Bound states of multi-nucleon channels in $N_f = 2 + 1$ lattice QCD

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We calculate the energies for multi-nucleon ground states with the nuclear mass number less than or equal to 4 in 2+1 flavor QCD at the lattice spacing of $a = 0.09$ fm employing a relatively heavy quark mass corresponding to $m_{\pi} = 0.51$ GeV. We investigate the volume dependence of the energy shift of the ground state and the state of free nucleons to distinguish a bound state from attractive scattering states. From the investigation we conclude that $^4$He, $^3$He, deuteron and dineutron are bound at $m_{\pi} = 0.51$ GeV. We compare their binding energies with those in our quenched studies and also with some recent investigations.
1. Introduction

Lattice QCD has a potential ability to quantitatively understand the nature of nuclei, whose characteristic feature is a hierarchical structure in the strong interaction. The nuclear binding energy is experimentally known to be about 10 MeV per nucleon, which is much smaller than the typical energy scale of hadrons. A measurement of the binding energies is therefore the first step for direct investigation of nuclei in lattice QCD.

In this direction we carried out a first attempt to measure the binding energies of the $^4$He and $^3$He nuclei in quenched QCD with a rather heavy quark mass corresponding to $m_\pi = 0.80$ GeV, thereby avoiding heavy computational cost [1]. We followed this work by a renewed investigation of the bound state for the two-nucleon channel in quenched QCD at the same quark mass, which found that not only the deuteron in the $^3S_1$ channel but also the dineutron in the $^1S_0$ channel is bound [2]. However, the bound state in the $^1S_0$ channel has not been observed in the experiment.

The situation of the two-nucleon channel is little complicated. There are two approaches to study the two-nucleon channel, such as direct calculation of the ground state energy [3, 4, 5, 6, 7, 8] and indirect calculation using the effective potential [9]. The studies with former approach, which is same as in our previous work, reported a possibility of the bound state in both the channels at $m_\pi = 0.39$ GeV in 2+1 flavor QCD [7], and the bound state formations at $m_\pi = 0.81$ GeV in 3-flavor QCD [8]. The pion mass of the 3-flavor case is comparable to the one of our quenched case, but the binding energies in the 3-flavor are about twice larger than ours. To understand the situation of the two-nucleon channel, we need further investigations with less systematic errors.

In order to reduce systematic errors, such as the quenched effect and heavier quark mass, we extend our previous works to the dynamical quark calculation with a lighter mass. In this report we present our results of the binding energies of the helium nuclei, the deuteron and the dineutron on 2+1 flavor QCD with the degenerate $u, d$ quark mass corresponding to $m_\pi = 0.51$ GeV. The details of this work have been already published in Ref. [10].

2. Simulation details

We generate 2+1 flavor gauge configurations with the Iwasaki gauge action [11] and the non-perturbative $O(a)$-improved Wilson quark action at $\beta = 1.90$ with $c_{SW} = 1.715$ [12]. The lattice spacing is $a = 0.8995(40)$ fm, corresponding to $a^{-1} = 2.194(10)$ GeV, determined with $m_\Omega = 1.6725$ GeV [13]. We take four lattice sizes, $L^3 \times T = 32^3 \times 48, 40^3 \times 48, 48^3 \times 48$ and $64^3 \times 64$, to investigate the spatial volume dependence of the ground state energy shift between the multi-nucleon system and the free nucleons. The physical spatial extents are 2.9, 3.6, 4.3 and 5.8 fm, respectively. From the investigation we distinguish a bound state from an attractive scattering state [14, 15, 16, 17]. Since it becomes harder to obtain a good signal-to-noise ratio at lighter quark masses for multi-nucleon systems [18, 8], we employ heavier $u, d$ quark mass corresponding to $m_\pi = 0.51$ GeV and $m_N = 1.32$ GeV. On the other hand, the strange quark mass is close to the physical value. The hopping parameters are $(\kappa_{ud}, \kappa_s) = (0.1373316, 0.1367526)$ which are chosen based on the previous results for $m_\pi$ and $m_s$ obtained by PACS-CS Collaboration [19, 13].
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We extract the ground state energies of the multi-nucleon systems and the nucleon state from

the correlation functions $G_O(t) = \langle 0 | O(t) \overline{O}(0) | 0 \rangle$ with $O$ being appropriate operators for $^4$He, $^3$He, two-nucleon $^3S_1$ and $^1S_0$ channels, and the nucleon state $N$.

