Nuclear Force from Monte Carlo Simulations of Lattice Quantum Chromodynamics

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Abstract.
The nuclear force acting between protons and neutrons is studied in the Monte Carlo simulations of the fundamental theory of the strong interaction, the quantum chromodynamics defined on the hypercubic space-time lattice. After a brief summary of the empirical nucleon-nucleon (NN) potentials which can fit the NN scattering experiments in high precision, we outline the basic formulation to derive the potential between the extended objects such as the nucleons composed of quarks. The equal-time Bethe-Salpeter amplitude is a key ingredient for defining the NN potential on the lattice. We show the results of the numerical simulations on a 32^4 lattice with the lattice spacing \( a \simeq 0.137\text{fm} \) (lattice volume \((4.4\text{ fm})^4\)) in the quenched approximation. The calculation was carried out using the massively parallel computer Blue Gene/L at KEK. We found that the calculated NN potential at low energy has basic features expected from the empirical NN potentials; attraction at long and medium distances and the repulsive core at short distance. Various future directions along this line of research are also summarized.

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1. Introduction

One of the long standing problems in particle and nuclear physics is the origin of the strong nuclear force which holds the nucleons (protons and neutrons) inside atomic nuclei. For the past half century, phenomenological fits of the proton-proton (pp) and neutron-proton (np) scattering data assuming empirical nucleon-nucleon (NN) potentials have been attempted [1, 2]: The potentials, which can fit more than 2000 data points of the NN phase shift with $\chi^2/\text{dof} \simeq 1$ for $T_{\text{lab}} < 300\text{MeV}$, include the CD-Bonn potential [3], Argonne $v_{18}$ potential [4] and Nijmegen potentials [5]. Alternative approach on the basis of the chiral perturbation theory has been also developed [6].

Shown in Fig.1 are three examples of the empirical NN potentials in the $^1S_0$ channel.‡ From this figure, some characteristic features of the nuclear force can be seen:

I. The long range part of the nuclear force ($r > 2$ fm) is dominated by the one pion exchange originally introduced by Yukawa [8].

II. The medium range part ($1$ fm $< r < 2$ fm) receives significant contributions from the exchange of multi-pions and heavy mesons ($\rho$, $\omega$, and $\sigma$). In particular, the spin-isospin independent attraction of about $-50 \sim -100$ MeV in this region plays an essential role for binding the atomic nuclei.

III. The short range part ($r < 1$ fm) behaves as a repulsive core originally introduced by Jastrow [9] to explain the pp and np scattering phase shifts simultaneously. Such a short range repulsion is relevant to the stability of atomic nuclei, to the maximum mass of neutron stars, and to the ignition of the Type II supernova explosions [10].

It is now well established that the nucleons are made of quarks and gluons which obey the law of quantum chromodynamics (QCD) [11]. Therefore, it is tempting to derive the strong nuclear force from the quark-gluon degrees of freedom. Two nucleons have a sizable overlap at distance $r < 1$ fm since the proton’s charge radius is about 0.86 fm. Therefore, the nuclear force at short distances must be described by taking into account the direct exchange of quarks and gluons between the nucleons. So far, there have been numerous theoretical attempts to understand the nuclear force from the quark structure of the nucleon [12]. However, conclusive results have not been obtained because of the highly non-perturbative nature of QCD.

Recently, the present authors have developed a new approach to this long standing problem of nuclear force on the basis of QCD defined on a space-time lattice (LQCD) [13, 14]. In LQCD, physical quantities are expressed by highly multi-dimensional integrals which can be carried out by importance sampling method. Our idea is to define the NN potential in the coordinate space from the equal-time Bethe-Salpeter amplitude calculated on the lattice: The first results on the central NN potential in the $^1S_0$ and $^3S_1$ channels have been reported with the quenched lattice QCD simulations in

‡ A system of two nucleons with total spin $s = (0, 1)$, orbital angular momentum $L = (S, P, D, \cdots)$ and total angular momentum $J = (0, 1, 2, \cdots)$ is denoted as $^{2s+1}L_J$. 
Figure 1. Three examples of the high-precision NN potentials in the $^1S_0$ channel. AV18 stands for the Argonne $v_{18}$ potential [4], Reid93 stands for one of the Nijmegen potentials [5] and Bonn stands for the Bonn potential [7]. I, II and III correspond to the long range part, medium range part and the short range part, respectively, as discussed in the text.

