_0\, T_{2-2}(\mathbf{q}; \mathbf{k})}{E_k - E_q + i\epsilon}, \tag{12}$$

$$\left|\mathbf{k}^B = \mathbf{0}\right\rangle_{\rm in} = \left|\mathbf{k}^B = \mathbf{0}\right\rangle_0 + \frac{1}{2\pi}\int d^3q \frac{|\mathbf{q}, -\mathbf{q}\rangle_0\, T_{2-1}(\mathbf{q}; \mathbf{0})}{m_B - E_q}, \tag{13}$$

with $E_k = 2\sqrt{k^2 + m^2}$ ($E_q = 2\sqrt{q^2 + m^2}$), where we have defined the half off-shell T-matrices as

$$\begin{aligned} T_{\mathbf{q}_B;\mathbf{k},-\mathbf{k}} &= \delta(\mathbf{q}_B) T_{1-2}(\mathbf{0}; \mathbf{k}), \\ T_{\mathbf{q}_a,\mathbf{q}_b;\mathbf{k},-\mathbf{k}} &= \delta(\mathbf{q}_a + \mathbf{q}_b) T_{2-2}(\mathbf{q}; \mathbf{k}), \\ T_{\mathbf{q}_a,\mathbf{q}_b;\mathbf{k}^B=\mathbf{0}} &= \delta(\mathbf{q}_a + \mathbf{q}_b) T_{2-1}(\mathbf{q}; \mathbf{0}), \end{aligned} \tag{14}$$

with $\mathbf{q} = \mathbf{q}_a = -\mathbf{q}_b$. We have removed some of the "$i\epsilon$" if the corresponding denominator does not lead to any real poles. As mentioned before, $T_{2-2}(\mathbf{q}; \mathbf{k})$ has a pole at $\mathbf{k}^2 = \mathbf{q}^2 = m_B^2/4 - m^2 < 0$.

3. Asymptotic behaviors of the NBS wave functions for a two-body scalar system with a bound state

In this section we derive the asymptotic behavior of the equal-time NBS wave functions for two scalar fields, ϕ_a and ϕ_b, in the center of mass system as

$$\begin{aligned} \Psi^{\mathbf{k}}_{ab}(\mathbf{r}) &= {}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{k}, -\mathbf{k}\rangle_{\rm in}\,, \\ \Psi^{B}_{ab}(\mathbf{r}) &= {}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, \left|\mathbf{k}^B = \mathbf{0}\right\rangle_{\rm in}\,, \end{aligned} \tag{15}$$

with $\mathbf{r} = \mathbf{x}_a - \mathbf{x}_b$. By substituting Eqs. (12) and (13) into Eq. (15), we obtain

$$\begin{aligned} \Psi^{\mathbf{k}}_{ab}(\mathbf{r}) = {}& {}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{k}, -\mathbf{k}\rangle_0 + \frac{1}{2\pi}\frac{{}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, \left|\mathbf{q}^B = \mathbf{0}\right\rangle_0 T_{1-2}(\mathbf{0}; \mathbf{k})}{E_k - m_B} \\ &+ \frac{1}{2\pi}\int d^3q\, \frac{{}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{q}, -\mathbf{q}\rangle_0\, T_{2-2}(\mathbf{q}; \mathbf{k})}{E_k - E_q + i\epsilon}, \end{aligned} \tag{16}$$

$$\begin{aligned} \Psi^{B}_{ab}(\mathbf{r}) = {}& {}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, \left|\mathbf{k}^B = \mathbf{0}\right\rangle_0 \\ &+ \frac{1}{2\pi}\int d^3 q \frac{{}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{q}, -\mathbf{q}\rangle_0\, T_{2-1}(\mathbf{q}; \mathbf{0})}{m_B - E_q}. \end{aligned} \tag{17}$$

As shown in Appendix B, ${}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, \left|\mathbf{q}^B = 0\right\rangle_0$ is exponentially suppressed at large $|\mathbf{r}|$, while ${}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{q}, -\mathbf{q}\rangle_0$ behaves as

$${}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{q}, -\mathbf{q}\rangle_0 \simeq \frac{1}{Z(\mathbf{q})}{}_0\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{q}, -\mathbf{q}\rangle_0\,. \tag{18}$$

Consequently, in the asymptotic region, $\left|\mathbf{x}^a - \mathbf{x}^b\right| \gg 1$, the NBS wave functions reduce to

$$\begin{aligned} \Psi^{\mathbf{k}}_{ab}(\mathbf{r}) \simeq {}& \frac{1}{Z(\mathbf{k})}{}_0\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{k}, -\mathbf{k}\rangle_0 \\ &+ \frac{1}{2\pi}\int d^3q \frac{1}{Z(\mathbf{q})}\frac{{}_0\langle 0|\, \phi_a(\mathbf{x_a}, 0)\phi_b(\mathbf{x_b}, 0)\, |\mathbf{q}, -\mathbf{q}\rangle_0\, T_{2-2}(\mathbf{q}; \mathbf{k})}{E_k - E_q + i\epsilon} \end{aligned}$$

$$= \frac{1}{E_k Z(\mathbf{k})}\left[\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^3} + \frac{1}{2\pi}\int \frac{d^3q}{(2\pi)^3}\frac{Z(\mathbf{k})E_k}{Z(\mathbf{q})E_q}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}T_{2-2}(\mathbf{q};\mathbf{k})}{E_k - E_q + i\epsilon}\right], \tag{19}$$

$$\Psi^B_{ab}(\mathbf{r}) = \frac{1}{2\pi}\int d^3q \frac{1}{Z(\mathbf{q})}\frac{{}_0\langle 0|\,\phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,|\mathbf{q},-\mathbf{q}\rangle_0\, T_{2-1}(\mathbf{q};\mathbf{0})}{m_B - E_q}$$

$$= \frac{1}{2\pi}\int \frac{d^3q}{(2\pi)^3}\frac{1}{Z(\mathbf{q})E_q}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}T_{2-1}(\mathbf{q};\mathbf{0})}{m_B - E_q}. \tag{20}$$

The rotational invariance implies that $Z(\mathbf{q}) = Z_q$ with $q = |\mathbf{q}|$, and we can write the spherical expansions as

$$e^{i\mathbf{q}\cdot\mathbf{r}} = 4\pi\sum_{l,m} i^l j_l(qr)Y_{lm}(\Omega_\mathbf{r})Y^*_{lm}(\Omega_\mathbf{q}), \tag{21}$$

$$T_{2-2}(\mathbf{q};\mathbf{k}) = \sum_{l,m} T^{2-2}_l(q,k)Y_{lm}(\Omega_\mathbf{q})Y^*_{lm}(\Omega_\mathbf{k}), \tag{22}$$

$$T_{2-1}(\mathbf{q};\mathbf{0}) = T^{2-1}_0(q)Y_{00}(\Omega_\mathbf{q}), \tag{23}$$

$$\Psi^\mathbf{k}_{ab}(\mathbf{r}) = \sum_{l,m} i^l\Psi^{lm}_{ab}(r,k)Y_{lm}(\Omega_\mathbf{r})Y^*_{lm}(\Omega_\mathbf{k}), \tag{24}$$

$$\Psi^B_{ab}(\mathbf{r}) = \Psi^{B,00}_{ab}(r)Y_{00}(\Omega_\mathbf{r}). \tag{25}$$

After performing the integration over $\Omega_\mathbf{q}$, we obtain

$$\Psi^{lm}_{ab}(r,k) = \frac{4\pi}{(2\pi)^3E_kZ_k}\left[j_l(kr) + \int_0^\infty \frac{q^2dq}{2\pi}\frac{Z_kE_k}{Z_qE_q}\frac{j_l(qr)T^{2-2}_l(q,k)}{E_k - E_q + i\epsilon}\right], \tag{26}$$

$$\Psi^{B,00}_{ab}(r) = \frac{4\pi}{(2\pi)^3E_kZ_k}\int_0^\infty \frac{q^2dq}{2\pi}\frac{Z_kE_k}{Z_qE_q}\frac{j_0(qr)T^{2-1}_0(q)}{m_B - E_q}. \tag{27}$$

