PROCEEDINGS OF SCIENCE

Time-dependent Schrödinger-like Equation for Lattice Nuclear Potentials

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A generalization of the HAL QCD method for lattice construction of inter-nucleon (NN) potentials is presented. It enables us to construct the NN potentials in the presence of contamination of excited states in the Nambu-Bethe-Salpeter (NBS) wave functions. For this purpose, we derive a "time-dependent" Schrödinger-like equation which describes the time-evolution of normalized four-point nucleon correlators. It makes it possible to construct the NN potentials in a smaller t region without requiring the ground state saturation in the four-point nucleon correlators. The time-dependent Schrödinger-like equation is applied to the NN central potential in $^1S_0$ channel. The potentials obtained by using different two-nucleon source operators agree within the statistical errors.

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1. Introduction

Inter-nucleon (NN) potential is one of the most essential building blocks in nuclear physics. It is conveniently used to study not only two-nucleon scatterings but also multi-nucleon properties. Although it is an off-shell quantity, it is conveniently used to describe on-shell experimental observables, providing physics insights into nuclear structures and reactions in terms of the nucleon, the effective degrees of freedom at low energy. Enormous efforts have been devoted to the development of modern high precision NN potentials, all of which can describe a few thousands of NN scattering data with $\chi^2/\mathrm{NDF} \simeq 1$ [1, 2, 3, 4].

A Lattice QCD method to determine NN potentials has been proposed by HAL QCD, where Nambu-Bethe-Salpeter (NBS) wave functions are used [5, 6, 7, 8, 9, 10, 11, 12, 13]. It leads to potentials which are faithful to NN scatterings, because the scattering phase is embedded in the long distance part of the NBS wave functions. It has been applied to the central and tensor potentials in the even parity sectors and the qualitative properties are found to be reproduced successfully. For a quantitative use, the ground state saturation of the NBS wave function is important. To achieve the ground state saturation, a large t region is used in the four-point correlators, where, to suppress the statistical errors, huge numerical cost is required for two-nucleon system.

The aim of this paper is to present a method to overcome this problem. We derive an equation, which describes the time-evolution of (normalized) four-point nucleon correlators. It is a second-order differential equation (with respect to t) involving the NN potential defined from NBS wave functions. It enables us to construct NN potentials in the presence of contamination of excited states. Since it can be regarded as a generalization of the Schrödinger-like equation of the HAL QCD method, we will refer to it as the "time-dependent" Schrödinger-like equation.

The contents are organised as follows. In Sect. 2, we give a brief review of HAL QCD method for NN potential on the lattice. In Sect. 3, we derive the "time-dependent" Schrödinger-like equation which can be safely be used to construct the NN potentials in the presence of contamination of excited states. In Sect. 4, we present numerical results.

2. A Brief Review of HAL QCD Method

For NN potential, we consider the equal-time NBS wave functions

$$\psi_{\vec{k}}(\vec{x}-\vec{y}) \equiv Z^{-1}\langle 0|N(\vec{x})N(\vec{y})|N(\vec{k})N(-\vec{k}), in\rangle, \tag{2.1}$$

where $\langle 0|$ and $|N(\vec{k})N(-\vec{k}), in\rangle$ denote the vacuum and a two-nucleon state with an asymptotic momentum $\vec{k}$. $N(x)$ denotes a composite interpolating field for nucleon. Z denotes the normalization constant involved in the limit $N(x) \to Z^{1/2}N_{out}(x)$ as $x_0 \to +\infty$. As far as $N(x)$ is local, the reduction formula is used to establish a relation with the S-matrix element. The relation leads to the asymptotic behavior of NBS wave functions at long distance which is parametrized by the scattering phase $\delta(k)$ [14, 15, 6]

$$\psi_{\vec{k}}(\vec{r}) = e^{i\delta(k)}\frac{\sin(kr+\delta(k))}{kr} + \cdots. \tag{2.2}$$

