



Hadron–hadron interactions from imaginary-time Nambu–Bethe–Salpeter wave function on the lattice

HAL QCD Collaboration

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ABSTRACT

Imaginary-time Nambu–Bethe–Salpeter (NBS) wave function is introduced to extend our previous approach for hadron–hadron interactions on the lattice. Scattering states of hadrons with different energies encoded in the NBS wave function are utilized to extract non-local hadron–hadron potential. “The ground state saturation”, which is commonly used in lattice QCD but is hard to be achieved for multi-baryons, is not required. We demonstrate that the present method works efficiently for the nucleon–nucleon interaction (the potential and the phase shift) in the 1S_0 channel.

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1. Introduction

Euclidean correlation functions are dominated by contributions from the corresponding lowest-energy states at sufficiently large time separation t . This property, called the ground state saturation, is heavily used in lattice QCD to extract various hadronic observables such as masses, decay constants and other matrix elements. The ground state saturation, however, is difficult to be achieved for multi-baryon systems. For example, the signal-to-noise ratio for the correlation of n -nucleons reads [1]:

$$\left(\frac{S}{N}\right)_n \sim e^{-n(m_N - 3m_\pi/2)t}, \quad (1)$$

where m_N and m_π are the nucleon mass and the pion mass, respectively. This relative enhancement of statistical noise at large t for $m_N - 3m_\pi/2 > 0$ is a common problem for baryonic systems, even for a single baryon ($n = 1$).

In addition, there exists another problem for the multi-hadrons at large t caused by the small splitting between the ground and the 1st excited states for large volume. For example, in the nucleon–nucleon (NN) system, the minimum splitting is estimated as

$$\Delta E \simeq \frac{\mathbf{p}_{\min}^2}{m_N} = \frac{1}{m_N} \frac{(2\pi)^2}{L^2}, \quad (2)$$

where L is a spatial extension of the lattice. If $L \simeq 6$ fm and $m_N \simeq 1$ GeV, we have $\Delta E \simeq 43$ MeV $\simeq 1/(4.6$ fm). The ground state saturation requires $t \gg (\Delta E)^{-1} \simeq 4.6$ fm, which corresponds to $t/a \gg 46$ for the lattice spacing $a \simeq 0.1$ fm. It is very difficult to extract signals at such large t due to the bad behavior of statistical noise in Eq. (1). To avoid these problems, techniques such as the use of improved operators and/or the diagonalization of matrix correlation functions [2] have been employed.¹

Recently, a novel method to derive hadron–hadron interactions from lattice QCD was developed by HAL QCD Collaboration [5–11], where the Nambu–Bethe–Salpeter (NBS) wave function is utilized

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¹ For recent applications of these methods to multi-baryons, see e.g. Refs. [3,4].

to extract the hadron–hadron potentials. Since its extraction from hadronic correlation functions relies on the ground state saturation, the problems mentioned above may exist in principle. In this Letter, we introduce time-dependent Schrödinger-like equation which can utilize the information of moderate t and can avoid the problem of ground state saturation. This allows one to derive the hadron–hadron potentials as defined in the original HAL QCD method with less systematic errors. The key observation is that the scattering states with “different” energies on the lattice are governed by the “same” non-local potential $U(\vec{r}, \vec{r}')$. The present time-dependent method has already been applied successfully to the baryon–baryon (BB) potentials in the flavor-SU(3) limit [12,13]. In the following, we give a full theoretical account of this imaginary-time HAL QCD method by taking the NN scattering with $(2+1)$ -flavor lattice QCD as a concrete example.

