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Helium nuclei in quenched lattice QCD

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We present results for the binding energies for ^{4}He and ^{3}He nuclei calculated in quenched lattice QCD at the lattice spacing of $a = 0.128$ fm with a heavy quark mass corresponding to $m_\pi = 0.8$ GeV. Enormous computational cost for the nucleus correlation functions is reduced by avoiding redundancy of equivalent contractions stemming from permutation symmetry of protons or neutrons in the nucleus and various other symmetries. To distinguish a bound state from an attractive scattering state, we investigate the volume dependence of the energy difference between the nucleus and the free multinucleon states by changing the spatial extent of the lattice from 3.1 to 12.3 fm. A finite energy difference left in the infinite spatial volume limit leads to the conclusion that the measured ground states are bounded. It is also encouraging that the measured binding energies and the experimental ones show the same order of magnitude.

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The atomic nuclei have been historically treated as collections of protons and neutrons. The great success of the nuclear shell model since 1949 [1,2], explaining the nuclear magic numbers and detailed spectroscopy, has established that protons and neutrons are very good effective degrees of freedom at the nuclear energy scale of a few MeV. Nonetheless, 60 years later, we know for certain that protons and neutrons are made of quarks and gluons whose laws are governed by QCD. It is a great challenge to quantitatively understand the structure and property of known nuclei based on the first principle of QCD. This direct approach will be more important and indispensable if we are to extract reliable predictions for experimentally unknown nuclei in the neutron-rich regions of the nuclear chart. In this article, we address the fundamental question in the research in this direction, namely, the binding energies of nuclei.

Interacting multibaryon systems have been investigated by several studies in lattice QCD. Nucleon-nucleon scattering was first studied in quenched QCD [3,4]. This work was followed by a partially quenched mixed action simulation in Ref. [5]. Extraction of nuclear force between two nucleons has been investigated in quenched and $2+1$ flavor QCD [6–8]. All these studies assumed that the deuteron channel is not bound for the heavy pion mass, $m_\pi \gtrsim 0.3$ GeV, employed in the calculations. Very recently, NPLQCD Collaboration has tried a feasibility study of the three-baryon system, focusing on the quantum number of $\Xi^0\Xi^0 n$. They found the interaction to be repulsive [9]. So far, no evidence supporting bound-state formation in multibaryon systems has been observed in lattice QCD. In this article, we examine the helium nuclei, ^{4}He and ^{3}He, in quenched lattice QCD using a heavy quark mass at a single lattice spacing.

The binding energy ΔE of the nucleus, consisting of N_N nucleons with the mass m_N, is very tiny compared with the mass M of the nucleus: $\Delta E/M \sim O(10^{-3})$ with $\Delta E = N_N m_N - M$. This causes a complicated situation in that it is difficult to distinguish the physical binding energy from the energy shift due to the finite volume effect in the attractive scattering system [10]. One way to solve the problem is to investigate the volume dependence of the measured energy shift: In the attractive scattering system, the energy shift is proportional to $1/L^3$ at the leading order in the $1/L$ expansion [10,11], while the physical binding energy remains at a finite value at the infinite spatial volume limit. In our simulation, we choose three spatial extents corresponding to 3.1, 6.1, and 12.3 fm, which are much larger than those employed in current numerical simulations so as to provide sufficient room for the interacting multinucleon system.

A major computational problem with multinucleon systems in lattice QCD is a factorially large number of Wick contractions of quark-antiquark fields required for evaluations of the nucleus correlation functions. A naive counting would give $(2N_p + N_n)!(2N_n + N_p)!$ for a nucleus composed of N_p protons and N_n neutrons, which quickly becomes prohibitively large beyond a three-nucleon system, e.g., 2880 for ^{3}He and 518 400 for ^{4}He.

This number, however, contains equivalent contractions under the permutation symmetry in terms of the protons or the neutrons in the interpolating operator. We can reduce the computational cost by avoiding the redundancy. In case of the ^{4}He nucleus, which consists of the same number of protons and neutrons, the isospin symmetry also helps us reduce the necessary contractions. After a scrutiny of the remaining equivalent contractions by a computer, we find that only 1107 (93) contractions are required for the ^{4}He (^{3}He) nucleus correlation function. We have made a numerical test that the result with the reduced contractions reproduces the one with the full contractions on a configuration.