15, 16, 17. Also the first results of the hyperon-nucleon potential have been reported in 18, 19.

In the following, we will outline the field theoretical derivation of the NN potential from QCD [20] in Sec.2 and Sec.3. Then, we show how to define the potential in LQCD formalism in Sec.4. The basic setup and the method of our numerical simulations are shown in Sec.5. Some numerical results of the low energy NN potential taken from 15, 16 are shown in Sec.6. The last section is devoted to summary and concluding remarks with a discussion on the future directions.

2. Bethe-Salpeter wave function and the NN potential

Let us start with the definition of the Bethe-Salpeter (BS) amplitude for the proton-neutron system,

$$\Psi_{\alpha\beta}(x, y) = \langle 0 | T[\hat{n}_\beta(y)\hat{p}_\alpha(x)] | p(\vec{q}, s)n(\vec{q}', s'); in \rangle, \quad (1)$$

$$\hat{n}_\beta(y) = \varepsilon_{abc} \left( \hat{u}_a(y)C\gamma_5\hat{d}_b(y) \right) \hat{d}_c(y), \quad (2)$$

$$\hat{p}_\alpha(x) = \varepsilon_{abc} \left( \hat{u}_a(x)C\gamma_5\hat{d}_b(x) \right) \hat{u}_{c\alpha}(x), \quad (3)$$

where $(\vec{q}, s)$ and $(\vec{q}', s')$ denote the spatial momentum and the spin-state of the incoming proton and those of the neutron, respectively. The local composite operator for the neutron (proton) are denoted by $\hat{n}_\beta(y)$ ($\hat{p}_\alpha(x)$) with the operators for the up-quark $\hat{u}(x)$ and the down-quark $\hat{d}(x)$. Also, $\alpha$ and $\beta$ denote the Dirac indices, $a$, $b$ and $c$ the color
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indices, and $C$ the charge conjugation matrix in the spinor space.

One of the advantages to use local operator for the nucleon is that the Nishijima and Zimmermann (NZ) reduction formula [21] for local composite fields can be utilized. In particular, in and out nucleon fields are defined through the Yang-Feldman equation,

$$\sqrt{Z} \hat{N}_{\text{in/out}}(x) = \hat{N}(x) - \int S_{\text{adv/ret}}(x - x'; m_N) \hat{J}(x') dx',$$

where $\hat{N}(x)$ is the nucleon composite operator ($\hat{n}(x)$ or $\hat{p}(x)$ in Eqs.(2,3)), $\hat{N}_{\text{in/out}}(x)$ is the associated in/out field, $m_N$ is the physical nucleon mass, and $\hat{J}(x) \equiv (i \partial_x - m_N) \hat{N}(x)$. The advanced/retarded propagator for the free nucleon field with the mass $m_N$ is denoted by $S_{\text{adv/ret}}(x - x'; m_N)$. The normalization factor, $\sqrt{Z}$, is the coupling strength of the composite operator $\hat{N}(x)$ to the physical nucleon state.

Through the NZ reduction formula, the BS amplitude in Eq.(1) is related to the four-point Green’s function $G_4$ of the composite nucleons which is decomposed into the free part and the scattering part, $G_4 = Z^2 (G_4^{(0)} + G_4^{(sc)})$, where $G_4^{(0)}$ is proportional to a product of the free nucleon propagators. After taking the equal time limit, $x^0 = y^0 = t$, with $\vec{r} \equiv \vec{x} - \vec{y}$, it is straightforward to rewrite Eq.(1) to the following integral equation in the c.m. frame ($\vec{q}' = -\vec{q}$) [20],