2. Potential with ground state saturation

In the original HAL QCD method, the “time-independent” NBS wave function was shown to satisfy the following “time-independent” Schrödinger equation [7]:

$$(\vec{k}^2/m_N - H_0)\psi_{\vec{k}}(\vec{r}) = \int d^3r' U(\vec{r}, \vec{r}')\psi_{\vec{k}}(\vec{r}'), \quad (3)$$

where $H_0 \equiv -\Delta/m_N$ with m_N being the nucleon mass. The potential $U(\vec{r}, \vec{r}')$ is non-local but independent on k [7,14]. The equal-time NBS wave function is given by

$$\psi_{\vec{k}}(\vec{x} - \vec{y}) \equiv \langle 0|N(\vec{x})N(\vec{y})|N(\vec{k})N(-\vec{k}); in\rangle, \quad (4)$$

where $|0\rangle$ and $|N(\vec{k})N(-\vec{k}); in\rangle$ denote the vacuum and a two-nucleon state with an asymptotic momentum \vec{k} , respectively, and $N(x)$ denotes a composite interpolating field for the nucleon. For $N(x)$ being local, the reduction formula for local composite operators [15] can be used to establish the relation between the NBS wave function and the S-matrix: The asymptotic behavior of the NBS wave function at long distance reads [7,16,17]

$$\psi_{\vec{k}}(\vec{r}) = e^{i\delta(k)} \frac{\sin(kr + \delta(k))}{kr} + \dots, \quad (5)$$

where $\delta(k)$ denotes the (scattering) phase of the S-matrix. Therefore the NN potential in Eq. (3) gives correct phase shift $\delta(k)$ for all k in the elastic region $E < E_{\text{th}} \equiv 2m_N + m_\pi$, by construction.

In lattice QCD calculations, NBS wave functions are extracted from the NN correlation function using the ground state saturation as

$$\begin{aligned} C_{NN}(\vec{x} - \vec{y}; t) &\equiv \frac{1}{V} \sum_{\vec{r}} \langle 0|T[N(\vec{x} + \vec{r}, t)N(\vec{y} + \vec{r}, t) \cdot \vec{J}(0)]|0\rangle \\ &= \sum_n \psi_n(\vec{x} - \vec{y}) \cdot a_n e^{-E_n t} \\ &\rightarrow \psi_0(\vec{x} - \vec{y}) a_0 e^{-E_0 t} \quad (t \rightarrow \infty), \end{aligned} \quad (6)$$

where $\vec{J}(0)$ is a two-nucleon source located at $t=0$, V denotes the spatial volume, $\psi_n(\vec{x} - \vec{y}) \equiv \langle 0|N(\vec{x})N(\vec{y})|n\rangle$ denotes an NBS wave function for an intermediate state $|n\rangle$ with the energy E_n , and $a_n \equiv \langle n|\vec{J}(0)|0\rangle$. In the spin-singlet sector, for example, the central potential $V_C(r)$ in the leading order of the velocity expansion, $U(\vec{r}, \vec{r}') = V(\vec{r}, \vec{\nabla}_r)\delta^3(\vec{r} - \vec{r}') = \{V_C(r) + O(\nabla^2)\}\delta^3(\vec{r} - \vec{r}')$, is given by

$$V_C(r) = \frac{\vec{k}^2}{m_N} - \lim_{t \rightarrow \infty} \frac{H_0 C_{NN}(\vec{r}, t)}{C_{NN}(\vec{r}, t)}, \quad (7)$$

where \vec{k} denotes the “asymptotic momentum” for the ground-state. The ground state saturation is crucial here to extract the potential.

3. Potential without ground state saturation

In this section, we propose an alternative derivation of potential without using the ground state saturation. For this purpose, we consider the normalized NN correlation function

$$R(t, \vec{r}) \equiv C_{NN}(\vec{r}, t)/(e^{-m_N t})^2. \quad (8)$$

We here assume that t is moderately large such that elastic contributions (at $E < E_{\text{th}} = 2m_N + m_\pi$) dominate $C_{NN}(t, \vec{r})$.

