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Lattice effective field theory for medium-mass nuclei

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ABSTRACT

We extend Nuclear Lattice Effective Field Theory (NLEFT) to medium-mass nuclei, and present results for the ground states of alpha nuclei from ^{4}He to ^{28}Si, calculated up to next-to-next-to-leading order (NNLO) in the EFT expansion. This computational advance is made possible by extrapolations of lattice data using multiple initial and final states. For our soft two-nucleon interaction, we find that the overall contribution from multi-nucleon forces must change sign from attractive to repulsive with increasing nucleon number. This effect is not produced by three-nucleon forces at NNLO, but it can be approximated by an effective four-nucleon interaction. We discuss the convergence of the EFT expansion and the broad significance of our findings for future *ab initio* calculations.

1. Introduction

Several *ab initio* methods are being used to study nuclear structure. These include coupled-cluster expansions [1], the no-core shell model [2,3], the in-medium similarity renormalization group approach [4], self-consistent Green's functions [5], and Green's function Monte Carlo [6]. The use of soft chiral nuclear EFT interactions has stimulated much of the recent progress in *ab initio* nuclear structure calculations. By "soft" interactions, we refer to the absence of strong repulsive forces at short distances. In this letter, we address a central question in nuclear structure theory: How large a nucleus can be calculated from first principles using the framework of chiral nuclear EFT, and what are the remaining challenges?

We address this question by using Nuclear Lattice Effective Field Theory (NLEFT) to calculate the ground states of alpha nuclei from ^{4}He to ^{28}Si. NLEFT is an *ab initio* method where chiral nuclear EFT is combined with Auxiliary-Field Quantum Monte Carlo (AFQMC) lattice calculations. NLEFT differs from other *ab initio* methods in that it is an unconstrained Monte Carlo calculation, which does not require truncated basis expansions, many-body perturbation theory, or any constraint on the nuclear wave function. Our NLEFT results are thus truly unbiased Monte Carlo calculations. The results presented here form an important benchmark for *ab initio* calculations of larger nuclei using chiral nuclear EFT. Any deficiencies are indicative of shortcomings in the specific nuclear interactions, rather than of errors generated by the computational method. Such a definitive analysis would be difficult to achieve using other methods.

The lattice formulation of chiral nuclear EFT is described in Ref. [7], a review of lattice EFT methods can be found in Ref. [9], and Refs. [10,11] provide a comprehensive overview of chiral nuclear EFT. We have recently applied NLEFT to describe the structure of the Hoyle state [12,13] and the dependence of the triple-alpha process on the fundamental parameters of nature [14]. These studies show that NLEFT is successful up to $A \simeq 12$ nucleons. In this letter, we report the first NLEFT results for medium-mass nuclei. We compute the ground state energies for all nuclei in the alpha ladder up to ^{28}Si using the lattice action established in Refs. [13, 12,15].

2. Chiral nuclear EFT for medium-mass nuclei

According to chiral nuclear EFT, our calculations are organized in powers of a generic soft scale Q associated with factors of momenta and the pion mass. We label the $\mathcal{O}(Q^0)$ contributions to the nuclear Hamiltonian as leading order (LO), $\mathcal{O}(Q^2)$ as next-to-leading order (NLO), and $\mathcal{O}(Q^3)$ as next-to-next-to-leading order

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(NNLO). The present calculations are performed up to NNLO. Our LO lattice Hamiltonian includes a significant part of the NLO and higher-order corrections by making use of smeared contact interactions [7,8,15]. See Ref. [15] for a discussion of the interactions used in this work. As discussed in Ref. [15], we are using a low-momentum power counting scheme where there are no additional two-nucleon corrections at NNLO beyond the terms already appearing at NLO.

The NLEFT calculations reported here are performed with a lattice spacing of $a = 1.97$ fm in a periodic cube of length $L = 11.82$ fm. Our trial wave function is denoted $|\Psi_A^{\text{init}}\rangle$, which is a Slater-determinant state composed of delocalized standing waves in the periodic cube, with A nucleons and the desired spin and isospin quantum numbers. For simplicity, we describe our calculations using the language of continuous time evolution. The actual AFQMC calculations use transfer matrices with a temporal lattice spacing of $a_t = 1.32$ fm [9].

Before we enter into the main part of the calculation, we make use of a low-energy filter based upon Wigner's SU(4) symmetry, where the spin–isospin degrees of freedom of the nucleon are all equivalent as four components of an SU(4) multiplet. Let us define

$$H_{\text{SU(4)}} \equiv H_{\text{free}} + \frac{1}{2} C_{\text{SU(4)}} \sum_{\vec{n},\vec{n}'} :\rho(\vec{n}) f(\vec{n}-\vec{n}') \rho(\vec{n}'):, \tag{1}$$

where $f(\vec{n}-\vec{n}')$ is a Gaussian smearing function with width set by the average effective range of the two S-wave interaction channels, and ρ is the total nucleon density. We then apply the exponential of $H_{\text{SU(4)}}$ to obtain

$$\left|\Psi_A(t')\right\rangle \equiv \exp\left(-H_{\text{SU(4)}} t'\right) \left|\Psi_A^{\text{init}}\right\rangle, \tag{2}$$

which we refer to as a "trial state". This part of the calculation is computationally inexpensive since it only requires a single auxiliary field and does not generate any sign oscillations in the Monte Carlo calculation.