$$\Psi_{\alpha\beta}(\vec{r}, t) = \psi_{\alpha\beta}(\vec{r}; \vec{q}, s, s') e^{-2i\sqrt{q^2 + m_N^2} t},$$

$$\psi_{\alpha\beta}(\vec{r}; \vec{q}, s, s') = Zu_{\alpha}(\vec{q}, s) u_{\beta}(-\vec{q}, s') e^{iq \cdot r}$$

$$+ Z \sum_{\gamma \delta} \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k} \cdot \vec{r}} F_{\alpha\beta,\gamma\delta}(\vec{k}; \vec{q}) u_{\gamma}(\vec{q}, s) u_{\delta}(-\vec{q}, s').$$

Here $u_{\alpha}(\vec{q}, s)$ is the positive-energy plain-wave solution of the Dirac equation and $F_{\alpha\beta,\gamma\delta}(\vec{k}; \vec{q})$ is an integral kernel obtained from $G_4^{(sc)}$ after carrying out the $k_0$-integration. Hereafter, we call $\psi_{\alpha\beta}(\vec{r}; \vec{q}, s, s')$ as the Bethe-Salpeter wave function. The differential form of the above equation is obtained by multiplying $(q^2 + \nabla^2) / m_N$ to Eq.(6);

$$\frac{1}{m_N} (q^2 + \nabla^2) \psi_{\alpha\beta}(\vec{r}; \vec{q}, s, s') = K_{\alpha\beta}(\vec{r}; \vec{q}, s, s').$$

Note that we have not made any non-relativistic approximation to derive Eq.(7). An important observation is that the plain wave component of $\psi_{\alpha\beta}(\vec{r}; \vec{q}, s, s')$ is projected out by the operator $(q^2 + \nabla^2)$ so that the function $K_{\alpha\beta}(\vec{r}; \vec{q}, s, s')$ is localized in coordinate space as long as $|\vec{q}|$ stays below the inelastic threshold as noted for pion-pion scattering in [22]. This is equivalently said that the Fourier transform of $K$ with respect to $\vec{r}$, which is proportional to the half off-shell $T$-matrix relating the the on-shell state with momentum $\vec{q}$ and the off-shell state with momentum $\vec{k}$, does not develop a real pole as a function of $|\vec{k}|$, if $|\vec{q}|$ is below the inelastic threshold.

3. The NN potential

In an abbreviated notation, $(\vec{r}, \alpha, \beta) \rightarrow x$, and $(\vec{q}, s, s') \rightarrow q$, Eq.(7) is written as

$$(E_q - H_0) \psi(x; q) = K(x; q),$$

(8)
where \( E_q = \frac{q^2}{m_N} \) and \( H_0 = -\nabla^2/m_N \). This equation defined in a finite box can be used to extract various information on the NN scattering from the lattice QCD simulations:

(i) Consider \( K(x; q) \) as a measure to identify the length \( R \) beyond which the two nucleons do not interact. If we stay in such a region where \( K(x > R; q) \approx 0 \), the wave function \( \psi(x > R; q) \) can be expanded by the solution of the Helmholtz equation inside a finite box. Then one can extract the phase shift given the incoming energy \( E_q \). This is the approach originally proposed in [23] and is later elaborated to study hadron-hadron scatterings on the lattice [24, 22, 25, 26].

(ii) Alternatively, one may extract the half off-shell \( T \)-matrix in momentum space by calculating the left-hand-side of Eq.(8) in the coordinate space and making Fourier transform with respect to \( x \).

(iii) One can go one-step further and define the non-local NN potential \( U(x, x') \) from \( K(x; q) \), so that Eq.(8) becomes the Schrödinger type equation.