As before, we write

$$R(t, \vec{r}) \simeq \sum_{\vec{k}} \psi_{\vec{k}}(\vec{r}) \cdot a_{\vec{k}} \exp(-t\Delta W(\vec{k})), \quad (9)$$

where

$$\Delta W(\vec{k}) \equiv 2\sqrt{m_N^2 + \vec{k}^2} - 2m_N$$

and

$$a_{\vec{k}} \equiv \langle N(\vec{k})N(-\vec{k}); in|\mathcal{J}(0)|0\rangle.$$

From an identity $\Delta W(\vec{k}) = \frac{\vec{k}^2}{m_N} - \frac{\Delta W(\vec{k})^2}{4m_N}$, it is easy to see

$$\begin{aligned} &-\frac{\partial}{\partial t} R(t, \vec{r}) \\ &= \sum_{\vec{k}} \left\{ \frac{\vec{k}^2}{m_N} - \frac{\Delta W(\vec{k})^2}{4m_N} \right\} \psi_{\vec{k}}(\vec{r}) \cdot a_{\vec{k}} \exp(-t\Delta W(\vec{k})), \\ &= \sum_{\vec{k}} \left\{ H_0 + U - \frac{1}{4m_N} \frac{\partial^2}{\partial t^2} \right\} \psi_{\vec{k}}(\vec{r}) \cdot a_{\vec{k}} \exp(-t\Delta W(\vec{k})), \end{aligned} \quad (10)$$

where U is the integration kernel associated with the non-local potential $U(\vec{r}, \vec{r}')$. Thanks to Eq. (3), \vec{k}^2/m_N in the first line can be replaced by $H_0 + U$ in the second line. We then arrive at the “time-dependent” Schrödinger-like equation,

$$\left\{ \frac{1}{4m_N} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right\} R(t, \vec{r}) = \int d^3r' U(\vec{r}, \vec{r}') R(t, \vec{r}'), \quad (11)$$

which shows that the same potential $U(\vec{r}, \vec{r}')$ as defined in Eq. (3) can be obtained from $R(t, \vec{r})$. An advantage of this method is that the ground state saturation (or more generally a single state saturation) is not required for $R(t, \vec{r})$ to satisfy Eq. (11).

Several comments are in order here:

- (i) For the present method to work, t has to be large enough such that elastic contributions at $E < E_{\text{th}} = 2m_N + m_\pi$ dominate $R(t, \vec{r})$. Note that such t is much smaller than that required for the ground state saturation. This is especially so for the large volume, since typical size of gaps between energy eigenvalues shrinks as $O(1/L^2)$. While it becomes more and more difficult to achieve the ground state saturation for larger volume, the requirement of the elastic dominance $E < E_{\text{th}}$ is less sensitive to the volume size.
- (ii) In the leading order of the velocity expansion, Eq. (11) leads to a generalization of Eq. (7)

$$\begin{aligned} V_C(r) &= -\frac{H_0 R(t, \vec{r})}{R(t, \vec{r})} - \frac{(\partial/\partial t)R(t, \vec{r})}{R(t, \vec{r})} \\ &\quad + \frac{1}{4m_N} \frac{(\partial/\partial t)^2 R(t, \vec{r})}{R(t, \vec{r})} \end{aligned} \quad (12)$$

for the spin-singlet sector. We can also include the higher order terms of the velocity expansion as discussed in Refs. [7,10].