If k^2 is below the four-particle threshold ($2\sqrt{k^2+m^2} < 4m$), the half off-shell T-matrix $T^{2S-2S}_l(q,k)$ does not have any poles or cuts on the real q axis. Then the integration in Eq. (26) can be performed at large r [3,4,6,36] by picking up the contribution from the pole at $E_q = E_k + i\epsilon$ as[1]

$$\Psi^{lm}_{ab}(r,k) \simeq \frac{4\pi}{(2\pi)^3E_kZ_k}\left[j_l(kr) - \frac{kE_k}{8}\left[n_l(kr) + ij_l(kr)\right]T^{2-2}_l(k,k)\right], \tag{28}$$

where the contributions from the singularities in the upper half-plane become exponentially small in the asymptotically large r region [36]. Using the relation between the T-matrix and the phase of the S-matrix in Appendix A, $\Psi^{lm}_{ab}(r,k)$ is expressed as

$$\Psi^{lm}_{ab}(r,k) \simeq \frac{4\pi}{(2\pi)^3E_kZ_k}\left[j_l(kr) + \left[n_l(kr) + ij_l(kr)\right]e^{i\delta^{2-2}_l(k)}\sin\delta^{2-2}_l(k).\right]$$

$$\simeq \frac{4\pi}{(2\pi)^3E_kZ_k}\frac{e^{i\delta^{2-2}_l(k)}}{kr}\sin\left(kr - l\pi/2 + \delta^{2-2}_l(k)\right), \tag{29}$$

[1] The condition for $T^{2S-2S}_l(q,k)$ at $q = 0$ assumed in Refs. [3,36] is found to be unnecessary.

which shows that the NBS wave function encodes the information of the scattering phase shift in its asymptotic behavior as if it were the wave function of quantum mechanics [3,4,36], so that the potential defined from the NBS wave functions can reproduce the scattering phases shift of QCD [6,7,9] even if the bound state exists in this channel.

The integral in Eq. (27), on the other hand, is evaluated at large r as

$$\Psi_{ab}^{B,00}(r) \simeq \frac{-T_0^{2-1}(iE_B)}{16\pi^2 Z_{iE_B}} \frac{e^{-\kappa_B r}}{r} + \text{other exponentially damping contributions,} \tag{30}$$

with $\kappa_B = \sqrt{m^2 - m_B^2/4}$. In the above, other exponentially damping contributions come from poles or cuts in $Z_q E_q$ or the half off-shell T-matrix $T_0^{2-1}(q)$ in the upper half-plane of the complex q, which are expected to be of the order of the typical mass scale of the system such as m. Therefore, $\Psi_{ab}^{B,00}(r)$ is dominated by the first term as long as κ_B is smaller than the typical mass scale, which is Λ_{QCD} or m_π in the case of QCD. Therefore, the potential constructed from the NBS wave functions including $\Psi_{ab}^{B,00}(r)$ can reproduce the binding energy of the bound state. This result ensures that the time-dependent HAL QCD method [38] works to extract the potential correctly from the correlation function, $\langle 0|\phi_a(\mathbf{x}_a,t)\phi_b(\mathbf{x}_b,t)\overline{\mathcal{J}}(0)|0\rangle$ with a source operator $\overline{\mathcal{J}}(0)$, which couples to the bound state together with scattering states. This is the main result of this paper.

4. Lippmann–Schwinger equation in the non-relativistic three-body scalar system with a bound state in a two-body subsystem

As an extension of the analysis in the previous sections, we consider the system of three complex scalar fields ϕ_i $(i = a, b, c)$ with the same mass m, where the interaction between ϕ_a and ϕ_b leads to one bound state denoted by ϕ_B with a mass $m_B(< 2m)$, and the other two-body interactions do not lead to any other bound states. We examine how interactions between the fundamental scalar particles and the bound particle are encoded in their NBS wave functions.

In this and the following sections, we consider

$$\left|\mathbf{k}^a, \mathbf{k}^b, \mathbf{k}^c\right\rangle_0 = a_a^\dagger(\mathbf{k}^a) a_b^\dagger(\mathbf{k}^b) a_c^\dagger(\mathbf{k}^c)|0\rangle_0, \quad \left|\mathbf{k}^c, \mathbf{k}^B\right\rangle_0 = a_c^\dagger(\mathbf{k}^c) a_B^\dagger(\mathbf{k}^B)|0\rangle_0, \tag{31}$$

which are eigenstates of the free Hamiltonian H_0 coupled with each other by the interaction, where the corresponding energies are given by

$$\begin{aligned} E_{\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^c} &= \sqrt{(k^a)^2 + m^2} + \sqrt{(k^b)^2 + m^2} + \sqrt{(k^c)^2 + m^2}, \\ E_{\mathbf{k}^c,\mathbf{k}^B} &= \sqrt{(k^c)^2 + m^2} + \sqrt{(k^B)^2 + m_B^2}. \end{aligned} \tag{32}$$

As before, the scalar fields in the Heisenberg representation at $t = 0$ can be expressed in terms of the creation and annihilation operators as

$$\phi_i(\mathbf{x}_i, 0) = \int \frac{d^3 k_i}{\sqrt{(2\pi)^3 2E_{\mathbf{k}^i}}} \left[a_i(\mathbf{k}_i) e^{i\mathbf{k}_i\cdot\mathbf{x}_i} + b_i^\dagger(\mathbf{k}_i) e^{-i\mathbf{k}_i\cdot\mathbf{x}_i}\right], \qquad i = a, b, c, B. \tag{33}$$

For the three-body system, it is convenient to introduce the modified Jacobi coordinates [9] as

$$\tilde{x}_i = \sqrt{\frac{i}{i+1}}\mathbf{x}_i^J, \;\; \tilde{\mathbf{k}}_i = \sqrt{\frac{i+1}{i}}\mathbf{k}_i^J \;\; (i = 1, 2), \tag{34}$$

where $\mathbf{x}_i^J$ and $\mathbf{k}_i^J$ are the standard Jacobi coordinates,

$$\mathbf{x}_1^J = \mathbf{x}_1 - \mathbf{x}_2,\ \mathbf{x}_2^J = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2) - \mathbf{x}_3,\ \mathbf{x}_3^J = \frac{1}{3}(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3),$$
$$\mathbf{k}_1^J = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2),\ \mathbf{k}_2^J = \frac{2}{3}\left\{\frac{1}{2}(\mathbf{k}_1 + \mathbf{k}_2) - \mathbf{k}_3\right\},\ \mathbf{k}_3^J = \mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3. \tag{35}$$

In the center-of-mass frame, we have

$$\sum_{i=1}^{3} \mathbf{k}_i \cdot \mathbf{x}_i = \sum_{i=1}^{2} \tilde{\mathbf{k}}_i \cdot \tilde{\mathbf{x}}_i,\ \ E_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \simeq 3m + \sum_{i=1}^{3} \frac{\mathbf{k}_i^2}{2m} = 3m + \frac{1}{2m}\sum_{i=1}^{2} (\tilde{\mathbf{k}}_i)^2 \equiv E_{\tilde{\mathbf{k}}_1,\tilde{\mathbf{k}}_2}, \tag{36}$$

where the non-relativistic approximation is used for the energy. In these coordinates, the three-body non-interacting state and in-state in the center-of-mass frame can be parametrized as

$$\left|\mathbf{k}^a, \mathbf{k}^b, \mathbf{k}^c\right\rangle_{0,\mathrm{in}} = |\tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b\ \rangle_{0,\mathrm{in}}. \tag{37}$$

