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First results of baryon interactions from lattice QCD with physical masses (1) – General overview and two-nucleon forces –

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We present the lattice QCD studies for baryon-baryon interactions for the first time with (almost) physical quark masses. $N_f = 2+1$ gauge configurations are generated with the Iwasaki gauge action and nonperturbatively $\mathcal{O}(a)$-improved Wilson quark action with stout smearing on the lattice of $(96a)^4 \simeq (8.2\text{fm})^4$ with $a \simeq 0.085$ fm, where $m_\pi \simeq 146$ MeV and $m_K \simeq 525$ MeV. Baryon forces are calculated from Nambu-Bethe-Salpeter (NBS) correlation functions using the time-dependent HAL QCD method. In this report, we first give the general overview of the theoretical frameworks essential to the physical point calculation of baryon forces. We then present the numerical results for the two-nucleon central and tensor forces in ${}^3S_1$-${}^3D_1$ coupled channel and the central force in ${}^1S_0$ channel. In particular, a clear signal is obtained for the tensor force.

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1. Introduction

Interactions among baryons (nuclear forces and hyperon forces) are one of the most fundamental constituents in nuclear physics. For nuclear forces, thanks to the extensive studies since the celebrated work by Yukawa 80 years ago [1], precision two-nucleon forces have been established. They have been, however, obtained phenomenologically from experimental scattering phase shifts and the relation to the underlying theory, Quantum Chromodynamics (QCD), is still hidden in a veil. For hyperon forces, even phenomenological information suffers from large uncertainties, since scattering experiments with hyperon(s) are very difficult. In the meantime, the comprehensive determination of baryon forces based on QCD has become an urgent issue in not only nuclear physics but also astrophysics, in the context of, e.g., the equation of state (EoS) of high dense matter. Therefore, it is most desirable to make a systematic determination of baryon forces by the first-principles calculations of QCD, such as lattice QCD simulations.

In lattice QCD, baryon interactions have been traditionally studied using the Lüscher's finite volume method [2]. (See, e.g., Refs. [3, 4, 5] for recent works.) Recently, a novel theoretical framework, HAL QCD method, is proposed where the interaction kernels (so-called "potentials") are determined from Nambu-Bethe-Salpeter (NBS) wave functions on a lattice [6]. In particular, with the extension to the "time-dependent" HAL QCD method, energy-independent (non-local) potentials can be extracted without relying on the ground state saturation [7]. The method has been successfully applied to nuclear forces, hyperon forces including coupled channel systems, three-nucleon forces and so on [8, 9]. Obtained interactions are also used to predict the properties of medium-heavy nuclei, EoS of nuclear matter and mass-radius relation of neutron stars [10].

Albeit the significant progress in recent years, existing lattice calculations for baryon interactions suffer from various systematic uncertainties, where the most critical one is associated with unphysically heavy quark masses. Under these circumstances, we have launched a new project under the HPCI (High Performance Computing Infrastructure) SPIRE (Strategic Program for Innovative REsearch) Field 5, which aims at the lattice calculations of nuclear and hyperon potentials with physically light quark masses on a large lattice volume, exploiting the capability of the latest supercomputers such as Japanese flagship K computer. In this paper, we present the latest status report for the baryon force calculations in this (on-going) project. We first give general overview of the theoretical framework. We then present numerical results for two-nucleon (2N) central and tensor forces in parity-even channel, namely, $^3S_1$-$^3D_1$ coupled channel and $^1S_0$ channel. The results for hyperon forces obtained in the same lattice setup are presented in Refs. [11]. Detailed account on the generation of gauge configurations used in this study is given in Ref. [12].