Another technique to save the computational cost is a modular construction of the nucleus correlation functions. We first make a block of three quark propagators where a nucleon operator with zero spatial momentum is constructed in the sink time slice. In this procedure, we can incorporate the permutation symmetry of two up (down) quarks in a proton (neutron) sink operator. This is a simple trick to calculate 2^{N_N} contractions simultaneously. We also prepare several combinations of the two blocks, which are useful for the construction of the nucleus correlators.

We carry out calculations on quenched configurations generated with the Iwasaki gauge action [12] at $\beta = 2.416$, whose lattice spacing is $a = 0.128$ fm determined with $r_0 = 0.49$ fm as an input [13]. We employ the hybrid Monte Carlo algorithm with the Omelyan-Mryglod-Folk integrator [14,15]. The step size is chosen to yield reasonable acceptance rate presented in Table I. We take three lattice sizes, $L^3 \times T = 24^3 \times 64$, $48^3 \times 48$, and $96^3 \times 48$, to investigate the spatial volume dependence of the energy difference between the nucleus and the free multinucleon states. The physical spatial extents are 3.1, 6.1, and 12.3 fm, respectively.

We use the tadpole-improved Wilson action with $c_{\rm SW} = 1.378$ [13]. Since it becomes harder to obtain a reasonable signal-to-noise ratio at lighter quark masses for the multinucleon system, we employ a heavy quark mass at $\kappa = 0.134\,82$, which gives $m_\pi = 0.8$ GeV for the pion mass and $m_N = 1.6$ GeV for the nucleon mass. Statistics are increased by repeating the measurement of the nucleus correlation functions with the source points in different time slices on each configuration. The numbers for the configurations and the measurements on each configuration are summarized in Table I. We separate 100 trajectories between each measurement with $\tau = 1$ for the trajectory length. The errors are estimated by the jackknife analysis, choosing 200 trajectories for the bin size.

TABLE I. Number of configurations ($N_{\rm conf}$), number of measurements on each configuration ($N_{\rm meas}$), acceptance rate in the hybrid Monte Carlo algorithm, pion mass (m_π), and nucleon mass (m_N).

L	$N_{\rm conf}$	$N_{\rm meas}$	Acceptance (%)	m_π [GeV]	m_N [GeV]
24	2500	2	93	0.8000(3)	1.619(2)
48	400	12	93	0.7999(4)	1.617(2)
96	200	12	68	0.8002(3)	1.617(2)

The quark propagators are solved with the periodic boundary condition in all the spatial and temporal directions, and using the exponentially smeared source $Ae^{-B|\vec{x}|}$ after the Coulomb gauge fixing. On each volume, we employ two sets of the smearing parameters: $(A, B) = (0.5, 0.5)$ and $(0.5, 0.1)$ for $L = 24$ and $(0.5, 0.5)$ and $(1.0, 0.4)$ for $L = 48$ and 96. Effective mass plots with different sources, which are shown later, help us confirm the ground state of the nucleus. Hereafter, the first and the second smearing parameter sets are referred to as "$S_{1,2}$," respectively.

The interpolating operator for the proton is defined as $p_\alpha = \varepsilon_{abc}([u_a]^t C\gamma_5 d_b)u_c^\alpha$, where $C = \gamma_4\gamma_2$ and α and a, b, and c are the Dirac index and the color indices, respectively. The neutron operator n_α is obtained by replacing u_c^α by d_c^α in the proton operator. To save the computational cost we use the nonrelativistic quark operator, in which the Dirac index is restricted to upper two components.