NN potential is defined as an energy-independent interaction kernel $U(\vec{r},\vec{r}')$ by demanding that the Schrödinger equation is satisfied by NBS wave functions in the elastic region $E < E_{\mathrm{th}} \equiv$

$2m_N + m_\pi$ as

$$\left(\vec{k}^2/m_N - H_0\right)\psi_{\vec{k}}(\vec{r}) = \int d^3r' U(\vec{r},\vec{r}')\psi_{\vec{k}}(\vec{r}'), \tag{2.3}$$

where $H_0 \equiv -\triangle/m_N$ with m_N being the nucleon mass. The NN potential so defined is faithful to the scattering phase, because the long distance part of NBS wave functions contains the scattering phase in exactly the same way as the non-relativistic quantum mechanics (see Eq.(2.2)).

To construct NN potentials, we need NBS wave functions as input. NBS wave functions are extracted from four-point nucleon correlators in the large t region by using

$$C_{NN}(\vec{x}-\vec{y};t) \equiv \langle 0|T[N(\vec{x},t)N(\vec{y},t)\cdot\bar{\mathscr{J}}(0)]|0\rangle = \sum_n \psi_n(\vec{x}-\vec{y})\cdot a_n e^{-E_n t} \tag{2.4}$$

where $\bar{\mathscr{J}}(0)$ denotes a two-nucleon source located at $t=0$. E_n denotes the energy of an intermediate state $|n\rangle$. $a_n \equiv \langle n|\bar{\mathscr{J}}(0)|0\rangle$, and $\psi_n(\vec{x}-\vec{y}) \equiv \langle 0|N(\vec{x})N(\vec{y})|n\rangle$ denotes an NBS wave function. For simplicity, we restrict ourselves to the spin-singlet sector. At the leading order of the derivative expansion $U(\vec{r},\vec{r}') = V(\vec{r},\vec{\nabla}_r)\delta^3(\vec{r}-\vec{r}') = \left\{V_{\rm C}(r) + O(\nabla^2)\right\}\delta^3(\vec{r}-\vec{r}')$, the central potential $V_{\rm C}(r)$ is obtained from Eq.(2.3) by using the ground-state NBS wave function as input. Since it is extracted from $C_{NN}(\vec{r},t)$ in the large t region, we have

$$V_{\rm C}(r) = \frac{\vec{k}^2}{m_N} - \lim_{t\to\infty}\frac{H_0 C_{NN}(\vec{r},t)}{C_{NN}(\vec{r},t)}, \tag{2.5}$$

where $\vec{k}$ represents the "asymptotic momentum" of the ground-state.

3. Time-dependent Schrödinger-like equation

Eq.(2.5) has to be used in the large t region so that the contamination of excited state is sufficiently suppressed. We seek for a generalization of Eq.(2.5) so that we can construct the potentials in a smaller t region where the ground state saturation is not achieved. For this purpose, we consider a normalized four-point nucleon correlator

$$R(t,\vec{x}) \equiv C_{NN}(t,\vec{x})/(e^{-m_N t})^2. \tag{3.1}$$

We restrict ourselves to a moderately large t region where elastic contributions ($E < E_{\rm th} = 2m_N + m_\pi$) dominate $C_{NN}(t,\vec{x})$. We rewrite $R(t,\vec{x})$ by inserting the complete set as

$$R(t,\vec{x}) = \sum_{\vec{k}} \psi_{\vec{k}}(\vec{x})\cdot a_{\vec{k}} \exp\left(-t\Delta W(\vec{k})\right), \tag{3.2}$$

where $\Delta W(\vec{k}) \equiv 2\sqrt{m_N^2+\vec{k}^2} - 2m_N$ and $a_{\vec{k}} \equiv \langle N(\vec{k})N(-\vec{k}), in|\mathscr{J}(0)|0\rangle$. By using an identity $\Delta W(\vec{k}) = \frac{\vec{k}^2}{m_N} - \frac{\Delta W(\vec{k})^2}{4m_N}$, the time derivative of $R(t,\vec{x})$ is arranged as