If we are interested only in the NN scattering phase shift in the free space, the procedure (i) is certainly enough. On the other hand, if we are interested in applying Eq.(8) to the problems of bound states and the nuclear many-body system, (ii) and (iii) are useful since they give us the off-shell information in a well-defined manner in QCD. To see this explicitly for the case (iii), we introduce a set of functions labeled by \( q \), \{\( \tilde{\psi}(x; q) \)\}, which is dual to the set \{\( \psi(x; q) \)\} in the following sense:

\[
\int dx \tilde{\psi}(x; q)\psi(x; p) = \delta_{q,p}. \tag{9}
\]

As long as the dimensions of the \( x \)-space and \( p \)-space are the same and the elements in \{\( \psi(x; p) \)\} are linearly independent, such a dual basis exists and is unique. If the dimension of \( p \)-space is less than that of \( x \)-space, the dual basis exists but is not unique.\(^\S\)

Assuming the existence (but not necessarily the uniqueness) of the dual basis, the non-local potential can be defined as

\[
U(x, x') = \int dp \, K(x, p)\tilde{\psi}(x'; p). \tag{10}
\]

The Eqs.(9,10) lead to the formula, \( K(x; q) = \int dx' \, U(x, x')\psi(x'; q) \), so that Eq.(8) becomes

\[
-\nabla^2 \psi_{\alpha\beta}(\vec{r}, \vec{q}, s, s') + \int d^3r' \, U_{\alpha\beta;\gamma\delta}(\vec{r}, \vec{r}'; \vec{q}, s, s') \psi_{\gamma\delta}(\vec{r}', \vec{q}, s, s') = E_q \psi_{\alpha\beta}(\vec{r}: \vec{q}, s, s'). \tag{11}
\]

Note that the non-local potential \( U \) can be rewritten in the form,

\[
U(\vec{r}, \vec{r}') = V(\vec{r}, \nabla)\delta(\vec{r} - \vec{r}'). \tag{12}
\]

\(^\S\) This is easily seen as follows. Let us introduce a basis \( \{e_{(1)}, e_{(2)}, \ldots, e_{(N)}\} \) in the \( N \)-dimensional vector space. The BS wave function in discretized coordinates \( \psi(x; p) \equiv \psi(i; \alpha) \) corresponds to \( e_{(\alpha)}^i \) with \( 1 \leq i \leq N \) and \( 1 \leq \alpha \leq M \leq N \). If \( M = N \), there exits a unique dual basis, \( \{\tilde{e}_{(1)}, \tilde{e}_{(2)}, \ldots, \tilde{e}_{(N)}\} \) satisfying \( \tilde{e}_{(\alpha)} \cdot e_{(\beta)} = \delta_{\alpha\beta} \) (see any textbook of linear algebra). If \( M < N \), there is still a dual basis \( \{\tilde{e}_{(1)}, \tilde{e}_{(2)}, \ldots, \tilde{e}_{(M)}\} \) satisfying the above condition for \( \alpha \leq M \) and \( \beta \leq M \). However, it is not unique because one always has a freedom to add linear combinations of \( \tilde{e}_\gamma \) \( (M + 1 \leq \gamma \leq N) \) to the above dual basis.
The general structure of $V(\vec{r}, \nabla)$ under various symmetry constraints in the non-relativistic kinematics has been worked out by Okubo and Marshak [27]. If we further make the derivative expansion at low energies [28], we obtain the expression familiar in the phenomenological potentials acting on the upper components of the wave function:

$$
V(\vec{r}, \nabla) = V_0(r) + V_T(r)(\vec{\tau}_1 \cdot \vec{\tau}_2) + V_{TS}(r)(\vec{\tau}_1 \cdot \vec{\tau}_2) + V_{LS}(r)(\vec{L} \cdot \vec{S}) + V_{LS}(r)(\vec{L} \cdot \vec{S})(\vec{\tau}_1 \cdot \vec{\tau}_2) + O(\nabla^2).
$$

(13)

Here $S_{12} = 3(\vec{\sigma}_1 \cdot \vec{n})(\vec{\sigma}_2 \cdot \vec{n}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$ is the tensor operator with $\vec{n} = \vec{r}/|\vec{r}|$, $\vec{S} = (\vec{\sigma}_1 + \vec{\sigma}_2)/2$ the total spin operators, $\vec{L} = -i\vec{r} \times \nabla$ the orbital angular momentum operator, and $\vec{\tau}_1, \vec{\tau}_2$ are the isospin operators for the nucleons. Each component of the potential in Eq.(13) can be obtained by appropriate spin, isospin and angular momentum projection of the BS wave function. Also, the higher derivative terms of the potential in Eq.(13) can be deduced by combining the BS wave functions for different incident energies.