The Lippmann–Schwinger equations in the center-of-mass frame for $\left|\tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b\right\rangle_{\mathrm{in}}$ and $\left|\mathbf{k}^c, \mathbf{k}^B = -\mathbf{k}^c\right\rangle_{\mathrm{in}}$ are given within the non-relativistic approximation as

$$|\tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b\ \rangle_{\mathrm{in}} \simeq |\tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b\ \rangle_0 + \frac{1}{2\pi}\frac{1}{3^{3/2}}\int d^3\tilde{q}^a d^3\tilde{q}^b \frac{\left|\tilde{\mathbf{q}}^a, \tilde{\mathbf{q}}^b\right\rangle_0 T_{3-3}(\tilde{\mathbf{q}}^a, \tilde{\mathbf{q}}^b; \tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b)}{E_{\tilde{\mathbf{k}}^a,\tilde{\mathbf{k}}^b} - E_{\tilde{\mathbf{q}}^a,\tilde{\mathbf{q}}^b} + i\epsilon}$$
$$+ \frac{1}{2\pi}\int d^3q^c \frac{\left|\mathbf{q}^c, \mathbf{q}^B = -\mathbf{q}^c\right\rangle_0 T_{2-3}(\mathbf{q}^c; \tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b)}{E_{\tilde{\mathbf{k}}^a,\tilde{\mathbf{k}}^b} - E^B_{\mathbf{q}^c} + i\epsilon}, \tag{38}$$

$$\left|\mathbf{k}^c, \mathbf{k}^B = -\mathbf{k}^c\right\rangle_{\mathrm{in}} \simeq \left|\mathbf{k}^c, \mathbf{k}^B = -\mathbf{k}^c\right\rangle_0 + \frac{1}{2\pi}\int d^3q^c \frac{\left|\mathbf{q}^c, \mathbf{q}^B = -\mathbf{q}^c\right\rangle_0 T_{2-2}(\mathbf{q}^c; \mathbf{k}^c)}{E^B_{\mathbf{k}^c} - E^B_{\mathbf{q}^c} + i\epsilon}$$
$$+ \frac{1}{2\pi}\frac{1}{3^{3/2}}\int d^3\tilde{q}^a d^3\tilde{q}^b \frac{\left|\tilde{\mathbf{q}}^a, \tilde{\mathbf{q}}^b\right\rangle_0 T_{3-2}(\tilde{\mathbf{q}}^a, \tilde{\mathbf{q}}^b; \mathbf{k}^c)}{E^B_{\mathbf{k}^c} - E_{\tilde{\mathbf{q}}^a,\tilde{\mathbf{q}}^b} + i\epsilon}, \tag{39}$$

where $E^B_{\mathbf{k}^c} \simeq m_B + m + \frac{(\mathbf{k}^c)^2}{2m_{\mathrm{red}}}$ with $1/m_{\mathrm{red}} = 1/m + 1/m_B$, and

$$T_{\mathbf{q}^a,\mathbf{q}^b,\mathbf{q}^c;\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^c} = \delta(\mathbf{q}^a + \mathbf{q}^b + \mathbf{q}^c) T_{3-3}(\tilde{\mathbf{q}}^a, \tilde{\mathbf{q}}^b; \tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b), \tag{40}$$
$$T_{\mathbf{q}^c\mathbf{q}^B;\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^c} = \delta(\mathbf{q}^c + \mathbf{q}^B) T_{2-3}(\mathbf{q}^c; \tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b), \tag{41}$$
$$T_{\mathbf{q}^c\mathbf{q}^B;\mathbf{k}^c,\mathbf{k}^B} = \delta(\mathbf{q}^c + \mathbf{q}^B) T_{2-2}(\mathbf{q}^c; \mathbf{k}^c), \tag{42}$$
$$T_{\mathbf{q}^a,\mathbf{q}^b,\mathbf{q}^c;\mathbf{k}^c,\mathbf{k}^B} = \delta(\mathbf{q}^a + \mathbf{q}^b + \mathbf{q}^c) T_{3-2}(\tilde{\mathbf{q}}^a, \tilde{\mathbf{q}}^b; \mathbf{k}^c). \tag{43}$$

For later convenience, by arranging the momenta as $\mathbf{Q}_2 = \mathbf{q}^c$, $\mathbf{K}_2 = \mathbf{k}^c$, $\mathbf{Q}_3 = (\tilde{\mathbf{q}}^a, \tilde{\mathbf{q}}^b)$, and $\mathbf{K}_3 = (\tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b)$, we rewrite the above coupled channel T-matrix (or S-matrix) compactly as $T_{l-m}(\mathbf{Q}_l; \mathbf{K}_m)$ (or $S_{l-m}(\mathbf{Q}_l; \mathbf{K}_m)$) with $l, m = 2, 3$.

5. Asymptotic behaviors of NBS wave functions for three-body non-relativistic scalar system with a bound state

The NBS wave functions in the coupled channel are compactly written as

$$\Psi(\mathbf{X}_l|\mathbf{K}_m) = {}_{\mathrm{in}}\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{K}_m\rangle_{\mathrm{in}}, \tag{44}$$

where $\mathbf{X}_2 \equiv \mathbf{x}_c - \mathbf{x}_B$, $\mathbf{X}_3 \equiv (\tilde{\mathbf{x}}_a, \tilde{\mathbf{x}}_b)$, and

$$\Phi_2(\mathbf{x}_2) \equiv \phi_c(\mathbf{x}_c, 0)\phi_B(\mathbf{x}_B, 0), \quad \Phi_3(\mathbf{x}_3) \equiv \phi_a(\mathbf{x}_a, 0)\phi_b(\mathbf{x}_b, 0)\phi_c(\mathbf{x}_c, 0),$$
$$|\mathbf{K}_2\rangle_{\text{in}} = |\mathbf{k}^c, \mathbf{k}^B = -\mathbf{k}^c\rangle_{\text{in}}, \qquad |\mathbf{K}_3\rangle_{\text{in}} = |\tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b\rangle_{\text{in}}. \tag{45}$$

By using the Lippmann–Schwinger equation given in Eqs. (38) and (39), the NBS wave functions within the non-relativistic approximation can be written as

$$\Psi(\mathbf{X}_l|\mathbf{K}_m) = {}_{\text{in}}\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{K}_m\rangle_0 + \frac{1}{2\pi}\sum_{n=2,3}\int [d\mathbf{P}]_n \frac{{}_{\text{in}}\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{P}_n\rangle_0 T_{n-m}(\mathbf{P}_n; \mathbf{K}_m)}{E_{K_m} - E_{P_n} + i\epsilon}, \tag{46}$$

where

$$[d\mathbf{P}]_n \equiv 3^{(6-3n)/2} d^{(3n-3)}\mathbf{P}_n = 3^{(6-3n)/2} P_n^{3n-4} dP_n\, d\Omega_{\mathbf{P}_n}, \quad P_n = |\mathbf{P}_n|, \tag{47}$$

$$E_{P_2} = m_B + m + \frac{P_2^2}{2m_{\text{red}}}, \quad E_{P_3} = 3m + \frac{P_3^2}{2m}. \tag{48}$$

As shown in Appendix B, we have

$${}_{\text{in}}\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{K}_m\rangle_0 \simeq \delta_{lm} D_l(\mathbf{K}_l) e^{i\mathbf{K}_l\cdot\mathbf{X}_l} + \delta_{l2}\delta_{m3} D_{23}(\mathbf{K}_3) e^{i\mathbf{K}_2\cdot\mathbf{X}_2} \tag{49}$$

in the asymptotic region, $|\mathbf{x}_i - \mathbf{x}_j| \gg 1$ for $i, j = a, b, c$ or $|\mathbf{x}_c - \mathbf{x}_B| \gg 1$, where

$$D_2(\mathbf{K}_2) = \frac{1}{Z_B(\mathbf{k}^c)(2\pi)^3\sqrt{E_{\mathbf{k}^c}E^B_{\mathbf{k}^c}}}, \quad D_3(\mathbf{K}_3) = \frac{1}{Z(\tilde{\mathbf{k}}^a, \tilde{\mathbf{k}}^b)}\prod_{j=a,b,c}\frac{1}{\sqrt{(2\pi)^3 2E_{\mathbf{k}^j}}},$$

$$D_{23}(\mathbf{K}_3) = \frac{1}{2\pi}\frac{T^\dagger_{0-ab\bar{B}}(0; \mathbf{k}^a, \mathbf{k}^b, \mathbf{k}^c)}{(2\pi)^3(4E_{\mathbf{k}^c}E^B_{\mathbf{k}^c})^{1/2}(-E_{\mathbf{k}^a,\mathbf{k}^b,\mathbf{q}^B=\mathbf{k}^c})},$$

$$E_{\mathbf{k}} \simeq m + \frac{\mathbf{k}^2}{2m}, \quad E^B_{\mathbf{k}} \simeq m_B + \frac{\mathbf{k}^2}{2m_B},$$

$$\mathbf{K}_2 \cdot \mathbf{X}_2 = \mathbf{k}_c \cdot (\mathbf{x}_c - \mathbf{x}_B), \quad \mathbf{K}_3 \cdot \mathbf{X}_3 = \tilde{\mathbf{k}}_a \cdot \tilde{\mathbf{x}}_a + \tilde{\mathbf{k}}_b \cdot \tilde{\mathbf{x}}_b.$$