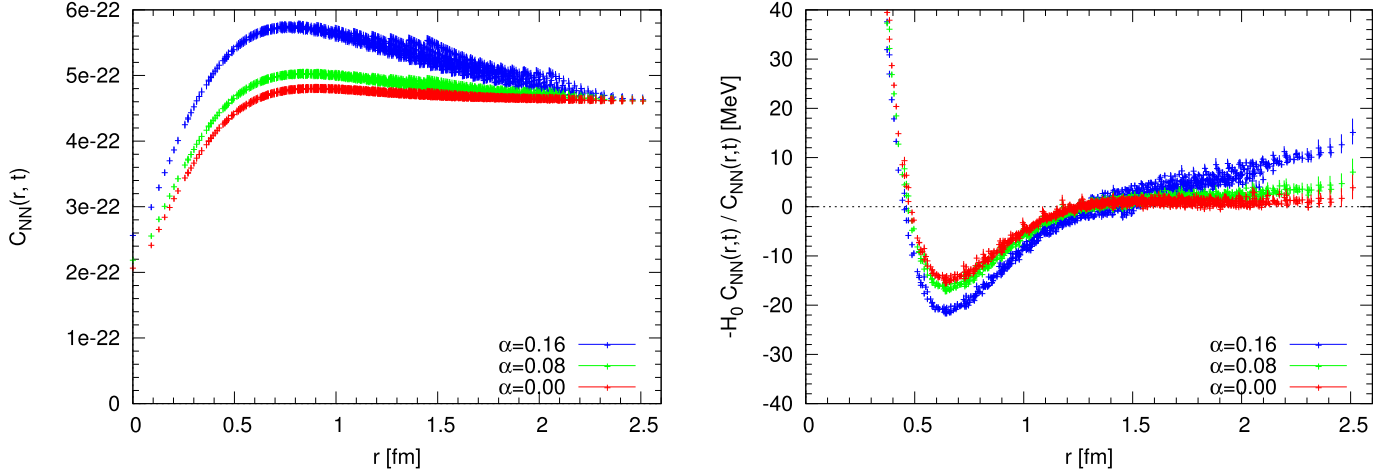


Fig. 1. (Left) $C_{NN}(\vec{r}, t)$ at $t = 9$. (Right) $-H_0 C_{NN}(\vec{r}, t) / C_{NN}(\vec{r}, t)$ at $t = 9$.

Convergence of the velocity expansion in the original HAL QCD method can be examined by comparing local potentials at two different energies as discussed in Ref. [10]. Equivalently, in the present method, the convergence can be examined by comparing the local potentials obtained for different t 's.

(iii) $D \equiv \frac{1}{4m_N} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t}$ in Eq. (11) plays a role of \vec{k}^2/m_N in Eq. (3). For $\Delta E \cdot t \gg 1$ where the ground state saturation is achieved, Eq. (11) reduces to Eq. (3). We therefore can regard the “time-dependent” Schrödinger-like equation as an extension of the time-independent Schrödinger equation (Eq. (3)).

(iv) In the non-relativistic limit where $\Delta W(\vec{k}) \equiv 2\sqrt{m_N^2 + \vec{k}^2} - 2m_N \simeq \frac{\vec{k}^2}{m_N}$, “time-dependent” Schrödinger-like equation leads to

$$\left\{ -\frac{\partial}{\partial t} - H_0 \right\} R(t, \vec{r}) = \int d^3r' U(\vec{r}, \vec{r}') R(t, \vec{r}'). \quad (13)$$

Therefore, the 2nd derivative term of t in Eq. (11) corresponds to the relativistic effect.

4. Numerical results

To test the present method, we employ (2 + 1)-flavor QCD gauge configurations generated by PACS-CS Collaboration [18] on $32^3 \times 64$ lattice with the RG improved Iwasaki gauge action at $\beta = 1.9$ and the non-perturbatively $O(a)$ improved Wilson quark action at $(\kappa_{ud}, \kappa_s) = (0.13700, 0.13640)$ and $C_{SW} = 1.715$. This parameter set corresponds to the lattice spacing $a \simeq 0.091$ fm ($a^{-1} = 2.176(31)$ GeV), the spatial extent $L = 32a \simeq 2.90$ fm, $m_\pi \simeq 701$ MeV and $m_N \simeq 1583$ MeV.

The periodic boundary condition is used for spatial directions, while the Dirichlet boundary condition is taken for the temporal direction at $t_{\text{DBC}} = 32a$ and $-32a$, to avoid opposite propagations of two nucleons in temporal direction, i.e., one propagates forward and the other propagates backward. From time-reversal and charge conjugation symmetries, we can average over forward propagation at $t > 0$ and backward propagation at $t < 0$ with a source at $t = 0$. By temporally shifting gauge configurations, 21 source points are used per one configuration and 390 gauge configurations are employed in total. Statistical errors are estimated by the Jackknife method with a bin size of 10 configurations. Composite operators for the proton and the neutron are taken to be $p(x) \equiv \epsilon_{abc} u_a^T(x) C \gamma_5 d_b(x) u_c(x)$ and $n(x) \equiv \epsilon_{abc} u_a^T(x) C \gamma_5 d_b(x) d_c(x)$, respectively. In our actual calculation, we replace $e^{-m_N t}$ in Eq. (8) by