It is in order here to remark that the structure of the non-local potential $U(x, x')$ is directly related to the nucleon interpolating operator adopted in defining the Bethe-Salpeter wave function. Different choices of the interpolating operator would give different forms of the NN potential at short distance, although they give the same phase shift at asymptotic large distance. The advantage of working in QCD is that we can unambiguously trace the connection between the NN potential and the interpolating operator.

4. Effective central potential on the lattice

The BS wave function in the $S$-wave on the lattice with the lattice spacing $a$ and the spatial lattice volume $L^3$ is obtained by

$$
\psi(r) = \frac{1}{24} \sum_{R \in O} \frac{1}{L^3} \sum_{\vec{x}} P_{\alpha\beta}^{\sigma} \langle 0 | \hat{n}_\beta (R[\vec{r}] + \vec{x}) \hat{p}_\alpha (\vec{x}) | pn; q \rangle.
$$

(14)

The summation over $R \in O$ is taken for the cubic transformation group to project out the $S$-wave. The summation over $\vec{x}$ is to select the state with zero total momentum. We take the upper components of the Dirac indices to construct the spin singlet (triplet) channel by $P_{\alpha\beta}^{\sigma = \text{singlet}} = (\sigma_2)_{\alpha\beta}$ ($P_{\alpha\beta}^{\sigma = \text{triplet}} = (\sigma_1)_{\alpha\beta}$). The BS wave function $\psi(\vec{r})$ is understood as the probability amplitude to find “neutron-like” three-quarks located at point $\vec{x} + \vec{r}$ and “proton-like” three-quarks located at point $\vec{x}$.

In the actual simulations, the BS wave function is obtained from the four-point correlator,

$$
G_4(\vec{x}, \vec{y}; t; t_0) = \left< 0 | \hat{n}_\beta (\vec{y}, t) \hat{p}_\alpha (\vec{x}, t) J_{pn}(t_0) | 0 \right> = \sum_n A_n \langle 0 | \hat{n}_\beta (\vec{y}) \hat{p}_\alpha (\vec{x}) | n \rangle e^{-En(t-t_0)}.
$$

(15)

Here $J_{pn}(t_0)$ is a wall source located at $t = t_0$, which is defined by $J_{pn}(t_0) = P_{\alpha\beta}^{\sigma} \sum_{\vec{x}, \vec{y}} \hat{p}_\alpha (\vec{x}, t_0) \hat{n}_\beta (\vec{y}, t_0)$. The eigen-energy and the eigen-state of the six quark system

|| In principle, this projection cannot remove possible contamination from the higher orbital waves with $L \geq 4$, although these contributions are expected to be negligible.
are denoted by $E_n$ and $|n\rangle$, respectively, with the matrix element $A_n(t_0) = \langle n|\mathcal{J}_{pn}(t_0)|0\rangle$. For $(t-t_0)/a \gg 1$, the $G_4$ and hence the wave function $\psi$ are dominated by the lowest energy state.

The lowest energy state created by the wall source $\mathcal{J}_{pn}(t_0)$ contains not only the $S$-wave component but also the $D$-wave component induced by the tensor force. In principle, they can be disentangled by preparing appropriate operator sets for the sink. Study along this line to extract the mixing between the $S$-wave and the $D$-wave at low energies has been put forward recently in [29]. In the present paper, instead of making such decomposition, we define an “effective” central potential $V_C(r)$ according to Refs.[15, 16]:

$$V_C(r) = E_q + \frac{1}{m_N} \nabla^2 \psi(r).$$  \hspace{1cm} (16)

Note that one can test the non-locality of the potential $U(x,x')$ by evaluating the effective central potential for different energies. If there arises appreciable energy dependence in $V_C(r)$, it is a signature of the necessity of high derivative terms in Eq.(13).