Thus the asymptotic behaviors of NBS wave functions reduce to

$$\Psi(\mathbf{X}_l|\mathbf{K}_m) \simeq D_l(\mathbf{K}_l)\left[\delta_{lm}e^{i\mathbf{K}_l\cdot\mathbf{X}_l} + \frac{1}{2\pi}\int [d\mathbf{P}]_l \frac{D_l(\mathbf{P}_l)}{D_l(\mathbf{K}_l)}\frac{e^{i\mathbf{P}_l\cdot\mathbf{X}_l}T_{l-m}(\mathbf{P}_l; \mathbf{K}_m)}{E_{K_m} - E_{P_l} + i\epsilon}\right]$$
$$+ D_{23}(\mathbf{K}_3)\delta_{l2}\left[\delta_{m3}e^{i\mathbf{K}_2\cdot\mathbf{X}_2} + \frac{1}{2\pi}\int [d\mathbf{P}]_3 \frac{D_{23}(\mathbf{P}_3)}{D_{23}(\mathbf{K}_3)}\frac{e^{i\mathbf{P}_2\cdot\mathbf{X}_2}T_{3-m}(\mathbf{P}_3; \mathbf{K}_m)}{E_{K_m} - E_{P_3} + i\epsilon}\right]. \tag{50}$$

Note that the third and fourth terms appear due to the transition from vacuum to the state with anti-bound particle and the a- and b-particles. They do not appear in the coupled channel three-body system in the absence of bound states, as was studied in Ref. [9]. We introduce the hyperspherical expansion as

$$e^{i\mathbf{K}_l\cdot\mathbf{X}_l} = d_{3l-3}\sum_{[L]_l} i^L j_L^{3l-3}(K_l X_l) Y_{[L]_l}(\Omega_{\mathbf{X}_l}) Y^*_{[L]_l}(\Omega_{\mathbf{K}_l}), \tag{51}$$

$$T_{l-m}(\mathbf{P}_l; \mathbf{K}_m) = \sum_{[L]_l, [M]_m} T^{l-m}_{[L]_l, [M]_m}(P_l, K_m) Y_{[L]_l}(\Omega_{\mathbf{P}_l}) Y^*_{[M]_m}(\Omega_{\mathbf{K}_m}), \tag{52}$$

$$\Psi(\mathbf{X}_l|\mathbf{K}_m) = \sum_{[L]_l,[M]_m} \Psi_{[L]_l,[M]_m}(X_l, K_m) Y_{[L]_l}(\Omega_{\mathbf{X}_l}) Y^*_{[M]_m}(\Omega_{\mathbf{K}_m}), \tag{53}$$

where $X_l = |\mathbf{X}_l|$,

$$d_D = (D-2)!! \frac{2\pi^{D/2}}{\Gamma\left(\frac{D}{2}\right)}, \tag{54}$$

and j_L^D is the hyperspherical Bessel function of the first kind, defined by

$$j_L^D(x) = \frac{\Gamma\left(\frac{D-2}{2}\right) 2^{\frac{D-4}{2}}}{(D-4)!! x^{\frac{D-2}{2}}} J_{L_D}(x), \tag{55}$$

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

$$j_L^3(x) \equiv \sqrt{\frac{\pi}{2x}} J_{L+1/2}(x) = j_L(x), \quad j_L^6(x) \equiv \frac{J_{L+2}(x)}{x^2}, \tag{56}$$

where $j_L(x)$ is the spherical Bessel function of the first kind. Here, $Y_{[L]_l}$ is the $3l-3$-dimensional hyperspherical harmonic function, which satisfies

$$\int d\Omega\, Y_{[L]_l}(\Omega) Y^*_{[M]_l}(\Omega) = \delta_{[L]_l,[M]_l}, \tag{57}$$

and $Y_{[L]_2}$ corresponds to the spherical harmonic function Y_{lm}. Within the non-relativistic approximation, we can write $D_l(\mathbf{K}_l)$ and $D_{23}(\mathbf{K}_3)$ as $D_l(\mathbf{K}_l) \simeq D_l(K_l)$, $D_{23}(\mathbf{K}_3) \simeq D^2_{23}(K_2) D^3_{23}(K_3)$ with $K_l = |\mathbf{K}_l|$.

The integration over $d\Omega_{\mathbf{P}_l}$ gives

$$\begin{aligned}\Psi_{[L]_l,[M]_m}(X_l, K_m) = d_{3l-3} i^L D_l(K_l) \Bigg[& j_L^{3l-3}(K_l X_l) \delta_{[L]_l,[M]_l} \delta_{lm} \\ & + \frac{3^{(6-3l)/2}}{2\pi} \int dP_l P_l^{3l-4} \frac{D_l(P_l)}{D_l(K_l)} \frac{j_L^{3l-3}(P_l X_l) T^{l-m}_{[L]_l,[M]_m}(P_l, K_m)}{E_{K_m} - E_{P_l} + i\epsilon} \Bigg] \\ & + d_3 i^L \delta_{l2} D^3_{23}(K_3) \Bigg[\delta_{m3} J_{[L]_2[M]_3}(K_3, X_2) \\ & + \frac{3^{-3/2}}{2\pi} \int dP_3 P_3^5 \frac{D^3_{23}(P_3)}{D^3_{23}(K_3)} \frac{\sum_{[N]_3} J_{[L]_2[N]_3}(P_3, X_2) T^{3-m}_{[N]_3,[M]_m}(P_3, K_m)}{E_{K_m} - E_{P_3} + i\epsilon} \Bigg], \end{aligned} \tag{58}$$

where

$$J_{[L]_2[M]_3}(K_3, X_2) = \int d\Omega_{\mathbf{K}_3} D^2_{23}(K_2) j_L^3(K_2 X_2) Y_{[M]_3}(\Omega_{\mathbf{K}_3}) Y^*_{[L]_2}(\Omega_{\mathbf{K}_2}). \tag{59}$$

In the nonrelativistic expansion, $D_{23}(\mathbf{K}_3)$ starts from $O\left(T^\dagger_{0-ab\bar{B}}/(m^{3/2} m_B^{1/2})\right)$, while $D_2(\mathbf{K}_2)$ starts from $O(1/m)$. Assuming that $T^\dagger_{0-ab\bar{B}} \simeq O(1)$, we therefore drop the third and fourth terms in our analysis hereafter.

The integration over P_l for the large X_l in the second term can be performed by picking up the poles inside the closed contour in a complex plane, as has been done in Ref. [9],

$$\Psi_{[L]_l,[M]_m}(X_l,K_m) \simeq i^L D_l(K_l)\frac{(2\pi)^{\frac{3l-3}{2}}}{(K_lX_l)^{\frac{3l-5}{2}}}\Bigg[J_{L_{3l-3}}(K_lX_l)\delta_{[L]_l,[M]_l}\delta_{l,m}$$
$$- \frac{1}{2}\frac{K_l^{3l-5}m_l}{3^{(3l-6)/2}}\left[N_{L_{3l-3}}(K_lX_l)+iJ_{L_{3l-3}}(K_lX_l)\right]T^{l-m}_{[L]_l,[M]_m}(K_l,K_m)\Bigg], \quad (60)$$

where K_l and K_m satisfy $E_{K_l} = E_{K_m} = E$ for a given total energy E, and $N_L(x)$ is the Bessel function of the second kind. Explicitly, K_2 and K_3 are written as $K_2 = \sqrt{2m_{\rm red}(E - m_B - m)}$ and $K_3 = \sqrt{2m(E-3m)}$.