2. Formalism

We explain the HAL QCD method for the 2N system as an illustration. We consider the (equal-time) NBS wave function in the center-of-mass frame, $\phi_W^{2N}(\vec{r}) \equiv 1/Z_N \cdot \langle 0|N(\vec{r},0)N(\vec{0},0)|2N,W\rangle_{\rm in}$, where N is the nucleon operator with its wave-function renormalization factor $\sqrt{Z_N}$ and $|2N,W\rangle_{\rm in}$ denotes the asymptotic in-state of the 2N system at the total energy of $W = 2\sqrt{k^2+m_N^2}$ with the relative momentum $k \equiv |\vec{k}|$, and we consider the elastic region, $W < W_{\rm th} = 2m_N + m_\pi$. The NBS wave function may be extracted from the four-point correlation function $G^{2N}(\vec{r},t) \equiv \frac{1}{L^3}\sum_{\vec{R}}\langle 0|(N(\vec{R}+\vec{r})N(\vec{R}))(t)\ \overline{(NN)}(t=0)|0\rangle$. The most important property of the NBS wave function is that it has a desirable asymptotic behavior at $r \equiv |\vec{r}| \to \infty$, $\phi_W^{2N}(\vec{r}) \propto \sin(kr - l\pi/2 + \delta_W^l)/(kr)$, where δ_W^l is the scattering phase shift with the orbital angular momentum l [2, 6, 13]. Exploiting this feature, we define the (non-local) 2N potential, $U^{2N}(\vec{r},\vec{r}')$, through the Schrödinger equation,

$$(E_W^{2N} - H_0)\phi_W^{2N}(\vec{r}) = \int d\vec{r}' U^{2N}(\vec{r},\vec{r}')\phi_W^{2N}(\vec{r}') \tag{2.1}$$

where $H_0 = -\nabla^2/(2\mu)$ and $E_W^{2N} = k^2/(2\mu)$ with the reduced mass $\mu = m_N/2$. It is evident that $U^{2N}(\vec{r},\vec{r}')$ is faithful to the phase shift by construction. In addition, it has been proven that one can construct $U^{2N}(\vec{r},\vec{r}')$ in an energy-independent way [6, 8]. Therefore, once $U^{2N}(\vec{r},\vec{r}')$ are obtained on a (finite volume) lattice, we can determine the phase shifts at arbitrary energies below the inelastic threshold by solving the Schrödinger equation with $U^{2N}(\vec{r},\vec{r}')$ in the infinite volume.

In the practical lattice calculations, several additional developments are necessary, in particular when calculations with physically light quark masses and larger volumes are of interest. In the following, we present three crucial developments: (1) extension to the "time-dependent" HAL QCD method (2) extension to coupled channel formalism above inelastic threshold and (3) development in computational scheme called the unified contraction algorithm.

2.1 Time-dependent HAL QCD method

In the original HAL QCD method described above, it is necessary to isolate each energy eigenstate on a lattice (most typical example is the so-called ground state saturation). Unfortunately, this is very difficult due to the existence of nearby elastic scattering states. For instance, on a lattice with the spacial extent of $L = 8.2$ fm and with physical quark masses (which is the lattice setup in this study), the first excited state of elastic 2N scattering state has $\sim (2\pi/L)^2/m_N \sim 25$ MeV excitation energy. Correspondingly, ground state saturation requires $t \gg (25\text{MeV})^{-1} \sim \mathcal{O}(10)$fm, where S/N may be suppressed by a factor of $\exp[-2(m_N - 3/2m_\pi)t] \sim 10^{-32}$.

The time-dependent HAL QCD method [7] is a suitable framework to avoid this problem. By noting that $U^{2N}(\vec{r},\vec{r}')$ is energy-independent below $W_{\rm th}$, one can show that the following "time-dependent" Schrödinger equation holds even without the ground state saturation,

$$\left(-\frac{\partial}{\partial t} + \frac{1}{4m_N}\frac{\partial^2}{\partial t^2} - H_0\right) R^{2N}(\vec{r},t) = \int d\vec{r}' U^{2N}(\vec{r},\vec{r}') R^{2N}(\vec{r}',t), \tag{2.2}$$

where $R^{2N}(\vec{r},t)$ is the NBS correlation function given by $R^{2N}(\vec{r},t) \equiv G^{2N}(\vec{r},t)/\{G^N(t)\}^2$ with $G^N(t)$ being the single nucleon correlator. It is still necessary to achieve "elastic state saturation" (suppression of contaminations from inelastic states), but it can be fulfilled by much easier condition, $t \gg (W_{\rm th} - W)^{-1} \sim m_\pi^{-1} \sim \mathcal{O}(1)$fm. This is in contrast to the Lüscher's method, which inevitably relies on the ground state saturation. (For detailed comparison between the Lüscher's method and the time-dependent HAL QCD method, see Refs. [14, 15].)