$$\begin{aligned} -\frac{\partial}{\partial t}R(t,\vec{x}) &= \sum_{\vec{k}}\left\{\frac{\vec{k}^2}{m_N} - \frac{\Delta W(\vec{k})^2}{4m_N}\right\}\psi_{\vec{k}}(\vec{x})\cdot a_{\vec{k}}\exp\left(-t\Delta W(\vec{k})\right), \\ &= \sum_{\vec{k}}\left\{H_0 + U - \frac{1}{4m_N}\frac{\partial^2}{\partial t^2}\right\}\psi_{\vec{k}}(\vec{x})\cdot a_{\vec{k}}\exp\left(-t\Delta W(\vec{k})\right). \end{aligned} \tag{3.3}$$

Here, U denotes the integration operator associated with the kernel $U(\vec{r},\vec{r}')$ which is defined through Eq.(2.3). To obtain the second line, we used Eq.(2.3) to replace $\vec{k}^2/m_N$ by H_0+U. We finally arrive at the "time-dependent" Schrödinger-like equation:

$$\left\{\frac{1}{4m_N}\frac{\partial^2}{\partial t^2}-\frac{\partial}{\partial t}-H_0\right\}R(t,\vec{r})=\int d^3r' U(\vec{r},\vec{r}')R(t,\vec{r}'). \tag{3.4}$$

Note that Eq.(3.4) is valid even if the ground state saturation is not achieved in $R(t,\vec{r})$. It follows that the potential defined in Eq.(2.3) can be obtained by Eq.(3.4) even in the presence of contamination of excited states.

Several comments are in order.

(i) At the leading order of the derivative expansion, by restricting ourselves to the spin-singlet sector, Eq.(3.4) leads to a generalization of Eq.(2.5)

$$V_{\rm C}(\vec{x})=-\frac{H_0R(t,\vec{x})}{R(t,\vec{x})}-\frac{(\partial/\partial t)R(t,\vec{x})}{R(t,\vec{x})}+\frac{1}{4m_N}\frac{(\partial/\partial t)^2R(t,\vec{x})}{R(t,\vec{x})}. \tag{3.5}$$

We emphasize that Eq.(3.5) is valid even if the ground state saturation is not achieved in $R(t,\vec{x})$.

(ii) To use Eq.(3.5), t has to be large enough so that the elastic contribution $E<E_{\rm th}\equiv m_N+m_\pi$ can dominate $R(t,\vec{x})$. Note that such t is much smaller than those which can achieve the ground state saturation. This is especially the case for the large volume. Since typical size of gaps between energy eigenvalues shrinks as $O(1/L^2)$, it becomes more difficult to achieve the ground state saturation as the volume becomes the larger. In contrast, the requirement of the elastic dominance $E<E_{\rm th}$ is less sensitive to the large volume limit.

(iii) In Ref. [11], convergence of derivative expansion is examined by using a result obtained from a different energy eigenstate. In our new prescription, the convergence may be examined by carefully studying t dependence, which may be used to arrange relative weights of intermediate states appearing in $R(t,\vec{x})$.

(iv) $D\equiv\frac{1}{4m_N}\frac{\partial^2}{\partial t^2}-\frac{\partial}{\partial t}$ in Eq.(3.4) plays the role of $\vec{k}^2/m_N$ in Eq.(2.3). For $t\gg 0$, where the ground state saturation is achieved, Eq.(3.4) reduces to Eq.(2.3). Thus, we may regard the "time-dependent" Schrödinger-like equation as a generalization of the Schrödinger-like equation Eq.(2.3).

4. Numerical Results

We use 2+1 flavor QCD gauge configurations on $32^3\times 64$ lattice by PACS-CS collaboration [16]. They are generated by employing Iwasaki gauge action at $\beta=1.9$ together with $O(a)$ improved Wilson quark action at $(\kappa_{ud},\kappa_s)=(0.13700,0.13640)$ with a non-perturbatively improved coefficient $C_{\rm SW}=1.715$. It leads to the lattice spacing $a\simeq 0.091$ fm ($a^{-1}=2.176(31)$ GeV) with $m_\pi\simeq 701$ MeV ($m_\pi a=0.32242(65)$) and $m_N\simeq 1583$ MeV ($m_N a=0.7277(22)$). The spatial extent amounts to $L=32a\simeq 2.90$ fm.

