Medium-Mass Nuclei from Chiral Nucleon-Nucleon Interactions

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We compute the binding energies, radii, and densities for selected medium-mass nuclei within coupled-cluster theory and employ a bare chiral nucleon-nucleon interaction at next-to-next-to-next-to-leading order. We find rather well-converged results in model spaces consisting of 15 oscillator shells, and the doubly magic nuclei ^{40}Ca, ^{48}Ca, and the exotic ^{48}Ni are underbound by about 1 MeV per nucleon within the coupled-cluster singles-doubles approximation. The binding-energy difference between the mirror nuclei ^{48}Ca and ^{48}Ni is close to theoretical mass table evaluations. Our computation of the one-body density matrices and the corresponding natural orbitals and occupation numbers provides a first step to a microscopic foundation of the nuclear shell model.

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Introduction.—Ab initio nuclear structure calculations have made great progress in the past decade. Light nuclei up to carbon or so can now be described in terms of their nucleonic degrees of freedom and realistic nucleon-nucleon (NN) forces (i.e., those that include pion exchange and fit the NN phase shifts up to 350 MeV lab energy with a $\chi^2 \approx 1$ per datum) augmented by a three-nucleon force (3NF) [1–3]. One of the major advances is due to the systematic construction of nuclear forces within chiral effective field theory (EFT) [4,5]. In this EFT, unknown short-ranged physics of the nuclear force is systematically parametrized in terms of contact terms and their low-energy constants, while the long-range part of the interaction stems from pion exchange. One of the hallmarks of this approach is the ''power counting'', i.e., an expansion of the nuclear Lagrangian in terms of the momentum ratio Q/Λ. Here, Q denotes the typical momentum scale at which the nucleus is probed, while Λ denotes the high-momentum cutoff scale that limits the applicability of the EFT. Within this approach, three-nucleon forces appear naturally at order $(Q/\Lambda)^3$, and four-nucleon forces appear at order $(Q/\Lambda)^4$ [6–8].

The chiral interactions have been probed in light systems up to mass 13 [9–12]. Fujii *et al.* have employed chiral NN interactions for studies of ^{16}O [13] within the unitary-model-operator approach (UOMA). Unfortunately, virtually nothing is known about chiral interactions in heavier nuclei. In particular, a study of their saturation properties is missing, and the contributions of chiral NN interactions to nuclear binding and structure in medium-mass nuclei needs to be determined. It is the purpose of the present Letter to fill this gap.

Ab initio methods began to explore medium-mass nuclei only very recently. Gandolfi *et al.* [14] employed the auxiliary field diffusion Monte Carlo method for a computation of the binding-energy of ^{40}Ca. However, this impressive calculation is not entirely realistic since the employed Argonne v_6' potential lacks the spin-orbit interaction. Roth and Navrátil [15] employed softer renormalized NN interactions and computed the binding energy of ^{40}Ca within an importance truncated no-core shell-model approach. However, this calculation was criticized [16,17] for its convergence properties, the violation of Goldstone's linked cluster theorem and the corresponding lack of size extensivity. In this Letter, we employ the bare chiral NN interaction with a cutoff of $\Lambda = 500$ MeV by Entem and Machleidt [7], and use the size-extensive coupled-cluster method [18–23] for the computation of various properties of the medium-mass nuclei ^{40}Ca, ^{48}Ca, and the exotic ^{48}Ni. The use of a bare NN interaction has the advantage that it avoids the introduction of additional many-body forces that are typically generated in secondary renormalization procedures of the two-body force. While our calculation includes the chiral NN interaction [7] at next-to-next-to-next-to-leading order (NNNLO), it neglects the contributions of any 3NFs.

This Letter is organized as follows. First, we briefly introduce spherical coupled-cluster theory. Second, we compute the binding energies of the nuclei ^{4}He, ^{16}O, ^{40}Ca, ^{48}Ca, and ^{48}Ni from a bare chiral NN potential.

Spherical coupled-cluster theory.—Coupled-cluster theory [18–23] is based on the similarity transform

$$\bar{H} = e^{-\hat{T}} \hat{H} e^{\hat{T}} \tag{1}$$

of the normal-ordered Hamiltonian $\hat{H}$. Here, the Hamiltonian is normal ordered with respect to a product state $|\phi\rangle$ which serves as a reference. Likewise, the particle-hole cluster operator $\hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$ is defined with respect to the reference state. The k-particle k-hole ($kp - kh$) cluster operator is

$$\hat{T}_k = \frac{1}{(k!)^2} \sum_{i_1,\ldots,i_k;a_1,\ldots,a_k} t^{a_1\ldots a_k}_{i_1\ldots i_k} \hat{a}^\dagger_{a_1} \ldots \hat{a}^\dagger_{a_k} \hat{a}_{i_k} \ldots \hat{a}_{i_1}. \tag{2}$$

