Medium-heavy Nuclei from Lattice Quantum Chromodynamics

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Mass and structure of ^{16}O and ^{40}Ca are deduced from the quantum chromodynamics (QCD), the fundamental theory of the strong interaction. We derive two-nucleon potentials in lattice QCD simulations by the HAL QCD method. Then we apply the potentials to the nuclei using the Brueckner-Hartree-Fock theory. We find that these two nuclei are bound and possess shell structures, for a heavy quark mass corresponding to a pseudo-scalar meson mass of 469 MeV (a nucleon mass of 1161 MeV). Obtained total binding energies, 35 MeV for ^{16}O and 113 MeV for ^{40}Ca, are rather smaller than the experimental data indeed, but it is due to the unrealistic quark mass in our lattice QCD simulations.

1 Introduction

It is established that QCD is the fundamental theory of the strong interaction. However, explaining properties of nuclei starting from QCD still remains one of the most challenging problem in physics. There are several attempts to obtain mass of nuclei from lattice QCD simulations at heavy quark masses [1, 2], but direct calculations are limited only to very light nuclei, *i.e.* mass number $A \leq 4$, due to computation costs and, more severely, due to several fundamental difficulties. In this paper, we employ an alternative approach to study mass and structure of medium heavy nuclei starting from QCD.

The HAL QCD method was proposed to extract the nucleon-nucleon interaction from lattice QCD [3]. In this method, a non-local but energy independent potential of the interaction is defined and determined through the Nambu-Bethe-Salpeter wave function of the system which can be measured in lattice QCD numerical simulations. This method has been developed further and applied to many other systems [4]. The HAL QCD approach has several advantages over the direct calculations for multi-hadron system. First of all, this method does not require the ground-state saturation, which is unavoidable in the direct calculation but is usually very difficult or even impossible to achieve for multi-baryon systems, in particular on a large spacial-volume. Secondly, this method does not require the infinite-volume extrapolation, since the potential is insensitive to the lattice volume, as long as the spatial extension is larger than the interaction range between hadrons. On top of these advantages, there is one significant advantage, namely, one can extract many physical observables in this approach. For example, solving the two-body Schrödinger equation with the potential, one can obtain scattering phase-shifts as a function of energy as well as the scattering length. Moreover, combining the lattice QCD potentials with sophisticated many-body theories, one can study nuclei or even nucleon matters based on QCD [5]. In this paper, we investigate ^{16}O and ^{40}Ca nuclei starting from QCD for the first time in history.

2 Method

There are several methods to investigate nuclei based on a free-space nucleon-nucleon interaction. The Green's function Monte Carlo method and the no-core shell model are successfully applied to nuclei around ^{12}C, but exact application to nuclei with $A > 14$ seems difficult at this moment. To study larger A nuclei, the Hartree-Fock mean field approximation has been applied traditionally. Since the Brueckner theory explains the independent particle nature of nuclei, which is a foundation of the mean field theory and shell models, the Brueckner-Hartree-Fock (BHF) theory became a standard framework for heavy nuclei [6]. In this paper, we adopt the lowest order BHF theory for our first study of medium heavy nuclei from QCD.

To study finite nuclei in the BHF theory, G matrix in a single-particle-orbit basis is needed and obtained by solving the integral Bethe-Goldstone equation

$$G(\omega)_{ij,kl} \;=\; V_{ij,kl} \;+\; \frac{1}{2}\sum_{m,n}^{>e_F} \frac{V_{ij,mn}\,G(\omega)_{mn,kl}}{\omega - e_m - e_n + i\epsilon} \tag{1}$$