We use periodic boundary condition for spatial directions and Dirichlet boundary condition for the temporal direction. The latter is to avoid an artifact arising from the separate propagation of two nucleons in temporal direction, i.e, one propagates forward, while the other propagates backward. By locating Dirichlet boundary on the time-slice $t=\pm 32$, we use the time-reversal and the charge

conjugation symmetries to combine the correlators for $t > 0$ and $t < 0$. We use 390 gauge configurations with 21 source points, where statistical data are split into bins of size 10. Statistical errors are obtained based on the jackknife prescription. For composite operators of proton and neutron, we employ $p(x) \equiv \varepsilon_{abc}\left(u_a^T(x)C\gamma_5 d_b(x)\right)u_c(x)$ and $n(x) \equiv \varepsilon_{abc}\left(u_a^T(x)C\gamma_5 d_b(x)\right)d_c(x)$, respectively. We use the two-point nucleon correlator $C_N(t) \equiv \sum_{\vec{x}}\langle 0|T[N(x)\bar{N}(0)]|0\rangle$ instead of $e^{-m_N t}$ in Eq.(3.1) in expectation of the cancellation of the statistical noise. The temporal derivatives in Eq.(3.5) are evaluated after applying the polynomial interpolation of degree 5.

To arrange how excited states appear in the NBS wave function, we introduce a source function with a single real parameter α by $f(x,y,z) \equiv 1+\alpha\left(\cos(2\pi x/L)+\cos(2\pi y/L)+\cos(2\pi z/L)\right)$, which reduces to the wall source at $\alpha = 0$. We use it to define a two-nucleon source by $\bar{\mathscr{J}}(f) \equiv \bar{p}(f)\cdot\bar{n}(f)$, where $\bar{p}(f) \equiv \varepsilon_{abc}\left(\bar{u}_a(f)C\gamma_5\bar{d}_b(f)\right)\bar{u}_c(f)$ and $\bar{d}(f) \equiv \varepsilon_{abc}\left(\bar{u}_a(f)C\gamma_5\bar{d}_b(f)\right)\bar{d}_c(f)$ with $\bar{u}(f) \equiv \sum_{\vec{x}}\bar{u}(\vec{x})f(\vec{x})$ and $\bar{d}(f) \equiv \sum_{\vec{x}}\bar{d}(\vec{x})f(\vec{x})$.

Figure 1 (left) shows $C_{NN}(\vec{r},t)$ at $t = 9$ for $\alpha = 0.00$, 0.08 and 0.16. At around $t = 9$, contamination of excited states is seen to be unavoidable, which leads to α dependence of $C_{NN}(\vec{r},t)$. (If the ground state saturation were achieved, they should agree up to overall normalization factors.) The α dependence is seen to be transferred to $[H_0 C_{NN}(\vec{r},t)]/C_{NN}(\vec{r},t)$ in Figure 1(right).

Figure 2(left) shows $V_C(r)$ obtained by our new formula Eq.(3.5) for the three values of α. We see that α dependence seen in Figure 1 disappears within the statistical errors. Figure 2(right) shows the three contributions in Eq.(3.5) for $\alpha = 0$. We see that the first term determines the main trend, to which the second term gives an important correction. The third term gives a negligible contribution, which implies that the non-relativistic approximation $\Delta W(\vec{k}) \simeq \vec{k}^2/m_N$, if we apply, turns out to work well in our NN system. Note that the second term can be regarded as a point-wise effective mass plot by $m_{\rm eff}(t;\vec{x}) \equiv \frac{\partial \log(R(t,\vec{x}))}{\partial t} = \frac{(\partial/\partial t)R(t,\vec{x})}{R(t,\vec{x})}$. Its deviation from a constant can be used as a measure of contamination of excited states.