5. Setup of the lattice simulations

In lattice QCD simulations, the vacuum expectation value of an operator $O(q,\bar{q},U)$ is defined as

$$\langle O \rangle = Z^{-1} \int \prod_\ell dU(\ell) \prod_x dq(x) d\bar{q}(x) \ O(q,\bar{q},U) \ e^{-S_1(q,\bar{q},U) - S_6(U)}$$

$$= Z^{-1} \int \prod_\ell dU(\ell) \ Q(U) \det M(U) \ e^{-S_6(U)}. \hspace{1cm} (17)$$

where $Z = \int \prod_\ell dU(\ell) \prod_x dq(x) d\bar{q}(x) \ e^{-S_1(q,\bar{q},U) - S_6(U)}$ is the QCD partition function, $S_1 = \sum_{x,x'} \bar{q}(x)M_{xx'}(U)q(x')$ is the quark part of the action, and $S_6$ is the gluon part of the action. The quark field $q(x)$ is defined on each site $x$ of the hypercubic space-time lattice, while the gluon field $U(\ell)$ denoted by $3 \times 3$ special unitary matrix is defined on each link $\ell$. In Eq.(18), the integration of the quark fields is carried out analytically. In the quenched approximation adopted in our simulation, the virtual fermion loop denoted by $\det M(U)$ is set to be 1 and the integration over link variables $U$ is performed using the importance sampling method [30].

We employ the standard plaquette gauge action on a $32^4$ lattice with the bare QCD coupling constant $\beta = 6/g^2 = 5.7$. The corresponding lattice spacing is determined to be $1/a = 1.44(2)$ GeV ($a \simeq 0.137$ fm) from the $\rho$ meson mass in the chiral limit [31]. Then, the physical size of our lattice becomes $L \simeq 4.4$ fm. For the fermion action, we adopt the standard Wilson quark action with the hopping parameter ($\kappa = 0.1640, 0.1665$ and 0.1678) which controls the quark masses. The periodic (Dirichlet) boundary condition is imposed on the quark fields along the spatial (temporal) direction. To generate the quenched gauge configurations, we adopt the heatbath algorithm with overrelaxation and sample configurations are taken in every 200 sweeps after skipping 3000 sweeps for thermalization.
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| $\kappa$ | $N_{\text{conf}}$ | $m_\pi$ [MeV] | $m_N$ [MeV] | $(t - t_0)/a$ | $E_q(^1S_0)$ [MeV] | $E_q(^3S_1)$ [MeV] |
|----------|-----------------|---------------|-------------|----------------|------------------|------------------|
| 0.1640   | 1000            | 732.1(4)      | 1558.4(63)  | 7              | -0.400(83)       | -0.480(97)       |
| 0.1665   | 2000            | 529.0(4)      | 1333.8(82)  | 6              | -0.509(94)       | -0.560(114)      |
| 0.1678   | 2021            | 379.7(9)      | 1196.6(32)  | 5              | -0.675(264)      | -0.968(374)      |

Table 1. The number of gauge configurations $N_{\text{conf}}$, the pion mass $m_\pi$, the nucleon mass $m_N$, time-slice $t - t_0$ on which BS wave functions are measured, and the non-relativistic energies $E_q \equiv q^2/m_N$ for $^1S_0$ and $^3S_1$ channels.

For our numerical simulations, we use IBM Blue Gene/L at KEK, which consists of 10,240 computation nodes with total theoretical performance of 57.3 TFlops. A modified version of the CPS++ (the Columbia Physics System) [33] is used to generate quenched gauge configurations and propagators of quarks. Most of the computational time is devoted to the calculation of the four-point function of nucleons, for which our code achieves 34–48 % of peak performance. Totally about 4000 hours are used by queues with 512 nodes for the calculations of the effective central potentials corresponding to the three values of hopping parameters. The number of sampled gauge configurations $N_{\text{conf}}$, the pion mass $m_\pi$, and the nucleon mass $m_N$ are summarized in Table 1. (For $\kappa = 0.1678$, we have removed 24 exceptional gauge configurations from the sample.)