Using the parametrization of the T-matrix derived in Appendix A as

$$T_{[L]_l,[M]_m}(K_l,K_m)$$
$$= -2C_l(E)\left\{\sum_{[N]_n} U_{[L]_l,[N]_n}(E)e^{i\delta_{[N]_n}(E)}\sin(\delta_{[N]_n}(E))U^\dagger_{[N]_n,[M]_m}(E)\right\}C_m(E) \quad (61)$$

with

$$C_l(E) = \sqrt{\frac{3^{(3l-6)/2}}{m_l(K_l)^{3l-5}}}, \quad (62)$$

and the asymptotic behaviors of $J_L(x)$ and $N_L(x)$ for large $|x|$ as

$$J_L(x) \simeq \sqrt{\frac{2}{\pi x}}\sin(x-\Delta_L), \quad N_L(x) \simeq \sqrt{\frac{2}{\pi x}}\cos(x-\Delta_L), \qquad \Delta_L = \frac{2L-1}{2}\pi, \quad (63)$$

we obtain the asymptotic forms related to the phase shifts as

$$\Psi_{[L]_l,[M]_m}(X_l,K_m) \simeq 2i^L D_l(K_l)\left(\frac{2\pi}{K_lX_l}\right)^{\frac{3l-4}{2}}\frac{C_m(E)}{C_l(E)}\sum_{[N]_n}U_{[L]_l,[N]_n}(E)e^{i\delta_{[N]_n}(E)}U^\dagger_{[N]_n,[M]_m}(E)$$
$$\times \sin(K_lX_l - \Delta_{L_{3l-3}} + \delta_{[N]_n}(E)) \quad (64)$$

for $l, m = 2$ (B, c) and $l, m = 3$ (a, b, c). The final result agrees with the one obtained in the absence of bound states [9].

6. Summary and concluding remarks

In this paper we have investigated the asymptotic behaviors of the NBS wave functions in complex scalar systems in the presence of a bound state. We include a bound state in the asymptotic states of the theory and consider a coupled system of two scattering particles and one bound state. We have shown that the asymptotic form for the NBS wave function of the scattering state is related to the phase shifts of the S-matrix via its unitary, while the asymptotic form for the NBS function of the bound state decays exponentially with its binding energy as long as the binding energy is smaller than other mass scales such as the mass of the scattering particle. This result establishes that the potential extracted via the time-dependent HAL QCD method [38] from the four-point correlation functions, which couple to the bound state as well as scattering states, can correctly reproduce both binding energy and scattering phase shift. This is the main result of this paper.

As an extension of our analysis, we have considered the three complex scalar systems, two of which can form a bound state. In addition to the the elastic scattering of the three-particles, three particles are scattered into one fundamental particle plus one bound state and vice versa. Although the analysis becomes rather involved in this case, the final result in the non-relativistic limit becomes almost identical to the one for the coupled two- and three-particle systems in Ref. [9].

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Appendix A. On-shell T-matrix and its parametrization

In this appendix, we parametrize the T-matrix, where $S = 1 - iT$, using the unitarity of the S-matrix, $S^\dagger S = 1$. We first discuss a simple two-body system and then consider a three-body system with a bound state.

A.1. Two-body case

In the center-of-mass frame such that $\mathbf{k}^a = -\mathbf{k}^b = \mathbf{k}$, the S-matrix is denoted as

$$ {}_0\left\langle \mathbf{q}^a, \mathbf{q}^b \middle| S \middle| \mathbf{k}^a = \mathbf{k}, \mathbf{k}^b = -\mathbf{k} \right\rangle_0 = \delta(E_q - E_k)\delta^{(3)}(\mathbf{q}^a + \mathbf{q}^b) S_{2-2}(\mathbf{q}; \mathbf{k}), \tag{A1} $$

where $\mathbf{q}^a = -\mathbf{q}^b = \mathbf{q}$, $E_q = 2\sqrt{q^2 + m^2}$, and $E_k = 2\sqrt{k^2 + m^2}$ with $q = |\mathbf{q}|$ and $k = |\mathbf{k}|$.

The unitarity of the S-matrix reads

$$ \delta(E_q - E_k) \int d^3p\, \delta(E_p - E_k) S_{2-2}(\mathbf{q}; \mathbf{p}) S^\dagger_{2-2}(\mathbf{p}; \mathbf{k}) = \delta^{(3)}(\mathbf{q} - \mathbf{k}). \tag{A2} $$

Introducing expansions in terms of the spherical harmonic functions as

$$ S_{2-2}(\mathbf{q}; \mathbf{p}) = \sum_{l,m} S_l^{2-2}(q; p) Y_{lm}(\Omega_{\mathbf{q}}) Y^*_{lm}(\Omega_{\mathbf{p}}), \tag{A3} $$

$$ \delta^{(3)}(\mathbf{q} - \mathbf{k}) = \sum_{l,m} \frac{1}{q^2} \delta(q - k) Y_{lm}(\Omega_{\mathbf{q}}) Y^*_{lm}(\Omega_{\mathbf{k}}), \tag{A4} $$

and

$$ \delta(E_p - E_k) = \frac{E_q}{4q} \delta(q - k), \qquad d^3p = p^2 dp d\Omega_{\mathbf{p}}, \tag{A5} $$

we obtain

$$ \left| S_l^{2-2}(q, q) \right|^2 = \frac{16}{q^2 E_q^2}, \tag{A6} $$

which is solved as

$$ S_l^{2-2}(q, q) = \frac{4e^{2i\delta_l^{2-2}(q)}}{qE_q}, \tag{A7} $$

with the phase shift $\delta_l^{2-2}(q)$. Thus, the T-matrix, defined from the S-matrix as $\delta(E_q - E_k) S_{2-2}(\mathbf{q};\mathbf{k}) = \delta(\mathbf{q}-\mathbf{k}) - i\delta(E_q - E_k) T_{2-2}(\mathbf{q};\mathbf{k})$, is expressed as

$$T_{2-2}(\mathbf{q};\mathbf{k}) = \sum_{l,m} T_l^{2-2}(q,q) Y_{lm}(\Omega_{\mathbf{q}}) Y_{lm}^*(\Omega_{\mathbf{k}}), \tag{A8}$$

where

$$T_l^{2-2}(q,q) = -\frac{8}{qE_q} e^{i\delta_l^{2-2}(q)} \sin \delta_l^{2-2}(q). \tag{A9}$$

A.2. Three-body case

We next consider the scattering of the three-body system, where not only the elastic scattering but also the bound particle production and its inverse process occur:

$$\phi_a + \phi_b + \phi_c \to \phi_a + \phi_b + \phi_c,\ \phi_B + \phi_c,$$
$$\phi_B + \phi_c \to \phi_a + \phi_b + \phi_c,\ \phi_B + \phi_c.$$

Denoting the corresponding S-matrix as $S_{l-m}(\mathbf{Q}_l;\mathbf{K}_m)$, as for the T-matrix in the main text, the unitarity condition is expressed as

$$\begin{aligned}
&\delta(E_{Q_l} - E_{K_m}) \sum_{n=2,3} \int d\mathbf{P}_n \delta(E_{Q_l} - E_{P_n}) S(\mathbf{Q}_l, \mathbf{P}_n) S^\dagger(\mathbf{P}_n, \mathbf{K}_m) \\
&= \delta_{l,m} 3^{(3l-6)/2} \delta^{(3l-3)}(\mathbf{Q}_l - \mathbf{K}_l),
\end{aligned} \tag{A10}$$

where $l, n, m = 2, 3$ represent a number of particles involved in the state,

$$\mathbf{P}_2 = \mathbf{p}, \quad \mathbf{P}_3 = \tilde{\mathbf{P}}, \quad E_{P_2} = m_B + m + \frac{P_2^2}{2m_{\rm red}}, \quad E_{P_3} = 3m + \frac{P_3^2}{2m}, \tag{A11}$$

$$d\mathbf{P}_n = 3^{(3n-6)/2} d^{(3n-3)}\mathbf{P}_n = 3^{(3n-6)/2} (P_n)^{3n-4} dP_n d\Omega_{\mathbf{P}_n}, \quad P_n = |\mathbf{P}_n|. \tag{A12}$$