We are interested in the energy shift between the ground state of the multi-nucleon system and the free nucleons on an $L^3$ box,

$$\Delta E_L = E_O - N_N m_N$$

with $E_O$ being the lowest energy level for the multi-nucleon channel, $N_N$ the number of nucleon and $m_N$ the nucleon mass. This quantity is directly extracted from the ratio of the multi-nucleon correlation function divided by the $N_N$-th power of the nucleon correlation function

$$R(t) = \frac{G_O(t)}{(G_N(t))^{N_N}},$$

when $t$ is large enough. The same source operator is chosen for the numerator and the denominator. We also define the effective energy shift as

$$\Delta E_L^{\text{eff}} = \ln \left( \frac{R(t)}{R(t+1)} \right),$$

from which we check the plateau region.

3. Results

3.1 $^4$He nucleus

The effective energy shift $\Delta E_L^{\text{eff}}$ defined in Eq. (2.3) is plotted in the left panel of Fig. 1. The signal is clear up to $t = 12$, beyond which the statistical error increases rapidly. The energy shift $\Delta E_L$ is extracted from $R(t)$ of Eq. (2.2) by an exponential fit. The fit result is denoted by the solid...
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Figure 2: Same as Fig. 1 for $^3$He channel.

The right panel of Fig. 1 shows the volume dependence of $\Delta E_L$ as a function of $1/L^3$. The inner bar denotes the statistical error and the outer bar represents the statistical and systematic errors combined in quadrature. The negative energy shifts are obtained in all the four volumes. We extrapolate the results to the infinite volume limit with a simple linear function of $1/L^3$,

$$\Delta E_L = \Delta E_\infty + \frac{C_L}{L^3}. \quad (3.1)$$

The systematic error is estimated from the variation of the results obtained by alternative fits which contain a constant fit of the data and a fit of the data obtained with a different fit range in $t$, where the minimum or maximum time slice is changed by $\pm 1$.

The non-zero negative value obtained for the infinite volume limit $\Delta E_\infty$ shown in the figure leads us to conclude that the ground state is bound in this channel for the quark mass. The binding energy $-\Delta E_\infty = 43(12)(8)$ MeV, where the first error is statistical and the second one is systematic, is consistent with the experimental result of 28.3 MeV and also with the previous quenched result at $m_\pi = 0.80$ GeV [2], although the error is still quite large.

A recent work in 3-flavor QCD at $m_\pi = 0.81$ GeV reported a value $110(20)(15)$ MeV for the binding energy of $^4$He nucleus [8]. This is about three times deeper than our value. Whether this difference can be attributed to the quark mass dependence in unquenched calculations needs to be clarified in future.

3.2 $^3$He nucleus

The left panel of Fig. 3 shows the effective energy shift $\Delta E^\text{eff}_L$ of Eq. (2.3). An exponential fit of $R(t)$ in Eq. (2.2) yields a negative value, which is denoted by the solid lines with the statistical error band in the figure.

The volume dependence is illustrated in the right panel of Fig. 2 as a function of $1/L^3$ with the inner and outer error bars as explained in the previous subsection. We carry out a linear extrapolation of Eq. (3.1). The systematic error is estimated in the same way as in the $^4$He channel. The right panel of Fig. 3 shows that the energy shift extrapolated to the infinite spatial volume limit is
non-zero and negative. This means that the ground state is a bound state in this channel. The value of $-\Delta E_\infty = 20.3(4.0)(2.0)$ MeV is roughly three times larger than the experimental result, 7.72 MeV, though consistent with our previous quenched result at $m_\pi = 0.80$ GeV [2].

In 3-flavor QCD $-\Delta E_\infty = 71(6)(5)$ MeV was reported [8] at a heavier quark mass corresponding to $m_\pi = 0.81$ GeV. Here again future work is needed to see if a quark mass dependence explains the difference from the experiment.