The ^{4}He nucleus has zero total angular momentum and positive parity $J^P = 0^+$ with the isospin singlet $I = 0$. We employ the simplest ^{4}He interpolating operator with the zero orbital angular momentum $L = 0$, and hence $J = S$ with S being the total spin. Such an operator was already given a long time ago in Ref. [16], $^4{\rm He} = (\bar{\chi}\eta - \chi\bar{\eta})/\sqrt{2}$, where $\chi = ([+-+-] + [-++-] - [+--+] - [-++-])/2$ and $\bar{\chi} = ([+-+-] + [-+-+] + [+--+] + [-++-] - 2[++--] - 2[--++])/\sqrt{12}$ with $+/-$ being the up/down spin of each nucleon. η, $\bar{\eta}$ are obtained by replacing $+/-$ in χ, $\bar{\chi}$ by p/n for the isospin. Each nucleon in the sink operator is projected to have zero spatial momentum. We also calculate the correlation function of the ^{3}He nucleus, whose quantum numbers are $J^P = \frac{1}{2}^+$, $I = \frac{1}{2}$, and $I_z = \frac{1}{2}$. We employ the interpolating operator in Ref. [17] with zero momentum projection on each nucleon in the sink operator.

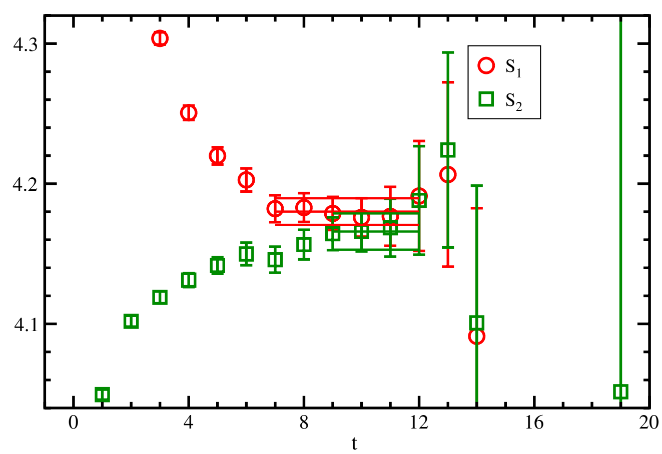

FIG. 1 (color online). Effective mass of ^{4}He nucleus with S_1 (circle) and S_2 (square) sources at $L = 48$ in lattice units. Fit results with one standard deviation error band are expressed by solid lines.

Let us first present the ^{4}He nucleus results. Figure 1 shows the effective mass plots of the ^{4}He nucleus correlators with the $S_{1,2}$ sources on the $(6.1\ \mathrm{fm})^3$ spatial volume. We find clear signals up to $t \approx 12$, beyond which statistical fluctuation dominates. The effective masses with the different sources show a reasonable agreement in the plateau region. The consistency is also shown in the exponential fit results in the plateau region as presented in the figure.

In order to determine the energy shift ΔE_L precisely, we define the ratio of the ^{4}He nucleus correlation function divided by the fourth power of the nucleon correlation function, $R(t) = G_{^4\mathrm{He}}(t)/(G_N(t))^4$, where $G_{^4\mathrm{He}}(t)$ and $G_N(t)$ are obtained with the same source. The effective energy shift is extracted as $\ln(R(t)/R(t+1)) = -\Delta E_L^{\mathrm{eff}}$, once the ground states dominate in both correlators. In Fig. 2 we present time dependence of $-\Delta E_L^{\mathrm{eff}}$ for the $S_{1,2}$ sources, both of which show negative values beyond the error bars in the plateau region of $8 \leq t \leq 11$. Note that this plateau region is reasonably consistent with that for the effective mass of the ^{4}He nucleus correlators in Fig. 1. The signals of $-\Delta E_L^{\mathrm{eff}}$ are lost beyond $t \approx 12$ because of the large fluctuations in the ^{4}He nucleus correlators. We determine ΔE_L by exponential fits of the ratios in the plateau region, $t = 8 - 12$ for S_1 and $t = 7 - 12$ for S_2, respectively. We estimate a systematic error of ΔE_L from the difference of the central values of the fit results, with the minimum or maximum time slice changed by ± 1.

The volume dependence of the energy shift ΔE_L is plotted as a function of $1/L^3$ in the upper panel of Fig. 3. Table II summarizes the numerical values of ΔE_L at three spatial volumes, where the statistical and systematic errors are presented in the first and second parentheses, respectively. The results for the $S_{1,2}$ sources are consistent within the error bars. In Fig. 3, we plot the combined error of the statistical and systematic ones added in quadrature. In the following discussions we use the combined error. We observe little volume dependence for ΔE_L indicating a bound state, rather than the $1/L^3$ dependence expected for a scattering state, for the ground state in the ^{4}He channel.