Introducing the hyperspherical expansion as [9]

$$S(\mathbf{Q}_l;\mathbf{K}_m) = \sum_{[L]_l,[M]_m} S_{[L]_l,[M]_m}(Q_l, K_m) Y_{[L]_l}(\Omega_{\mathbf{Q}_l}) Y_{[M]_m}^*(\Omega_{\mathbf{K}_m}), \tag{A13}$$

$$\delta^{(3l-3)}(\mathbf{Q}_l - \mathbf{K}_l) = \sum_{[L]_l} \frac{\delta(Q_l - K_l)}{Q^{3l-4}} Y_{[L]_l}(\Omega_{\mathbf{Q}_l}) Y_{[L]_l}^*(\Omega_{\mathbf{K}_l}), \tag{A14}$$

and using

$$\delta(E_{Q_l} - E) = \frac{m_l}{Q_l} \delta(Q_l - Q_l(E)), \tag{A15}$$

where $m_2 = m_{\rm red}$, $m_3 = m$, and $Q_l(E)$ is a solution of $E_{Q_l} = E$, the unitarity condition for a total energy E reads

$$\begin{aligned}
&C_l(E)^{-1} \sum_{[N]_n} S_{[L]_l,[N]_n}(Q_l(E), Q_n(E))\, C_n(E)^{-1} \\
&\times C_n(E)^{-1} \overline{S_{[M]_m,[N]_n}(Q_m(E), Q_n(E))}\, C_m(E)^{-1} = \delta_{[L]_l,[M]_m},
\end{aligned} \tag{A16}$$

where

$$C_l(E) = \sqrt{\frac{3^{(3l-6)/2}}{m_l\{Q_l(E)\}^{3l-5}}}. \tag{A17}$$

Thus we can parametrize the above S-matrix as

$$S_{[L]_l,[M]_m}(Q_l(E), Q_m(E)) = C_l(E)\left\{\sum_{[N]_n} U_{[L]_l,[N]_n}(E)e^{i2\delta_{[N]_n}(E)}U^\dagger_{[N]_n,[M]_m}(E)\right\}C_m(E), \tag{A18}$$

where $\delta_{[N]_n}(E)$ is the (generalized) scattering phase shift for the channel $[N]_n$ at the energy E, and $U(E)$ is the unitary matrix introduced for the diagonalization.

The corresponding T-matrix is then given by

$$T_{[L]_l,[M]_m}(Q_l(E), Q_m(E)) \\ = -2C_l(E)\left\{\sum_{[N]_n} U_{[L]_l,[N]_n}(E)e^{i\delta_{[N]_n}(E)}\sin(\delta_{[N]_n}(E))U^\dagger_{[N]_n,[M]_m}(E)\right\}C_m(E). \tag{A19}$$

Appendix B. Lippmann–Schwinger equation for the vacuum in-state

Using the Lippmann–Schwinger equation for the vacuum in-state,

$$|0\rangle_{\rm in} = |0\rangle_0 + \int d\beta \frac{|\beta\rangle_0 T_{\beta;0}}{-E_\beta + i\epsilon}, \qquad E_0 = 0, \tag{B1}$$

we evaluate the vacuum contribution to the two-body and three-body NBS wave functions. Extensions to the general n-body NBS wave functions are straightforward.

B.1. Two-body case

As seen in Eqs. (16) and (17),

$$\text{(i)} \quad {}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^B = 0\right\rangle_0$$

and

$$\text{(ii)} \quad {}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^a, \mathbf{q}^b\right\rangle_0$$

appear in the two-body NBS wave function.

(i) Using the Lippmann–Schwinger equation for the vacuum in-state in Eq. (B1), we have

$${}_{\rm in}\langle 0|\, \phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^B = 0\right\rangle_0 = \frac{1}{2\pi}\int d\beta\, T^\dagger_{0;\beta} \frac{{}_0\langle \beta|\, \phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^B = 0\right\rangle_0}{-E_\beta + i\epsilon}, \tag{B2}$$

since ${}_0\langle 0|\, \phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^B = 0\right\rangle_0 = 0$ from the definition of $\phi_i(\mathbf{x},0)$ in Eq. (4). The non-zero contribution in Eq. (B2), which comes from

$${}_0\langle \beta| = {}_0\langle 0|\, b_a(\mathbf{k}^a)b_b(\mathbf{k}^b)a_B(\mathbf{k}^B), \tag{B3}$$

is evaluated as

$$
\begin{aligned}
&{}_{\rm in}\langle 0|\,\phi_a(\mathbf{x}^a,0)\phi_b(\mathbf{x}^b,0)\,\left|\mathbf{q}^B=0\right\rangle_0 \\
&= \frac{1}{2\pi}\int d^3k^B d^3k^a d^3k^b\, T^\dagger_{0;\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^B}\frac{{}_0\langle 0|\, b_a(\mathbf{k}^a)b_b(\mathbf{k}^b)a_B(\mathbf{k}^B)\phi_a(\mathbf{x}^a,0)\phi_b(\mathbf{x}^b,0)\,\left|\mathbf{q}^B=0\right\rangle_0}{-E_{\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^B}} \\
&= \int d^3k^a\,\frac{T^\dagger_{0-2}(0;\mathbf{k}^a)\,e^{-i\mathbf{k}^a\cdot(\mathbf{x}^a-\mathbf{x}^b)}}{(2\pi)^4 2E_{\mathbf{k}^a}(-2E_{\mathbf{k}^a}-m_B)},
\end{aligned}
\tag{B4}
$$

where $T^\dagger_{0-2}(0;\mathbf{k}^a)$ is defined as $T^\dagger_{0;\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^B=0}=\delta^{(3)}(\mathbf{k}^a+\mathbf{k}^b)T^\dagger_{0-2}(0;\mathbf{k}^a)$. Since the integrand in the last line does not have any poles on the real axis of $|\mathbf{k}^a|$ as in the case of Sect. 3, this contribution vanishes exponentially in large $\left|\mathbf{x}^a-\mathbf{x}^b\right|$. Note that complex poles from the denominator appear at $k^2=-m^2$ or on the unphysical sheet of k^2 which satisfies $2E_{\mathbf{k}}+m_B=0$.

(ii) In the same manner, we obtain

$$
\begin{aligned}
{}_{\rm in}\langle 0|\,\phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^a,\mathbf{q}^b\right\rangle_0 &= {}_0\langle 0|\,\phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^a,\mathbf{q}^b\right\rangle_0 \\
&\quad + \frac{1}{2\pi}\int d\beta\, T^\dagger_{0;\beta}\frac{{}_0\langle\beta|\,\phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,\left|\mathbf{q}^a,\mathbf{q}^b\right\rangle_0}{-E_\beta+i\epsilon}.
\end{aligned}
\tag{B5}
$$

As shown in Appendix A of Ref. [9], this reduces to

$$
{}_{\rm in}\langle 0|\,\phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,|\mathbf{q};-\mathbf{q}\rangle_0 \simeq \frac{1}{Z(\mathbf{q})}\,{}_0\langle 0|\,\phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\,|\mathbf{q};-\mathbf{q}\rangle_0
\tag{B6}
$$

in the center-of-mass system, where $Z(\mathbf{q})$ corresponds to the renormalization factor for the vacuum, whose explicit form can be found in Ref. [9].

B.2. Three-body case

As seen in Eq. (46), we need to evaluate ${}_{\rm in}\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{K}_m\rangle_0$. Using the Lippmann–Schwinger equation for the vacuum state, we have

$$
{}_{\rm in}\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{K}_m\rangle_0 = {}_0\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{K}_m\rangle_0\delta_{lm} + \frac{1}{2\pi}\int d\beta T^\dagger_{0;\beta}\frac{{}_0\langle\beta|\,\Phi_l(\mathbf{x}_l)\,|\mathbf{K}_m\rangle_0}{-E_\beta+i\epsilon}.
\tag{B7}
$$

We first consider the case with $l=m$, which has already been analyzed in Appendix A of Ref. [9] for $n=2$ and $n=3$, and the result is given by

$$
{}_{\rm in}\langle 0|\Phi_l(\mathbf{x}_l)|\mathbf{K}_l\rangle_0 \simeq D_l(\mathbf{K}_l)e^{i\mathbf{K}_l\cdot\mathbf{X}_l}
\tag{B8}
$$

for the asymptotic region, where

$$
D_2(\mathbf{K}_2) = \frac{1}{Z(\mathbf{k}_c)(2\pi)^3\sqrt{4E_{\mathbf{k}^c}E_{\mathbf{k}^c}}},\qquad \frac{1}{Z(\mathbf{k}_c)} = 1+\sum_{i=c,B}\frac{T^\dagger_{0;i\bar{i}}(0;\mathbf{k}_i,-\mathbf{k}_i)}{-2\sqrt{k_i^2+m_i^2}},
\tag{B9}
$$

$$
D_3(\mathbf{K}_3) = \frac{1}{Z(\tilde{\mathbf{k}}^a,\tilde{\mathbf{k}}^b)}\prod_{j=a,b,c}\frac{1}{\sqrt{(2\pi)^3 2E_{\mathbf{k}^j}}},\qquad \frac{1}{Z(\tilde{\mathbf{k}}^a,\tilde{\mathbf{k}}^b)} = 1+\sum_{i=a,b,c}\frac{T^\dagger_{0;i\bar{i}}(0;\mathbf{k}_i,-\mathbf{k}_i)}{-2\sqrt{k_i^2+m_i^2}}.
\tag{B10}
$$

Here, $m_{a,b,c}=m$, $\mathbf{k}_c+\mathbf{k}_B=0$ ($\mathbf{k}_b+\mathbf{k}_b+\mathbf{k}_c=0$) for D_2 (D_3), and $T_{0;i\bar{i}}$ is the off-shell T-matrix from vacuum to a particle–antiparticle pair with a flavor i.