2.2 HAL QCD method for coupled channel systems

If we consider the hyperon forces, it is necessary to extend our framework so that it can be applied even above the inelastic threshold. For instance, in the calculation of $\Lambda\Lambda$ interactions, the inelastic threshold (the $N\Xi$ channel) is open only ~ 30 MeV above the $\Lambda\Lambda$ threshold. In addition, these coupled channel effects themselves are important subjects in hypernuclear physics.

The HAL QCD method can be extended to coupled channel systems thanks to the energy-independence of (coupled channel) potentials [8]. Considering the $\Lambda\Lambda$–$N\Xi$ coupled channel system

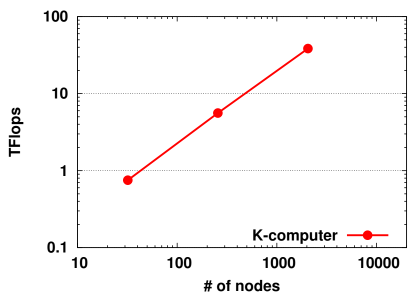

Figure 1: Weak scaling of the total flops performance for calculations of NBS correlators. Measured on K computer with excluding the I/O part.

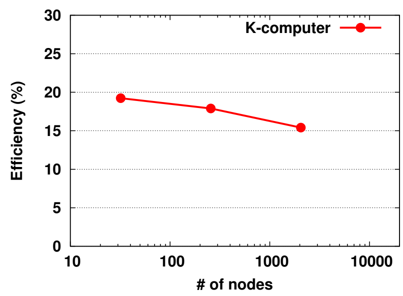

Figure 2: Same as Fig. 1, but for the performance efficiency.

as an example, coupled channel potentials $U^c{}_{c'}(\vec{r},\vec{r}')$ can be extracted from the following equations in the original (time-independent) HAL QCD method,

$$(E^c_W - H^c_0)\,\phi^c_W(\vec{r}) = \sum_{c'=a,b} \int d\vec{r}' U^c{}_{c'}(\vec{r},\vec{r}')\phi^{c'}_W(\vec{r}',t) \quad (c=a,b), \tag{2.3}$$

where a,b denotes $\Lambda\Lambda$ and $N\Xi$, respectively, and $W = 2\sqrt{m^2_\Lambda + (k^a)^2} = \sqrt{m^2_N + (k^b)^2} + \sqrt{m^2_\Xi + (k^b)^2}$, $H^c_0 = -\nabla^2/(2\mu^c)$ and $E^c_W = (k^c)^2/(2\mu^c)$ with μ^c being the reduced mass in the channel c. The NBS wave function ϕ^c_W is defined in a similar matter to the 2N case. The extension to the time-dependent HAL QCD method for coupled channel systems is straightforward [8].

2.3 Unified Contraction Algorithm (UCA)

In lattice QCD studies of multi-baryon systems, significant amount of computational resources are required for the calculation of correlation functions. The reasons are that (i) the number of Wick contractions grows factorially with mass number A, and (ii) the number of color/spinor contractions grows exponentially for larger A. In the case of the HAL QCD method, additional resources are necessary since (iii) each NBS correlation function has spacial degrees of freedom (L^3). Note also that there are many channels (correlation functions) to be calculated in order to obtain nuclear and hyperon forces. Specifically, in $N_f = 2+1$ flavor space, there exist 52 channels in particle base in the case of baryon forces between two-octet baryons in parity-even channel.