The physical binding energy ΔE defined in the infinite spatial volume limit is extracted by a simultaneous fit of the data for the $S_{1,2}$ sources employing a fit function of

TABLE II. Binding energies of ^{4}He and ^{3}He nuclei on each spatial volume. Extrapolated results to the infinite spatial volume limit are also presented. The first and second errors are statistical and systematic, respectively.

L	ΔE_L [MeV]			
	^{4}He(S_1)	^{4}He(S_2)	^{3}He(S_1)	^{3}He(S_2)
24	28(14)(11)	46.8(7.3)(1.6)	19.0(6.3)(6.0)	23.2(3.2)(0.5)
48	27(14)(05)	36(12)(04)	16.6(6.9)(3.2)	19.5(5.6)(2.3)
96	24(18)(12)	24(14)(03)	19.0(7.6)(4.9)	18.4(6.1)(1.9)
∞	27.7(7.8)(5.5)		18.2(3.5)(2.9)	

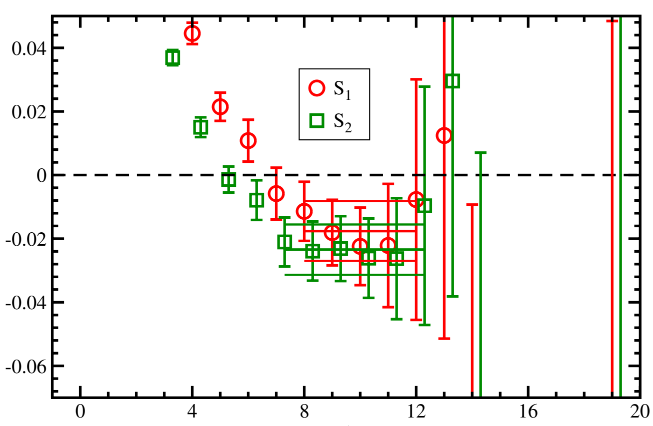

FIG. 2 (color online). Effective energy shift of ^{4}He nucleus in a convention of $-\Delta E_L^{\mathrm{eff}}$ with S_1 (circle) and S_2 (square) sources at $L = 48$ in lattice units. Square symbols are slightly shifted to positive direction in horizontal axis for clarity. Fit results with one standard deviation error band are expressed by solid lines.