where indices i to n stands for a single-particle energy-eigenstate and V is the two-nucleon interaction potential and the sum runs over excluding occupied states of the nucleus. With G matrix, single-particle potential U is given by $U_{ab} = \sum_{c,d} G(\tilde{\omega})_{ac,bd}\,\rho_{dc}$, where indices a, b, c, d corresponds to a basis-function for which we use a harmonic-oscillator wave function, and ρ is the density matrix in this basis, which is given with the wave function of energy-eigenstate Ψ^i by $\rho_{ab} = \sum_i^{occ} \Psi_a^i \Psi_b^{i*}$, where the sum runs over occupied states of the nucleus. While, the energy-eigenstates are given by solution of the Hartree-Fock equation $[K + U]\,\Psi^i = e_i \Psi^i$ with the potential U and the kinetic energy operator K. These equations are highly coupled, and self-consistent G, U, ρ, Ψ^i and e_i are determined in the iterative procedure. Finally, the Hartree-Fock ground state energy of the nucleus is given with the self-consistent U and ρ by,

$$E_0 = \sum_{a,b}\left[K_{ab} + \frac{1}{2}U_{ab}\right]\rho_{ba} - K_{\rm cm} \tag{2}$$

where $K_{\rm cm}$ is the kinetic energy of the spurious center-of-mass motion in the potential rest flame which is included in the first term.

The two-nucleon potential which we adopt at eq.(1) is the one which we derived from lattice QCD in ref. [5]. There, dynamical lattice QCD simulations ware carried out at five degenerated u, d, s-quark masses. Measured hadron masses $\{M_{\rm PS}\ , M_{\rm B}\}$ ranges from {1171, 2274} MeV to {469, 1161} MeV, where PS and B abbreviate the pseudo-scalar meson and the octet baryon, respectively. Extracted two-nucleon potentials in $^1S_0$, $^3S_1$ and $^3D_1$ channels, share common features with phenomenological ones, *i.e.* the strong repulsive core at short distance, the attractive pocket at intermediate distance, and the strong $^3S_1$-$^3D_1$ coupling, and accordingly, reproduce experimental phase-shifts qualitatively [5]. In this paper, we include two-nucleon interaction in these three channels and omit that in higher partial waves due to a lack of lattice QCD data. We ignore the Coulomb force between protons for simplicity. For details of numerical procedure of BHF calculation, we follow ref. [7].

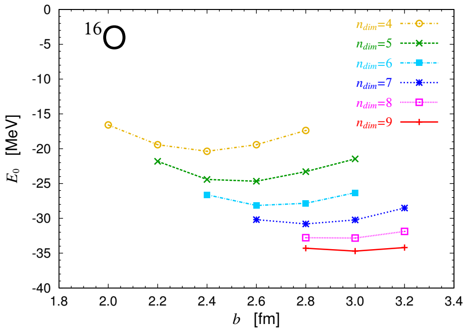

Figure 1: Ground state energy of ^{16}O at a quark mass of $M_{\rm PS} \simeq 469$ MeV

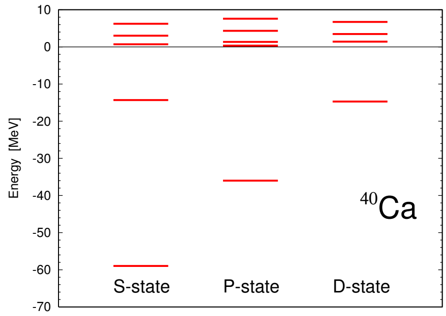

Figure 2: Single particle levels in the ^{40}Ca at a quark mass of $M_{\rm PS} \simeq 469$ MeV.

3 Results and discussion

Figure 1 shows obtained ground state energy of ^{16}O at the lightest quark mass corresponding to $M_{\rm PS} \simeq 469$ MeV, as a function of parameter b and number n_{dim} of the harmonic-oscillator wave function used as basis. We obtain a similar figure for ^{40}Ca at this quark mass. Consequently, we confirm that there are bound nuclei at this quark mass. While, we do not obtain any negative E_0 for both ^{16}O and ^{40}Ca at the other four quark masses, which at least exclude existence of tightly bound nucleus at these quark masses. In the following, we therefore consider only the lightest quark mass case, where pion mass is 469 MeV and nucleon mass is 1161 MeV. Since a computation of ^{40}Ca with $n_{dim} = 10$ is already tough on PC, we adopt $b = 3.0$ fm and $n_{dim} = 9$ for both ^{16}O and ^{40}Ca, according to the figure. Figure 2 shows obtained single particle levels of ^{40}Ca, where we can see a regular shell structure. These levels are already in good agreement with experimental data, but it could be accidental since quark masses are different.