We adopt the wall source on the time-slice $t/a = t_0/a = 5$. The BS wave functions are measured on the time-slice $(t - t_0)/a = 7, 6, 5$ for $\kappa = 0.1640, 0.1646, 0.1678$, respectively. The ground state saturation is examined by the $t$-dependence of the NN potential. We employ the nearest neighbor representation of the discretized Laplacian as $\nabla^2 f(\vec{x}) \equiv \sum_{i=1}^{3} \{ f(\vec{x} + a\vec{n}_i) + f(\vec{x} - a\vec{n}_i) \} - 6 f(\vec{x})$, where $\vec{n}_i$ denotes the unit vector along the $i$-th coordinate axis. BS wave functions are fully measured for $r < 0.7$ fm, where rapid change of the NN potential is expected. Since the change is rather modest for $r > 0.7$ fm, the measurement of BS wave functions is restricted on the coordinate axes and their nearest neighbors to reduce the calculational cost. The “asymptotic momentum” $q$ is obtained by fitting the BS wave function with the Green’s function in a finite and periodic box [23]:

$$G(\vec{r}; q^2) = \frac{1}{L^3} \sum_{\vec{n} \in \mathbb{Z}^3} \frac{e^{i(2\pi/L)\vec{n} \cdot \vec{r}}}{(2\pi/L)^2 \vec{n}^2 - q^2},$$

which satisfies $(-\nabla^2 + q^2)G(\vec{r}; q^2) = -\delta_L(\vec{r})$ with $\delta_L(\vec{r})$ being the periodic delta-function. In the actual calculation, Eq.(19) is rewritten in terms of the heat kernel $\mathcal{H}$ satisfying the heat equation, $\partial_t \mathcal{H}(t, \vec{r}) = \nabla^2 \mathcal{H}(t, \vec{r})$ with the initial condition, $\mathcal{H}(t \to 0+, \vec{r}) = \delta_L(\vec{r})$. The fits are performed outside the range of NN interaction determined by $\nabla^2 \psi(\vec{r})/\psi(\vec{r})$ [25].

6. Numerical results

Fig.2 (upper panel) shows the BS wave functions in $^1S_0$ and $^3S_1$ channels for $\kappa = 0.1665$. The suppression of the wave function in the region $r < 0.5$ fm indicate the existence of
Figure 2. (Upper panel) The NN wave functions in $^1S_0$ and $^3S_1$ channels. The inset is a 3D plot of the wave function $\phi(x, y, z = 0; ^1S_0)$. (Lower panel) The NN effective central potential in the $^1S_0$ and $^3S_1$ channels for $m_\pi = 529$ MeV ($\kappa = 0.1665$).

repulsion at short distance. Fig.2 (lower panel) shows the reconstructed NN potentials for $\kappa = 0.1665$, i.e., the effective central potentials for $^1S_0$ and $^3S_1$ channels. See Table 1, for the values of the non-relativistic energies $E_q \equiv q^2/m_N$ in Eq.(16).

We show the NN potentials for three different quark masses in $^1S_0$ channel in Fig. 3. As the quark mass decreases, the repulsive core at short distance is enhanced rapidly, whereas the attraction at medium distance is modestly enhanced. This indicates that it is important to perform the lattice QCD calculations for the lighter quark mass region in order to make quantitative comparison of our results with the observables in the real world.

Although there exist both attraction and repulsion, the net effect of our potential is attractive at low energies as shown by the scattering lengths calculated from
Central potentials in the $^1S_0$ channel for three different quark masses in the quenched QCD simulations on a (4.4 fm)$^4$ lattice.