5. Summary and Conclusion

We have generalized the HAL QCD method for the lattice determination of inter-nucleon (NN) potentials from Nambu-Bethe-Salpeter (NBS) wave functions so that it can safely be used even in the presence of contamination of excited states. For this purpose, we have derived the

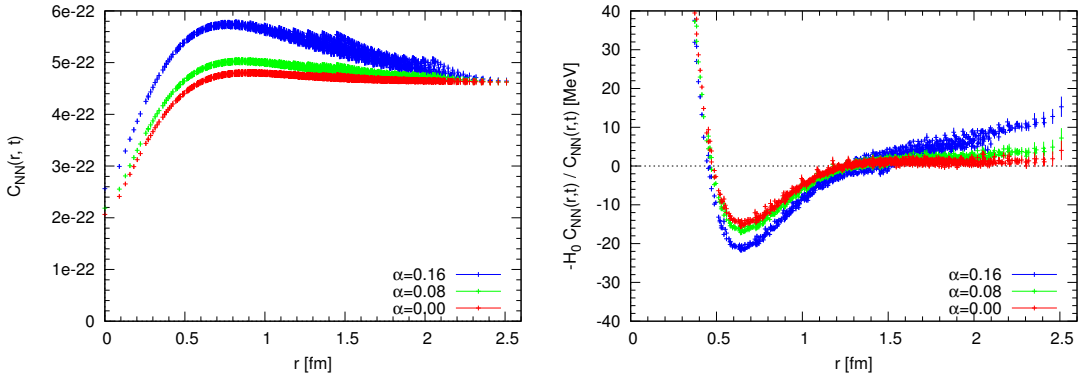

Figure 1: (left) $C_{NN}(\vec{r},t)$ at $t = 9$. (right) $-H_0 C_{NN}(\vec{r},t)/C_{NN}(\vec{r},t)$ at $t = 9$.

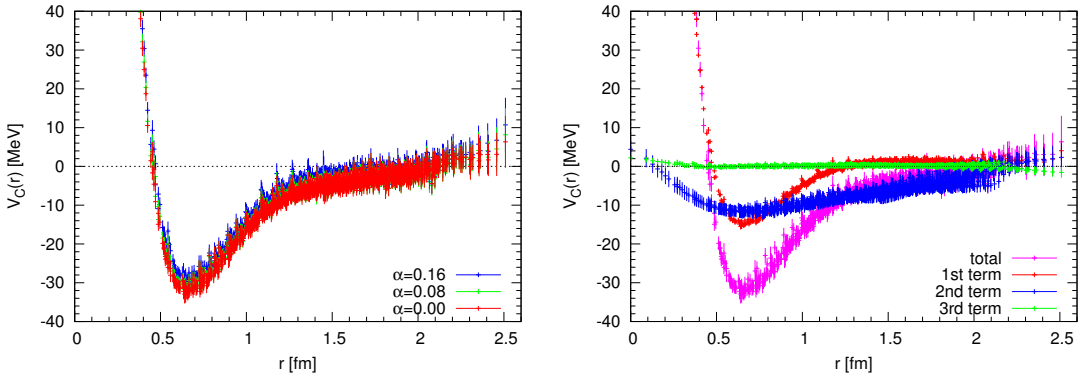

Figure 2: (left) Central potentials obtained by our new formula Eq.(3.5) at $t = 9$ for the three values of α. (right) Three contributions in Eq.(3.5) at $t = 9$ for $\alpha = 0$.

"time-dependent" Schrödinger-like equation, which is a second order differential equation in time describing time-evolution of the (normalized) four-point nucleon correlators. The equation enables us to construct NN potentials without requiring the ground state saturation in the four-point nucleon correlators. We have applied the time-dependent Schrödinger-like equation to the NN central potential in $^1S_0$ channel. We have seen that resulting potentials obtained with different two-nucleon source operators agree within the statistical errors.

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