Next, we use the LO Hamiltonian H_{LO} to construct the Euclidean-time projection amplitude

$$Z_A(t) \equiv \left\langle \Psi_A(t') \right| \exp(-H_{\text{LO}} t) \left| \Psi_A(t') \right\rangle, \tag{3}$$

from which we compute the "transient energy"

$$E_A(t) = -\partial \left[\ln Z_A(t)\right] / \partial t. \tag{4}$$

If the lowest eigenstate of H_{LO} that possesses a non-vanishing overlap with the trial state $|\Psi_A(t')\rangle$ is denoted $|\Psi_{A,0}\rangle$, the energy $E_{A,0}$ of $|\Psi_{A,0}\rangle$ is obtained as the $t \to \infty$ limit of $E_A(t)$.

The higher-order corrections to $E_{A,0}$ are evaluated using perturbation theory. We compute expectation values using

$$Z_A^{\mathcal{O}}(t) \equiv \left\langle \Psi_A(t') \right| \exp(-H_{\text{LO}} t/2) \times \mathcal{O} \exp(-H_{\text{LO}} t/2) \left| \Psi_A(t') \right\rangle, \tag{5}$$

for any operator $\mathcal{O}$. Given the ratio

$$X_A^{\mathcal{O}}(t) = Z_A^{\mathcal{O}}(t) / Z_A(t), \tag{6}$$

the expectation value of $\mathcal{O}$ for the desired state $|\Psi_{A,0}\rangle$ is again obtained in the $t \to \infty$ limit according to

$$X_{A,0}^{\mathcal{O}} \equiv \langle \Psi_{A,0} | \mathcal{O} | \Psi_{A,0} \rangle = \lim_{t\to\infty} X_A^{\mathcal{O}}(t), \tag{7}$$

which gives the corrections to $E_{A,0}$ induced by the NLO and NNLO contributions.

The closer $|\Psi_A(t')\rangle$ is to $|\Psi_{A,0}\rangle$, the less the required projection time t. The trial state can be optimized by adjusting both the SU(4) projection time t' and the strength of the coupling $C_{\text{SU(4)}}$ of $H_{\text{SU(4)}}$. Here, we show that the accuracy of the extrapolation $t \to \infty$ can be further improved by simultaneously incorporating data from multiple trial states that differ in the choice of $C_{\text{SU(4)}}$. This approach enables a "triangulation" of the asymptotic behavior as the common limit of several different functions of t.

3. Extrapolation in Euclidean time

The behavior of $Z_A(t)$ and $Z_A^{\mathcal{O}}(t)$ at large t is controlled by the low-energy spectrum of H_{LO}. Let $|E\rangle$ label the eigenstates of H_{LO} with energy E, and let $\rho_A(E)$ denote the density of states for a system of A nucleons. For simplicity, we omit additional labels needed to distinguish degenerate states. We can then express $Z_A(t)$ and $Z_A^{\mathcal{O}}(t)$ in terms of their spectral representations,

$$Z_A(t) = \int dE\, \rho_A(E) \left|\left\langle E \middle| \Psi_A(t') \right\rangle\right|^2 \exp(-Et), \tag{8}$$

$$Z_A^{\mathcal{O}}(t) = \int dE\, dE'\, \rho_A(E) \rho_A(E') \exp\left(-(E+E')t/2\right), \times \left\langle \Psi_A(t') \middle| E \right\rangle \langle E | \mathcal{O} | E' \rangle \left\langle E' \middle| \Psi_A(t') \right\rangle, \tag{9}$$

from which the spectral representations of $E_A(t)$ and $X_A^{\mathcal{O}}(t)$ are obtained using Eq. (4) and Eq. (6), respectively. We can approximate these to arbitrary accuracy over any finite range of t by taking $\rho_A(E)$ to be a sum of energy delta functions,

$$\rho_A(E) \approx \sum_{i=0}^{i_{\max}} c_i \delta(E - E_{A,i}), \tag{10}$$

where we use $i_{\max} = 4$ for the calculation of the ^{4}He ground state, and $i_{\max} = 3$ for $A \geqslant 8$. These choices give a good description over the full range of t for all trial states, without introducing too many free parameters. Using AFQMC data for different values of $C_{\text{SU(4)}}$, we perform a correlated fit of $E_A(t)$ and $X_A^{\mathcal{O}}(t)$ for all operators $\mathcal{O}$ that contribute to the NLO and NNLO corrections. We find that using 2–6 distinct trial states for each A allows for a much more precise determination of $E_{A,0}$ and $X_{A,0}^{\mathcal{O}}$ than hitherto possible. In particular, we may "triangulate" $X_{A,0}^{\mathcal{O}}$ using trial states that correspond to functions $X_A^{\mathcal{O}}(t)$ which converge both from above and below.

As the extent of our MC data in Euclidean time is relatively short, we discuss next the level of confidence that we can attribute to our results. In our "triangulation" method, the accuracy and reliability of the extrapolation $t \to \infty$ is increased by means of correlated fits to multiple trial states. We first note that the number of Euclidean time steps N_t available for the extrapolation does not decrease drastically with the number of nucleons A. This inspires confidence that our method, which has by now been successfully applied to the structure, spectrum and electromagnetic properties of ^{16}O in Ref. [16] should also be applicable to heavier systems. Nevertheless, "spurious early convergence" in Euclidean time extrapolations should be carefully guarded against. If only one trial state is used, this issue arises much more readily. In our "triangulation" method, the extrapolation is very strongly constrained by the requirement that all observables for all trial states should be described by the same exponential dependence on Euclidean time. Rapid convergence in t then translates into a small sensitivity to $C_{\text{SU(4)}}$ at large values of t. It is also encouraging to note that our new extrapolations are consistent with our earlier results for ^{12}C in Refs. [13,14], which were computed using delocalized plane-wave as well as alpha-cluster trial wave functions.

4. Lattice Monte Carlo results

In Fig. 1, we show the LO transient energy $E_A(t)$ as a function of the number of temporal lattice steps $N_t = t/a_t$, for ^{16}O