### 3.3 Two-nucleon channels

In the left panel of Fig. 3 we show the time dependence for $\Delta E^\text{eff}_L$ of Eq. (2.3) in the $^3S_1$ channel. The signals are lost beyond $t \approx 14$. We observe negative values beyond the error bars in the plateau region. We extract the value of $\Delta E_L$ from an exponential fit for $R(t)$ of Eq. (2.2).

The left panel of Fig. 4 shows the result for $\Delta E^\text{eff}_L$ in the $^1S_0$ channel. The value of $\Delta E^\text{eff}_L$ is again negative beyond the error bars in the plateau region, though the absolute value is smaller than in the $^3S_1$ case. The energy shift $\Delta E_L$ is obtained in the same way as for the $^3S_1$ channel.

The volume dependences of $\Delta E_L$ in the $^3S_1$ and $^1S_0$ channels are plotted as a function of $1/L^3$ in the right panel of Figs. 3 and 4, respectively. There is little volume dependence for $\Delta E_L$. 

**Figure 3:** Same as Fig. 1 for $^3S_1$ channel.

**Figure 4:** Same as Fig. 1 for $^1S_0$ channel. There is no experimental value.
indicating a non-zero negative value in the infinite volume and a bound state, rather than the $1/L^3$ dependence expected for a scattering state, for the ground state for both channels.

The binding energies in the infinite spatial volume limit are obtained by fitting the data with a function including a finite volume effect on the two-particle bound state \[\Delta E_L = -\frac{\gamma^2}{m_N} \left\{ 1 + \frac{C_T}{\gamma L} \sum_{\bar{n}}' \frac{\exp(-\gamma L \sqrt{\bar{n}^2})}{\sqrt{\bar{n}^2}} \right\}, \quad (3.2)\]

where $\gamma$ and $C_T$ are free parameters, $\bar{n}$ is three-dimensional integer vector, and $\sum_{\bar{n}}'$ denotes the summation without $|\bar{n}| = 0$. The binding energy $-\Delta E_\infty$ is determined from

\[-\Delta E_\infty = \frac{\gamma^2}{m_N} \approx 2m_N - 2\sqrt{m_N^2 - \gamma^2}. \quad (3.3)\]

The systematic error is estimated from the variation of the fit results choosing different fit ranges in the determination of $\Delta E_L$ and also using constant and linear fits as alternative fit forms. We obtain the binding energies $-\Delta E_\infty$=11.5(1.1)(0.6) MeV and 7.4(1.3)(0.6) MeV for the $^3S_1$ and $^1S_0$ channels, respectively. The result for the $^3S_1$ channel is roughly five times larger than the experimental value, 2.22 MeV. Our finding of a bound state in the $^1S_0$ channel contradicts the experimental observation. These features are consistent with our quenched results with a heavy quark mass corresponding to $m_\pi=0.80$ GeV \[3\].

The most recent study \[8\] at a heavier quark mass of $m_\pi=0.81$ GeV in 3-flavor QCD found large values for the binding energies: 25(3)(2) MeV for the $^3S_1$ channel and 19(3)(1) MeV for the $^1S_0$ channel. While all recent studies \[2, 7, 8\] are consistent with a bound ground state for both $^3S_1$ and $^1S_0$ channels when quark masses are heavy, quantitative details still need to be clarified.

4. Conclusion and discussion

We have calculated the binding energies for the helium nuclei, the deuteron and the dineutron in 2+1 flavor QCD with $m_\pi=0.51$ GeV and $m_N=1.32$ GeV. The bound states are distinguished from the attractive scattering states by investigating the spatial volume dependence of the energy shift $\Delta E_L$. While the binding energy for the $^4$He nucleus is comparable with the experimental value, those for the $^3$He nucleus and the deuteron are much larger than the experimental ones. Furthermore we detect the bound state in the $^1S_0$ channel as in the previous study with quenched QCD, which is not observed in nature. To understand the discrepancy from the experimental results we need further study of systematic errors in our results, especially for the heavier quark mass employed in the calculations.

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