For (iii), we can reduce the computational cost by considering the "baryon-block" in momentum space together with FFT technique. (A brief explanation is given as "block algorithm" in Ref. [16].) While (i) and (ii) have been significant bottlenecks in lattice studies for multi-baryon systems, we recently develop a novel algorithm called the unified contraction algorithm (UCA). This algorithm unifies the two contractions (i) and (ii) in a systematic way, and significantly reduces the computational cost [16]. We implement UCA with the use of OpenMP + MPI hybrid parallelism in our computational code for the NBS correlators, called "Hadron-Force code." In Figs. 1 and 2, we show the weak scaling of the total flops performance and its efficiency, respectively, for the Hadron-Force code excluding the I/O part. Good weak scaling with the efficiency of 15–20 % is achieved for 32–2048 nodes ($\times$ 8 cores/node) on K computer. Together with the efficient solver for quark propagators [17], the total measurement calculation (solver and Hadron-Force code as well as I/O) achieves $\sim$ 17% efficiency, or $\sim$ 45 TFlops sustained on 2048 nodes of K computer.

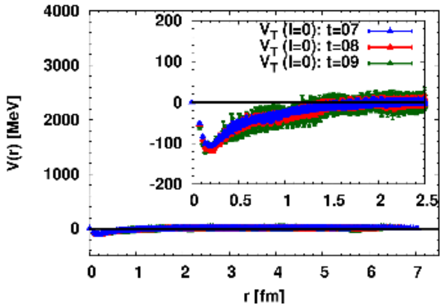

Figure 3: Nuclear tensor force $V_T(r)$ in ${}^3S_1$-${}^3D_1$ ($I=0$) channel obtained at $t = 7,8,9$.

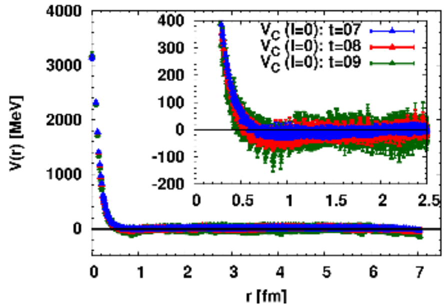

Figure 4: Nuclear central force $V_C(r)$ in ${}^3S_1$-${}^3D_1$ ($I=0$) channel obtained at $t = 7,8,9$.

3. Lattice QCD setup

$N_f = 2+1$ gauge configurations are generated with the Iwasaki gauge action at $\beta = 1.82$ and nonperturbatively $\mathscr{O}(a)$-improved Wilson quark action with $c_{sw} = 1.11$ [18] on the 96^4 lattice. We employ hopping parameters $(\kappa_{ud}, \kappa_s) = (0.126117, 0.124790)$ with APE stout smearing with $\alpha = 0.1$, $n_{\rm stout} = 6$ and the periodic boundary condition is used for all four directions. Domain-Decomposed HMC (DDHMC) is used for ud quarks and UV-filtered Polynomial HMC (UVPHMC) is used for s quark. Additional techniques such as even-odd preconditioning, mass preconditioning and multi-time scale integration are employed. Using K computer, about 2000 trajectories are generated after the thermalization, and preliminary studies show that $a^{-1} \simeq 2.33$ GeV ($a \simeq 0.085$ fm) and $m_\pi \simeq 146$ MeV, $m_K \simeq 525$ MeV [12]. This lattice setup enables us to study baryon forces with physically light quark masses on the large lattice volume of $(8.2\text{fm})^4$. For further details on the gauge configuration generation, see Ref. [12].

The measurements of NBS correlators are performed at the unitary point. We calculate all 52 channels relevant to two-octet baryon forces in parity-even channel. We employ wall quark source with Coulomb gauge fixing (which is performed after the stout smearing). The periodic boundary condition is used for spacial directions, while the Dirichlet boundary condition is used for temporal direction at $t - t_0 = 47, 48$ in order to avoid the wrapping-around artifact, and forward and backward propagations are averaged to reduce the statistical fluctuations. We pick 1 configuration per each 10 trajectories, and we make a use of the rotation symmetry to increase the statistics. The total statistics used in this report amounts to 203 configurations $\times$ 4 rotations $\times$ 20 wall sources.

4. Results

Baryon forces are determined in the time-dependent HAL QCD method in ${}^3S_1$-${}^3D_1$ and ${}^1S_0$ channels. We perform the velocity expansion [8] in terms of the non-locality of potentials, and obtain the leading order potentials, i.e., central and tensor forces. In this report, we present the results for nuclear forces: See Refs. [11] for hyperon forces. In this preliminary analysis shown below, the term which corresponds to the relativistic effects ($\partial^2/\partial t^2$-term in Eq. (2.2)) is neglected.