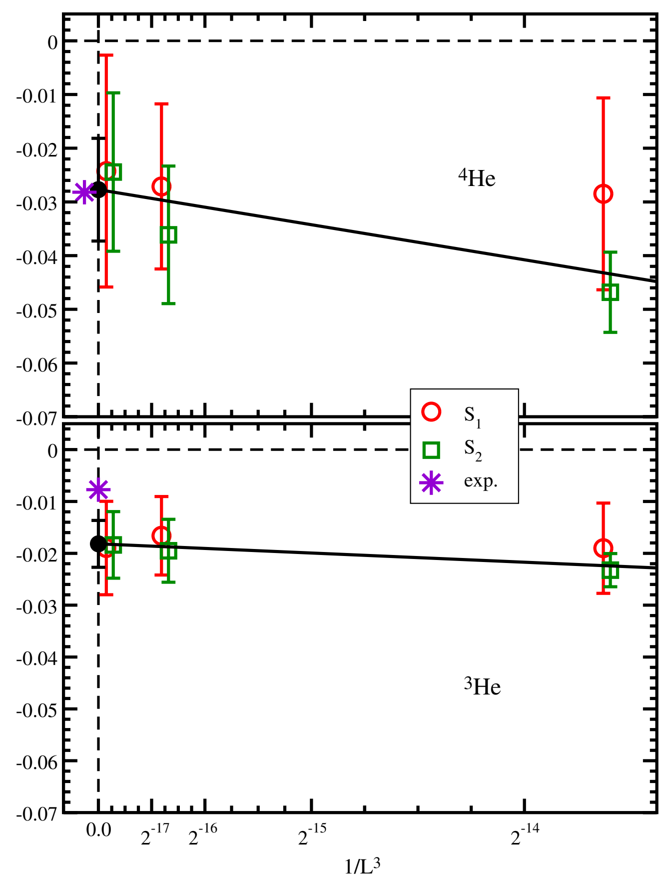

FIG. 3 (color online). Spatial volume dependence of $-\Delta E_L = M - N_N m_N$ in GeV units for ^{4}He (upper) and ^{3}He (lower) nuclei with S_1 (open circle) and S_2 (open square) sources. Statistical and systematic errors are added in quadrature. Square symbols are slightly shifted to positive direction in horizontal axis for clarity. Extrapolated results to the infinite spatial volume limit (filled circle) and experimental values (star) are also presented.

$\Delta E + C/L^3$ with ΔE and C free parameters. Since ΔE_L may be contaminated by the scattering states, which are $O(1/L^3)$ effects, we add a possible $1/L^3$ term. A systematic error is estimated from the difference of the central values of the fit results using the data with the different fit ranges in the determination of ΔE_L. The result for ΔE is 0.0180(62) in lattice units, which is 2.9σ away from zero as shown in Fig. 3. We also try a pure bound-state fit, allowing for an exponentially small finite size correction: ΔE and $\Delta E + C_1 e^{-C_2 L}$ with ΔE and $C_{1,2}$ free parameters. We find that all the results are in agreement with reasonable values of χ^2.

Based on these analyses, we conclude that the ground state of the measured four-nucleon system is bounded. An encouraging finding is that $\Delta E = 27.7(9.6)$ MeV with $a^{-1} = 1.54$ GeV agrees with the experimental value of 28.3 MeV. However, we do not intend to stress the consistency because our calculation is performed at the unphysically heavy pion mass, $m_\pi = 0.8$ GeV, and the electromagnetic interactions and the isospin symmetry breaking effects are neglected.

We also calculate ΔE_L for the ^{3}He nucleus with the $S_{1,2}$ sources, whose results are presented in Fig. 3 and Table II. The trend of the volume dependence is similar to the ^{4}He nucleus case. A simultaneous fit of the data for the $S_{1,2}$ sources with a fit function of $\Delta E + C/L^3$ yields a finite value of $\Delta E = 18.2(4.5)$ MeV, which means the existence of a bound state in the ^{3}He nucleus channel. Our result for ΔE is about twice larger than the experimental value of 7.72 MeV. A main reason could be the heavy pion mass employed in this calculation.

As an alternative way to view this result, we compare the binding energies normalized by the atomic number: $\Delta E/N_N = 6.9(2.4)$ MeV and 6.1(1.5) MeV for the ^{4}He and ^{3}He nuclei, respectively. At our unphysically heavy pion mass, the three- and four-nucleon system does not show the experimental feature that the binding is stronger for ^{4}He than for ^{3}He.

We have addressed the issue of nuclear binding for the ^{4}He and ^{3}He nuclei. We have shown that the current computational techniques and resources allow us to tackle this issue. Albeit in quenched QCD and for unphysically heavy pion mass, we are able to extract evidence for the bound-state nature of the ground state and the binding energies for these nuclei.

A future direction of primary importance is to investigate the quark mass dependence of the binding energies of the nuclei. There are several model studies of the quark mass dependence of the nuclear binding energies [18] which suggest that the quark masses play an essential role in a quantitative understanding of the binding energies. Another important issue is the development of a strategy to calculate nuclei with larger atomic numbers. The required number of the Wick contractions quickly diverges as the atomic number increases, even if the redundancies are removed with various symmetries. We leave it to future work.

Numerical calculations for the present work have been carried out on the HA8000 cluster system at the Information Technology Center of the University of Tokyo and on the PACS-CS computer under the Interdisciplinary Computational Science Program of the Center for Computational Sciences, University of Tsukuba. We thank our colleagues in the PACS-CS Collaboration for helpful discussions and providing us the code used in this work. This work is supported in part by Grants-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (No. 18104005, No. 18540250, No. 20105002, No. 21105501, No. 22244018).

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