Here and in the following, $i, j, k, \ldots$ label occupied single-particle orbitals, while $a, b, c, \ldots$ label unoccupied orbitals of the reference state; i.e., they should have significant overlap with the ground-state. Throughout this work we will restrict ourselves to the coupled-cluster singles-doubles (CCSD) approximation $\hat{T} \approx \hat{T}_1 + \hat{T}_2$. The unknown amplitudes t_i^a and t_{ij}^{ab} in this expression are determined from the solution of the coupled-cluster equations

$$0 = \langle \phi_i^a | \bar{H} | \phi \rangle \quad \text{and} \quad 0 = \langle \phi_{ij}^{ab} | \bar{H} | \phi \rangle. \tag{3}$$

Here $|\phi_i^a\rangle = \hat{a}_a^\dagger \hat{a}_i |\phi\rangle$ is a $1p-1h$ excitation of the reference state, and $|\phi_{ij}^{ab}\rangle$ is a similarly defined $2p-2h$ excited state. Once the CCSD equations are solved, the correlation energy of the ground state is computed as

$$E_{\text{corr}} = \langle \phi | \bar{H} | \phi \rangle. \tag{4}$$

Coupled-cluster theory fulfills Goldstone's linked cluster theorem and therefore yields size-extensive results. This is particularly important in applications to medium-mass nuclei. Within the CCSD approximation, the computational effort scales as $n_o^2 n_u^4$, where n_o and n_u denote the occupied and unoccupied orbitals of the reference state $|\phi\rangle$, respectively. This approximation typically captures more than 90% of the correlation energy [23]. This method has recently been employed in several *ab initio* nuclear structure calculations [24–28]. It is also able to compute lifetimes of unstable nuclei [29], to treat 3NFs [30], and it meets benchmarks [17].

For spherical reference states (i.e., nuclei with closed major shells or closed subshells), one can employ the spherical symmetry to further reduce the number of unknowns (i.e., the number of cluster amplitudes). For such nuclei, the cluster operator $\hat{T}$ is a scalar under rotation, and depends only on reduced amplitudes. A naive estimate shows that a model space of $n_o + n_u$ single-particle states consists of only $(n_o + n_u)^{2/3}$ j shells. Thus, the entire computational effort is approximately reduced by a power $2/3$ within the spherical scheme compared to the m scheme. We have derived and implemented the spherical scheme within the CCSD approximation. We tested that our m-scheme code and the spherical code give identical results for several cases.

Results.—The single-particle basis consists of wave functions of the spherical harmonic oscillator with the spacing $\hbar\omega$, the radial quantum number n, and angular momentum l, and we include single-particle states with $2n + l \leq N$ in our model space. The largest model space we consider ($N = 14$) consists of 15 oscillator shells. In such a large model space, configuration interaction becomes impossible as the proton space alone consists of about 10^{40} Slater determinants for ^{40}Ca. We first transform the Hamiltonian to the spherical Hartree-Fock basis, and the CCSD equations are solved in this basis. Fully converged observables must be independent of the parameters N and $\hbar\omega$ of our single-particle basis. In practice, we cannot go to infinitely large spaces, and the dependence of our results on these parameters serve to gauge the convergence.

As a test case, Fig. 1 shows that the CCSD results for ^{4}He are converged within a few keV with respect to increases in the size of the model space (denoted by N) and variation of the oscillator frequency. For the CCSD-T1 triples correction [31] we employ our m-scheme code for in model spaces up to $N = 7$. This yields another 1.3 MeV of binding, is very close to the virtually exact Faddeev-Yakubowski result $E = -25.41$ MeV quoted in Ref. [10] for the same chiral NN interaction. The experimental value is $E = -28.3$ MeV, and the additional binding is due to the missing 3NFs.

The CCSD energies for ^{16}O (see Fig. 2) are converged within the order of about 100 keV and change by less than 1 MeV over a considerable variation of the oscillator frequency. This result is in reasonably good agreement with the work by Fujii *et al.* who obtained -110 MeV as the ground-state energy from the UOMA [13]. Recall that both methods are approximations and based on similarity-transformed Hamiltonians.

We turn to nuclei in the mass-40 region. The CCSD results for ^{40}Ca are shown in Fig. 3. Increasing the model space from $N = 13$ to $N = 14$ yields an additional 0.9 MeV, and the $\hbar\omega$-dependence is less than 2.2 MeV over the considered range of oscillator frequencies. Thus, the convergence with respect to the parameters of our model space is very satisfactory, and we are missing about 10% of the experimental binding-energy of 342 MeV.