Let us first consider the ${}^3S_1$-${}^3D_1$ (iso-singlet) channel. The S-wave and D-wave components in NBS correlators are extracted by $\mathscr{P}$ and $(1-\mathscr{P})$-projection, respectively, where $\mathscr{P}$-projection denotes the A_1^+ projection in the cubic group and the higher partial wave mixings ($l \geq 4$) are neglected. By solving the coupled channel Schrödinger equation, we obtain the tensor and central forces. In Fig. 3, we show the tensor force $V_T(r)$ obtained at $t = 7,8,9$. Remarkably, it is clearly visible that $V_T(r) < 0$ with the long-range tail, qualitatively in accordance with phenomenological

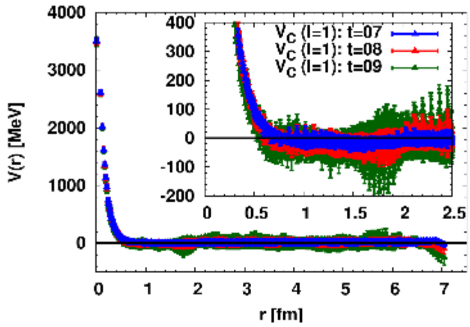

Figure 5: Nuclear central force $V_C(r)$ in $^1S_0$ $(I=1)$ channel obtained at $t=7,8,9$.

potentials and/or the structure of the one-pion-exchange potential. Compared to the lattice tensor forces obtained with heavier quark masses, the range of interaction is found to be longer. Since it is the tensor force which plays the most crucial role in the binding of deuteron, this is a very intriguing result. For more quantitative studies, it is desirable to take larger t by increasing the statistics, which is currently underway.

In Fig. 4, we show the central force $V_C(r)$ in $^3S_1$-$^3D_1$ channel obtained at $t=7,8,9$. In this case, the potentials suffer from much larger statistical fluctuations. However, the repulsive core at short-range is clearly obtained and it is also encouraging that mid- and long-range attraction tends to appear as we take larger t. Certainly, a study with larger t with larger statistics is desirable.

We then consider the $^1S_0$ (iso-triplet) channel. The S-wave components are extracted by $\mathscr{P}$-projection and the central force is obtained by solving the single channel Schrödinger equation. Shown in Fig. 5 is the obtained central force $V_C(r)$ at $t=7,8,9$. As was the case for the central force in $^3S_1$-$^3D_1$ channel, the results suffer from large statistical fluctuations. Yet, the repulsive core at short-range is observed and the tendency is seen that mid- and long-range attraction emerges as we take larger t. Investigations with larger t and larger statistics are under progress.

5. Summary

We have presented the first lattice QCD studies for baryon interactions which employ physically light quark masses. $N_f = 2+1$ gauge configurations have been generated with the Iwasaki gauge action and nonperturbatively $\mathscr{O}(a)$-improved Wilson quark action with stout smearing on the lattice of $(96a)^4 \simeq (8.2\text{fm})^4$ with $a \simeq 0.085$ fm, where $m_\pi \simeq 146$ MeV and $m_K \simeq 525$ MeV. Baryon forces have been calculated from NBS correlation functions in the HAL QCD method.

We have given a general overview of this project and presented three developments crucial for this study: (1) time-dependent HAL QCD method, by which notorious ground state saturation can be avoided (2) coupled channel HAL QCD formalism above inelastic threshold, which is particularly useful for hyperon forces and (3) unified contraction algorithm for the efficient computation.

Preliminary numerical results for the two-nucleon central and tensor forces in $^3S_1$-$^3D_1$ coupled channel and the central force in $^1S_0$ channel have been shown. In particular, we have observed a clear signal for the tensor force. Together with the results for hyperon forces [11] and with increased statistics available soon, we expect to mark a significant milestone which bridges particle physics and nuclear physics as well as astrophysics.

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