the single-nucleon $C_N(t) \equiv \sum_{\vec{x}} \langle 0 | T [N(x) \bar{N}(0)] | 0 \rangle$ to suppress statistical noises of $R(t, \vec{r})$. This replacement is permitted as long as the ground state saturation for $C_N(t)$ is achieved. Time derivatives in Eq. (12) are evaluated after applying the polynomial interpolation of degree 5 to $R(t, \vec{r})$.

In order to see how excited states of the two nucleons affect the final NN potential, we introduce a source function with a real parameter α as

$$f(x, y, z) \equiv 1 + \alpha (\cos(2\pi x/L) + \cos(2\pi y/L) + \cos(2\pi z/L)), \quad (14)$$

which reduces to the wall source at $\alpha = 0$. Two-nucleon source is then defined by $\vec{J}(f) \equiv \vec{p}(f) \cdot \vec{n}(f)$, where $\vec{p}(f) \equiv \epsilon_{abc} (\bar{u}_a(f) C \gamma_5 \bar{d}_b(f)) \bar{u}_c(f)$ and $\vec{n}(f) \equiv \epsilon_{abc} (\bar{u}_a(f) C \gamma_5 \bar{d}_b(f)) \bar{d}_c(f)$ with $\bar{u}(f) \equiv \sum_{\vec{x}} \bar{u}(\vec{x}) f(\vec{x})$ and $\bar{d}(f) \equiv \sum_{\vec{x}} \bar{d}(\vec{x}) f(\vec{x})$.

Fig. 1 (left) shows $C_{NN}(\vec{r}, t)$ at $t = 9$ for $\alpha = 0.00, 0.08$ and 0.16 . If the ground state saturation were achieved, results with different values of α should be the same up to overall normalizations. Fig. 1 (left) reveals that contamination from the excited states is non-negligible at $t = 9$. As shown in Fig. 1 (right), the contamination is transferred to the α dependence of $[H_0 C_{NN}(\vec{r}, t)] / C_{NN}(\vec{r}, t)$.

Fig. 2 (left) shows $V_C(r)$ obtained from our present method Eq. (12) for three values of α . The α dependence seen in Fig. 1 (right) disappears within statistical errors. Three contributions to $V_C(r)$ in Eq. (12) are separately shown in Fig. 2 (right) for $\alpha = 0$. We observe that the first term of Eq. (12) (the red points) determines the main trend, while the second term (the blue points) gives an important correction. The third term (the green points), on the other hand, is negligible, showing that the non-relativistic approximation $\Delta W(\vec{k}) \simeq \vec{k}^2/m_N$ works well in this case. Note that the \vec{r} -dependence of the second term in Eq. (12), $-\frac{(\partial/\partial t)R(t, \vec{r})}{R(t, \vec{r})} = -\frac{\partial \log(R(t, \vec{r}))}{\partial t}$, is a useful measure of the departure from the ground state saturation.

5. Scattering length and scattering phase shift

We now calculate the NN scattering phase shift, by solving the Schrödinger equation with the potential $V_C(r)$ in the infinite volume. For this purpose, as shown in Fig. 3 (left), the central potential $V_C(r)$ is fitted with multi-Gaussian functions as $g(r) \equiv \sum_{n=1}^{N_{\text{gauss}}} V_n \cdot \exp(-v_n r^2)$, where V_n and $v_n (> 0)$ are used as fit parameters, N_{gauss} denotes the number of Gaussian functions. We then solve the Schrödinger equation in 1S_0 channel [19].