We consider other cases with $l \neq m$.

(i) $l = 3$ and $m = 2$. Non-zero contributions to ${}_0\langle\beta|\,\phi_a(\mathbf{x_a},0)\phi_b(\mathbf{x_b},0)\phi_c(\mathbf{x_c},0)\,\left|\mathbf{k}^c,\mathbf{k}^B\right\rangle_0$ come from

$$ {}_0\langle\beta| = {}_0\langle 0|\,a_B(\mathbf{q}^B)b_a(\mathbf{q}^{\bar{a}})b_b(\mathbf{q}^{\bar{b}}) \;\text{ or }\; {}_0\langle 0|\,a_c(\mathbf{q}^c)a_B(\mathbf{q}^B)b_a(\mathbf{q}^{\bar{a}})b_b(\mathbf{q}^{\bar{b}})b_c(\mathbf{q}^{\bar{c}}). \tag{B11}$$

Equation (B7) thus reduces to

$$ \begin{aligned} &{}_{\text{in}}\langle 0|\Phi_l(\mathbf{x}_3)|\mathbf{K}_2\rangle_0 \\ &= \frac{1}{2\pi}\int d^3q^{\bar{a}}\frac{T^\dagger_{0-\bar{a}\bar{b}B}(0;\mathbf{q}^{\bar{a}},\mathbf{k}^c-\mathbf{q}^{\bar{a}},\mathbf{k}^B)e^{i\mathbf{q}^{\bar{a}}\cdot(\mathbf{x}_b-\mathbf{x}_a)}e^{i\mathbf{k}^c\cdot(\mathbf{x}_c-\mathbf{x}_b)}}{\{(2\pi)^3\}^{3/2}(8E_{\mathbf{q}^{\bar{a}}}E_{\mathbf{k}^c-\mathbf{q}^{\bar{a}}}E_{\mathbf{k}^c})^{1/2}(-E_{\mathbf{q}^{\bar{a}},\mathbf{k}^c-\mathbf{q}^{\bar{a}},\mathbf{k}^B})} \\ &+\frac{1}{2\pi}\int d^3q^{\bar{a}}d^3q^{\bar{b}}\frac{T^\dagger_{0-\bar{a}\bar{b}\bar{c}cB}(0;\mathbf{q}^{\bar{a}},\mathbf{q}^{\bar{b}},-\mathbf{q}^{\bar{a}}-\mathbf{q}^{\bar{b}},\mathbf{k}^c,\mathbf{k}^B)e^{i\mathbf{q}^{\bar{a}}\cdot(\mathbf{x}_c-\mathbf{x}_a)}e^{i\mathbf{q}^{\bar{b}}\cdot(\mathbf{x}_c-\mathbf{x}_b)}}{\{(2\pi)^3\}^{3/2}(8E_{\mathbf{q}^{\bar{a}}}E_{\mathbf{q}^{\bar{b}}}E_{\mathbf{q}^{\bar{a}}+\mathbf{q}^{\bar{b}}})^{1/2}(-E_{\mathbf{q}^{\bar{a}},\mathbf{q}^{\bar{b}},-\mathbf{q}^{\bar{a}}-\mathbf{q}^{\bar{b}},\mathbf{k}^c,\mathbf{k}^B})} \end{aligned} \tag{B12}$$

for $\mathbf{k}^c = -\mathbf{k}^B$. Since both integrands have no poles for real momenta $\mathbf{q}^{\bar{a}}$ and/or $\mathbf{q}^{\bar{b}}$, these terms vanish for asymptotically large $|\mathbf{x}_a-\mathbf{x}_b|$, $|\mathbf{x}_a-\mathbf{x}_c|$, and $|\mathbf{x}_c-\mathbf{x}_b|$.

(ii) $l = 2$ and $m = 3$. Non-zero contributions to ${}_0\langle\beta|\,\phi_c(\mathbf{x}_c,0)\phi_B(\mathbf{x}_B,0)\,\left|\tilde{\mathbf{k}}^a,\tilde{\mathbf{k}}^b\right\rangle_0$ come from

$$ {}_0\langle\beta| = {}_0\langle 0|\,b_B(\mathbf{q}^{\bar{B}})a_a(\mathbf{q}^a)a_b(\mathbf{q}^b) \;\text{ or }\; {}_0\langle 0|\,b_{\bar{c}}(\mathbf{q}^{\bar{c}})b_B(\mathbf{q}^{\bar{B}})a_a(\mathbf{q}^a)a_b(\mathbf{q}^b)a_c(\mathbf{q}^c). \tag{B13}$$

Equation (B7) thus becomes

$$ \begin{aligned} &{}_{\text{in}}\langle 0|\Phi_l(\mathbf{x}_2)|\mathbf{K}_3\rangle_0 \\ &= \frac{1}{2\pi}\frac{T^\dagger_{0-ab\bar{B}}(0;\mathbf{k}^a,\mathbf{k}^b,\mathbf{q}^{\bar{B}}=\mathbf{k}^c)e^{i\mathbf{k}^c\cdot(\mathbf{x}_c-\mathbf{x}_B)}}{(2\pi)^3(4E_{\mathbf{k}^c}E^B_{\mathbf{k}^B})^{1/2}(-E_{\mathbf{k}^a,\mathbf{k}^b,\mathbf{q}^{\bar{B}}=\mathbf{k}^c})} \\ &+\frac{1}{2\pi}\int d^3q^{\bar{c}}\frac{T^\dagger_{0-abc\bar{c}\bar{B}}(0;\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^c,\mathbf{q}^{\bar{c}},\mathbf{q}^{\bar{B}}=\mathbf{q}^{\bar{c}})e^{i\mathbf{q}^{\bar{c}}\cdot(\mathbf{x}_B-\mathbf{x}_c)}}{(2\pi)^3(4E_{\mathbf{q}^{\bar{c}}}E^B_{\mathbf{q}^{\bar{c}}})^{1/2}(-E_{\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^c,\mathbf{q}^{\bar{c}},\mathbf{q}^{\bar{B}}=\mathbf{q}^{\bar{c}}})}, \end{aligned} \tag{B14}$$

whose second term vanishes as $|\mathbf{x}_B-\mathbf{x}_c|\to\infty$. Thus we have

$$ {}_{\text{in}}\langle 0|\Phi_2(\mathbf{x}_l)|\mathbf{K}_3\rangle_0 \simeq D_{23}(\mathbf{K}_3)e^{i\mathbf{k}^c\cdot(\mathbf{x}^c-\mathbf{x}_B)}, \tag{B15}$$

$$ D_{23}(\mathbf{K}_3) = \frac{1}{2\pi}\frac{T^\dagger_{0-ab\bar{B}}(0;\mathbf{k}^a,\mathbf{k}^b,\mathbf{k}^c)}{(2\pi)^3(4E_{\mathbf{k}^c}E^B_{\mathbf{k}^c})^{1/2}(-E_{\mathbf{k}^a,\mathbf{k}^b,\mathbf{q}^B=\mathbf{k}^c})}. \tag{B16}$$

References

[1] M. Lüscher, Nucl. Phys. B **354**, 531 (1991).
[2] C.-J. D. Lin, G. Martinelli, C. T. Sachrajda, and M. Testa, Nucl. Phys. B **619**, 467 (2001) [arXiv:hep-lat/0104006] [Search INSPIRE].
[3] S. Aoki et al. [CP-PACS Collaboration], Phys. Rev. D **71**, 094504 (2005) [arXiv:hep-lat/0503025] [Search INSPIRE].
[4] N. Ishizuka, PoS **LATTICE2009**, 119 (2009) [arXiv:0910.2772 [hep-lat]] [Search INSPIRE].
[5] N. Ishii, S. Aoki, and T. Hatsuda, Phys. Rev. Lett. **99**, 022001 (2007) [arXiv:nucl-th/0611096] [Search INSPIRE].
[6] S. Aoki, T. Hatsuda, and N. Ishii, Prog. Theor. Phys. **123**, 89 (2010) [arXiv:0909.5585 [hep-lat]] [Search INSPIRE].