![Figure 3](image.png)

Table 2. Scattering lengths obtained from the Lüscher’s formula [23] in the spin-singlet and spin-triplet channels for different quark masses.

| $\kappa$  | $m_\pi$ [MeV] | $a_0(^1S_0)$ [fm] | $a_0(^3S_1)$ [fm] |
|-----------|----------------|-------------------|-------------------|
| 0.1640    | 732.1(4)       | 0.115(26)         | 0.140(31)         |
| 0.1665    | 529.0(4)       | 0.126(25)         | 0.140(31)         |
| 0.1678    | 379.7(9)       | 0.159(66)         | 0.252(104)        |

The Lüscher’s formula is qualitatively understood by the Born approximation formula for the scattering length $a_0 \simeq -m_N \int V_C(r) r^2 dr$. Owing to the volume factor $r^2 dr$, the attraction at medium distance can overcome the repulsive core at short distance. However, there is a considerable discrepancy between the scattering lengths in Table 2 and the empirical values, $a_0^{(exp)}(^1S_0) \sim 20$ fm and $a_0^{(exp)}(^3S_1) \sim -5$ fm. This is attributed to the heavy quark masses employed in our simulations.

If we can get closer to the physical quark mass, there appears an “unitary region” where the NN scattering length becomes singular and changes sign as a function of the quark mass [31, 32, 26]. The singularity is associated with the formation of the di-nucleon bound state. Because of this, the NN scattering length becomes a highly non-linear function of the light quark mass. One should note that the NN potential changes smoothly even in the unitary region in contrast to the scattering length. This is one of the reasons why the NN potential is much more appropriate quantity to be examined on the lattice instead of the NN scattering length.
7. Summary and concluding remarks

In this article, we have outlined the basic notion of the nucleon-nucleon potential and its field-theoretical derivation from the equal-time Bethe-Salpeter amplitude. Such a formulation allows us to extract the potential between extended objects by using the lattice QCD simulations. The central part of the NN potential at low energies was obtained in lattice QCD simulations with quenched approximation. It was found that the NN potential calculated on the lattice at low energy shows all the basic features expected from the empirical NN potentials determined from the NN scattering data; attraction at long and medium distances and the repulsion at short distance. This is the first step toward the understanding of atomic nuclei from the fundamental law of the strong interaction, the quantum chromodynamics.

There are a number of directions to be explored on the basis of our approach:

1. Energy dependence of the NN potential in Eq.(16) should be studied to test the non-locality of the potential $U(x,x')$ and the validity of its derivative expansion. This is currently under investigation by changing the spatial boundary condition of the fermion field [34].

2. The tensor force, which mixes the states with different orbital angular momentum by two units, is a unique feature of the nuclear force and plays an essential role for the deuteron binding. This is also under investigation by projecting out the $^3S_1$ component and $^3D_1$ component separately from the exact two-nucleon wave function with $J = 1$ on the lattice [29, 35]. The spin-orbit force, which is known to be strong at short distances in empirical NN force, should be also studied.

3. Three nucleon force is thought to play important roles in nuclear structure and also in the equation of state of high density matter. Since the experimental information is scarce, simulations of the three nucleons on the lattice combined with appropriate generalizations of the formulas in Section 2 may lead to the first principle determination of the three nucleon potential in the future. With these generalizations of the present approach, one may eventually make a firm link between QCD and the physics of nuclear structure [36].

4. The hyperon-nucleon (YN) and hyperon-hyperon (YY) potentials are essential for understanding the properties of hyper nuclei and the hyperonic matter inside the neutron stars. However, the experimental data are very limited due to the short lifetime of hyperons. On the lattice, NN, YN and YY interactions can be treated in the same footing since the difference is only the mass of the strange quark. Recently, the $\Xi N$ potential [18, 19] and the $\Lambda N$ potential [37] are examined as a first step toward systematic derivation of the hyperon interactions.

5. To compare the NN potential on the lattice with experimental observables, it is necessary to carry out full QCD simulations which take into account the dynamical quark loops. Study of the nuclear force with the use of the full-QCD configurations generated by PACS-CS Collaboration [38] is currently under
investigation [34, 35, 37].

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