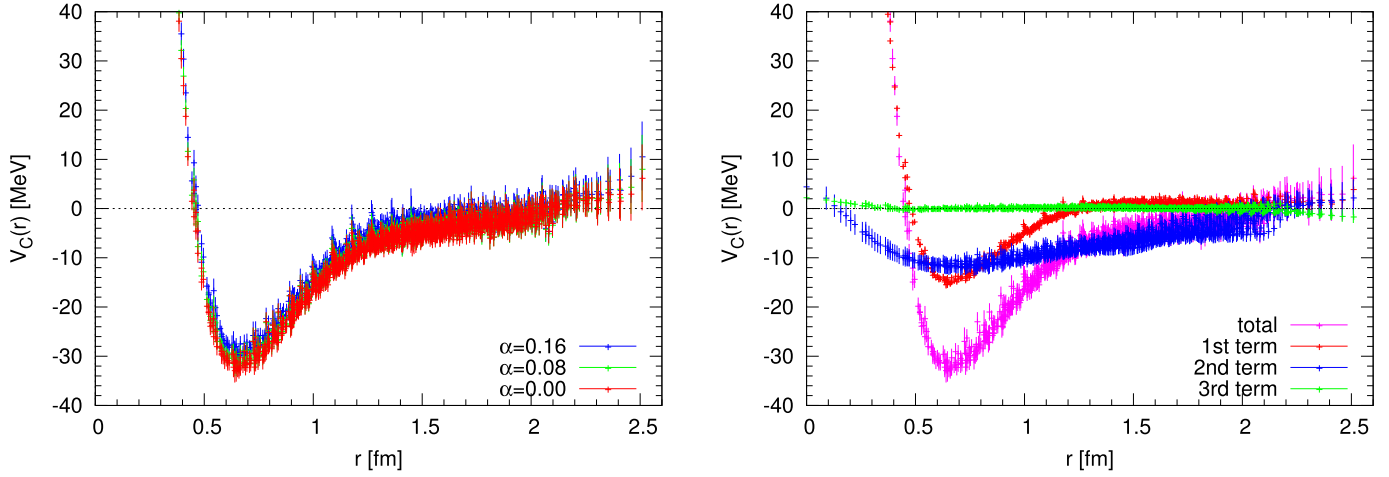


Fig. 2. (Left) Central potentials obtained by our new method Eq. (12) at $t=9$ for three values of α . (Right) Three contributions to $V_C(r)$ in Eq. (12) at $t=9$ for $\alpha=0$. (For interpretation of the references to color, the reader is referred to the web version of this Letter.)