[7] S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, K. Murano, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Prog. Theor. Exp. Phys. **2012**, 01A105 (2012) [arXiv:1206.5088 [hep-lat]] [Search INSPIRE].
[8] J. Carbonell and V. A. Karmanov, Phys. Lett. B **754**, 270 (2016) [arXiv:1601.00297 [hep-ph]] [Search INSPIRE].
[9] S. Aoki, N. Ishii, T. Doi, Y. Ikeda, and T. Inoue, Phys. Rev. D **88**, 014036 (2013) [arXiv:1303.2210 [hep-lat]] [Search INSPIRE].
[10] T. Iritani, T. Doi, S. Aoki, S. Gongyo, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, K. Murano, H. Nemura, and K. Sasaki [The HAL QCD collaboration], J. High Energy Phys. **1610**, 101 (2016) [arXiv:1607.06371 [hep-lat]] [Search INSPIRE].
[11] T. Iritani, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Phys. Rev. D **96**, 034521 (2017) [arXiv:1703.07210 [hep-lat]] [Search INSPIRE].
[12] T. Iritani, S. Aoki, T. Doi, S. Gongyo, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, H. Nemura, and K. Sasaki, arXiv:1805.02365 [hep-lat] [Search INSPIRE].
[13] H. Nemura, N. Ishii, S. Aoki, and T. Hatsuda, Phys. Lett. B **673**, 136 (2009) [arXiv:0806.1094 [nucl-th]] [Search INSPIRE].
[14] T. Inoue, N. Ishii, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, K. Murano, H. Nemura, and K. Sasaki, Prog. Theor. Phys. **124**, 591 (2010) [arXiv:1007.3559 [hep-lat]] [Search INSPIRE].
[15] T. Inoue, N. Ishii, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, K. Murano, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Phys. Rev. Lett. **106**, 162002 (2011) [arXiv:1012.5928 [hep-lat]] [Search INSPIRE].
[16] K. Murano, N. Ishii, S. Aoki, and T. Hatsuda, Prog. Theor. Phys. **125**, 1225 (2011) [arXiv:1103.0619 [hep-lat]] [Search INSPIRE].
[17] T. Doi, S. Aoki, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, K. Murano, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Prog. Theor. Phys. **127**, 723 (2012) [arXiv:1106.2276 [hep-lat]] [Search INSPIRE].
[18] T. Inoue, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, N. Ishii, K. Murano, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Nucl. Phys. A **881**, 28 (2012) [arXiv:1112.5926 [hep-lat]] [Search INSPIRE].
[19] K. Murano, N. Ishii, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Phys. Lett. B **735**, 19 (2014) [arXiv:1305.2293 [hep-lat]] [Search INSPIRE].
[20] T. Kurth, N. Ishii, T. Doi, S. Aoki, and T. Hatsuda, J. High Energy Phys. **1312**, 015 (2013) [arXiv:1305.4462 [hep-lat]] [Search INSPIRE].
[21] Y. Ikeda, B. Charron, S. Aoki, T. Doi, T. Hatsuda, T. Inoue, N. Ishii, K. Murano, H. Nemura, and K. Sasaki, Phys. Lett. B **729**, 85 (2014) [arXiv:1311.6214 [hep-lat]] [Search INSPIRE].
[22] F. Etminan, H. Nemura, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, K. Murano, and K. Sasaki [HAL QCD Collaboration], Nucl. Phys. A **928**, 89 (2014) [arXiv:1403.7284 [hep-lat]] [Search INSPIRE].
[23] M. Yamada, K. Sasaki, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, K. Murano, and H. Nemura [HAL QCD Collaboration], Prog. Theor. Exp. Phys. **2015**, 071B01 (2015) [arXiv:1503.03189 [hep-lat]] [Search INSPIRE].
[24] K. Sasaki, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, and K. Murano [HAL QCD Collaboration], Prog. Theor. Exp. Phys. **2015**, 113B01 (2015) [arXiv:1504.01717 [hep-lat]] [Search INSPIRE].
[25] Y. Ikeda, S. Aoki, T. Doi, S. Gongyo, T. Hatsuda, T. Inoue, T. Iritani, N. Ishii, K. Murano, and K. Sasaki [HAL QCD Collaboration], Phys. Rev. Lett. **117**, 242001 (2016) [arXiv:1602.03465 [hep-lat]] [Search INSPIRE].
[26] T. Miyamoto et al., Nucl. Phys. A **971**, 113 (2018) [arXiv:1710.05545 [hep-lat]] [Search INSPIRE].
[27] D. Kawai, S. Aoki, T. Doi, Y. Ikeda, T. Inoue, T. Iritani, N. Ishii, T. Miyamoto, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Prog. Theor. Exp. Phys. **2018**, 043B04 (2018) [arXiv:1711.01883 [hep-lat]] [Search INSPIRE].
[28] Y. Ikeda [HAL QCD Collaboration], J. Phys. G: Nucl. Part. Phys. **45**, 024002 (2018) [arXiv:1706.07300 [hep-lat]] [Search INSPIRE].
[29] S. Gongyo, K. Sasaki, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, T. Iritani, N. Ishii, T. Miyamoto, and H. Nemura [HAL QCD Collaboration] Phys. Rev. Lett. **120**, 212001 (2018) [arXiv:1709.00654 [hep-lat]] [Search INSPIRE].

[30] K. Sasaki, S. Aoki, T. Doi, S. Gongyo, T. Hatsuda, Y. Ikeda, T. Inoue, T. Iritani, N. Ishii, T. Miyamoto, and K. Murano, PoS **LATTICE2016**, 116 (2017) [arXiv:1702.06241 [hep-lat]] [Search INSPIRE].
[31] N. Ishii et al., PoS **LATTICE2016**, 127 (2017) [arXiv:1702.03495 [hep-lat]] [Search INSPIRE].
[32] T. Doi et al., PoS **LATTICE2016**, 110 (2017) [arXiv:1702.01600 [hep-lat]] [Search INSPIRE].
[33] H. Nemura et al., PoS **LATTICE2016**, 101 (2017) [arXiv:1702.00734 [hep-lat]] [Search INSPIRE].
[34] T. Doi, T. Iritani, S. Aoki, S. Gongyo, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, T. Miyamoto, H. Nemura, and K. Sasaki, Proc. 35th Int. Symp. Lattice Field Theory (Lattice 2017) Granada, Spain, June 18–24, 2017. (2017) [arXiv:1711.01952 [hep-lat]] [Search INSPIRE].
[35] H. Nemura, S. Aoki, T. Doi, S. Gongyo, T. Hatsuda, Y. Ikeda, T. Inoue, T. Iritani, N. Ishii, T. Miyamoto, and K. Sasaki, Proc. 35th Int. Symp. Lattice Field Theory (Lattice 2017) Granada, Spain, June 18–24, 2017 (2017) [arXiv:1711.07003 [hep-lat]] [Search INSPIRE].
[36] S. Aoki, Proc. 93rd Int. School: Modern Perspectives in Lattice QCD: Quantum Field Theory and High Performance Computing. Les Houches, France, August 3–28, 2009. (2010), pp. 591–628. [arXiv:1008.4427 [hep-lat]] [Search INSPIRE].
[37] S. Weinberg, *The Quantum Theory of Fields* (Cambridge, Cambridge University Press, 2005), Vol. 1.
[38] N. Ishii, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, K. Murano, H. Nemura, and K. Sasaki [HAL QCD Collaboration], Phys. Lett. B **712**, 437 (2012) [arXiv:1203.3642 [hep-lat]] [Search INSPIRE].