Table 1 shows mass and structure of ^{16}O and ^{40}Ca nuclei obtained at the lightest quark, where single particle levels, total energy, and mean radius are given. Experimental data of the total energies are -127.62 MeV for ^{16}O and -342.05 MeV for ^{40}Ca. We see that the obtained binding energies are rather smaller than the experimental ones, but this is principally due to the large u, d-quark mass in our calculation. The root-mean-square radii are calculated without taking nucleon form factor and correction for the center-of-mass motion. Contrary to large discrepancies of E_0 from experimental data, these radii are more of less similar to experimental charge radius, 2.73 fm for ^{16}O and 3.48 fm for ^{40}Ca, probably due to an accidental cancellation between contributions from weaker attraction of the nuclear force and heavier nucleon mass than experimental values in this study.

In our previous papers [5], we studied the ^{4}He nucleus and the symmetric nuclear matter (SNM) from lattice QCD. We obtained energy per particle E_0/A as -1.3 MeV for ^{4}He and -5.4 MeV for SNM at the same lightest quark mass. We can see in Table 1 that the present E_0/A of ^{16}O and ^{40}Ca lie between these two values, which means that obtained E_0 are consistent with the previous results and reasonable for the nuclei at the quark mass. Moreover, in the real world, it is known that binding energy of nuclei are well described by the semi-empirical Bethe-Weizsäcker formula $E_0(A) = a_V A + a_S A^{2/3} + \cdots$. We find that E_0/A obtained from QCD at the quark mass are well described by the formula with $a_V = -5.46$ MeV and $a_S = 6.56$ MeV, when $E_0(n_{dim})$ of ^{16}O and ^{40}Ca are extrapolated for $n_{dim} \to \infty$ with $E_0(n_{dim}) = E_0(\infty) + c/n_{dim}$.

	Single particle level [MeV]				Total energy [MeV]		Radius [fm]
	$1S$	$1P$	$2S$	$1D$	E_0	E_0/A	$\sqrt{\langle r^2 \rangle}$
^{16}O	-35.8	-13.8			-34.7	-2.17	2.35
^{40}Ca	-59.0	-36.0	-14.7	-14.3	-112.7	-2.82	2.78

Table 1: Mass and structure of ^{16}O and ^{40}Ca nuclei obtained from QCD at a quark mass corresponding to pseudo-scalar meson mass of 469 MeV and octet baryon mass of 1161 MeV. Single particle levels, total energy, and root-mean-square radius are listed.

In this paper, we've obtained mass and structure of ^{16}O and ^{40}Ca nuclei from QCD at a heavy quark mass for the first time in history. This success is certainly a significant progress in theoretical nuclear physics, and demonstrates that the HAL QCD approach is quite promising.

In this study, we neglected P, F and higher partial-wave nuclear forces, in particular the LS force. It is known that the LS force is important for structures of nuclei, such as the magic number, especially at the region of heavy nuclei $A > 40$. We will include in our next study the LS force recently extracted in lattice QCD [8]. It is also known that three-nucleon force is necessary for quantitative explanation of mass and structure of nuclei. Study toward three-nucleon force from QCD is in progress [9]. Masses of u, d-quark in this study are much heavies than physical values, but this limitation will be removed in a few years, as lattice QCD simulations at the physical quark mass are currently underway on the K-computer at RIKEN AICS in Japan. Nuclear force obtained in such simulations by the HAL QCD approach will open a new connection between QCD and nuclear physics.

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