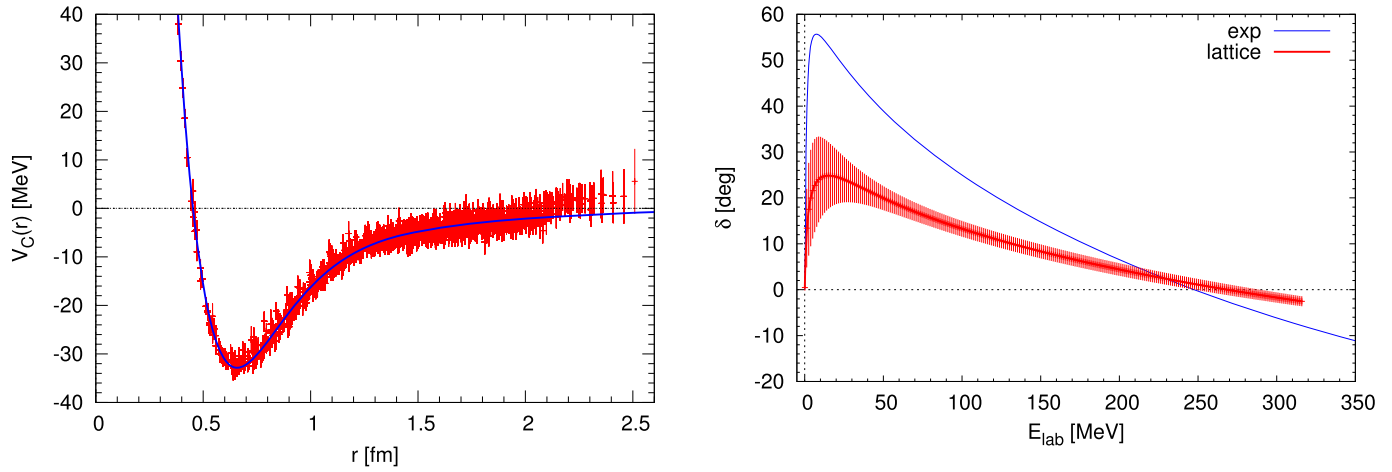


Fig. 3. (Left) The multi-Gaussian fit of the central potential $V_C(r)$ with $N_{\text{Gauss}} = 5$ for $\alpha = 0$ at $t=9$. (Right) The scattering phase in 1S_0 channel in the laboratory frame obtained from the lattice NN potential, together with experimental data [20].

Fig. 3 (right) shows the scattering phase $\delta(k)$ extracted from the long distance behavior of the solution $\psi_k(r)$, together with the experimental data for comparison. Qualitative feature of the phase shift as a function of k is well reproduced, though the strength is weaker, most likely due to the heavy pion mass ($m_\pi \simeq 701$ MeV) in this calculation. In fact, the recent 3-flavor QCD simulations show that the NN phase shift approaches toward the physical value as the quark mass decreases [13]. The scattering length for $m_\pi \simeq 701$ MeV in the present method, calculated from the derivative of the scattering phase shift at $E_{\text{lab}} = 0$, leads to $a(^1S_0) = \lim_{k \rightarrow 0} \tan \delta(k)/k = 1.6 \pm 1.1$ fm.

6. Non-local potential

By extending the present method further, one may directly extract the non-local potential. Let us introduce a more general NN correlation function,

$$R_{\vec{r}, \vec{r}'}(t) = \frac{1}{V^2} \sum_{\vec{x}, \vec{x}'} \frac{\langle 0 | T [N(\vec{x} + \vec{r}, t) N(\vec{x}, t) \bar{N}(\vec{x}' + \vec{r}', 0) \bar{N}(\vec{x}', 0)] | 0 \rangle}{(e^{-m_N t})^2}, \quad (15)$$

which is shown to satisfy

$$K(t) \equiv \left\{ \frac{1}{4m_N} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right\} R(t) = U \cdot R(t). \quad (16)$$

Here the matrix indices \vec{r}, \vec{r}' for $K(t)$, $R(t)$, U and a necessary integration over spatial coordinates are implicit. The non-local potential is then extracted as $\tilde{U} = K(t) \cdot \tilde{R}^{-1}(t)$, where an approximated inverse of the hermitian operator $R(t)$ is defined by $\tilde{R}^{-1}(t) = \sum_{\lambda_n(t) \neq 0} \lambda_n(t)^{-1} |n, t\rangle \langle n, t|$. Here $\lambda_n(t)$ and $|n, t\rangle$ are an eigenvalue of $R(t)$ and its eigenvector, respectively. Zero eigenvalues are removed in the summation. Note that U which satisfies Eq. (16) is not unique, since $U = \tilde{U} + \sum_{\lambda_n(t)=0} c_n |n, t\rangle \langle n, t|$ also satisfies the same equation for arbitrary $\{c_n\}$. This is related to the fact that the zero-modes or nearly zero-modes are associated with states above the inelastic threshold.

7. Summary and concluding remarks

A method to extract hadron–hadron interactions by generalizing the original HAL QCD method is proposed. We derived “time-dependent” Schrödinger-like equation, a second order differential equation in t , which enables us to construct NN potentials without assuming the ground state saturation in the elastic region

$E < E_{\text{th}} = 2m_N + m_\pi$. We have shown that this method works well for extracting the central NN potential in the 1S_0 channel: Identical potential is obtained for different source-operators within the statistical error. Also, resultant NN potential, the scattering phase shift and the scattering length are much improved both qualitatively and quantitatively from those obtained by assuming ground state saturation.

While we have considered the system only in the elastic region so far, an extension to the inelastic region is also possible. In Ref. [21], it has been shown that one can define and extract the hadronic potentials above inelastic threshold. Together with the framework proposed in this Letter, this could provide a novel prescription to solve the S -matrix in QCD.

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