We also computed the ground-state energies of the mirror nuclei ^{48}Ca and ^{48}Ni. For ^{48}Ca the convergence of the results is satisfactory as shown in Fig. 4, and the convergence is very similar for ^{48}Ni. ^{48}Ni was discovered only recently [32]. It is believed to be a two-proton emitter, and its lifetime is very large compared to a typical nuclear time scale (i.e., the "orbital period" of a nucleon inside the nucleus). Thus, we can describe ^{48}Ni in terms of a spherical

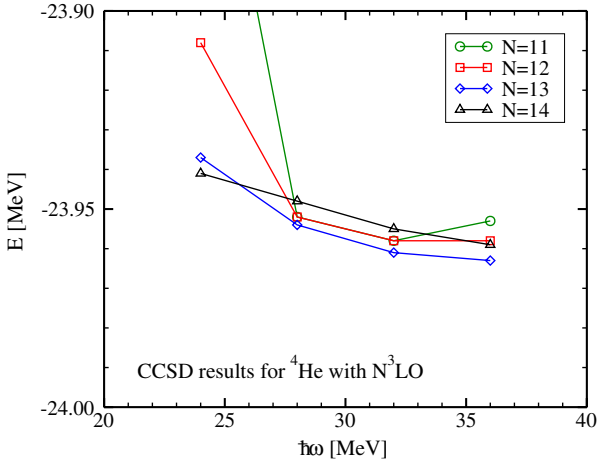

FIG. 1 (color online). CCSD ground-state energy for ^{4}He from a chiral NN potential at order NNNLO as a function of the oscillator spacing $\hbar\omega$ and the size of the model space.

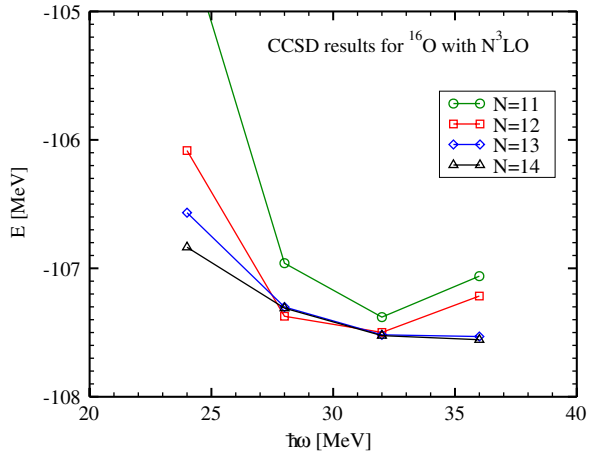

FIG. 2 (color online). Same as Fig. 1 but for ^{16}O.

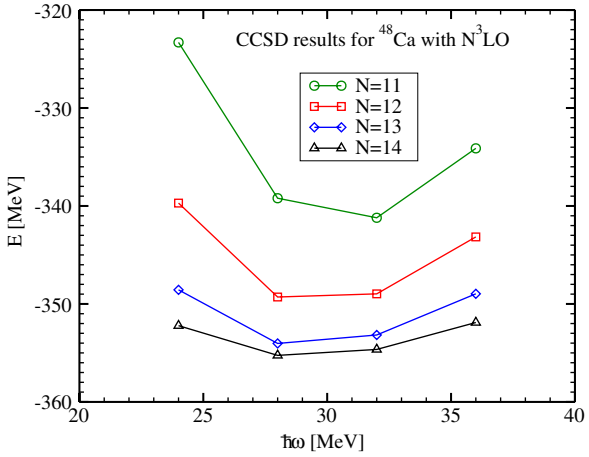

FIG. 4 (color online). Same as Fig. 1 but for ^{48}Ca.

Hartree-Fock basis based on the oscillator orbitals. Recall that the chiral interaction includes charge symmetry-breaking and charge independence-breaking effects, and we also included the Coulomb interaction. The difference of our CCSD results for the mirror nuclei ^{48}Ca and ^{48}Ni is 1.38 MeV per nucleon and stems from these combined effects. Theoretical mass table evaluations [33] suggest that the binding-energy of ^{48}Ni is 1.43 MeV per nucleon smaller than for ^{84}Ca. Our results are in good agreement with this estimate. The density of ^{48}Ca is shown in Fig. 5. The results still exhibit a dependence of the oscillator spacing $\hbar\omega$, and the central density decreases with decreasing $\hbar\omega$. This observable is less well converged than the energy with respect to the size of the model space. The convergence is slow with respect to the maximum radial quantum number n employed in our model space, while the single-particle angular momentum l could be limited to $l \leq 7$.

Table I summarizes some of our results which are taken at $\hbar\omega = 28$ MeV in the largest model spaces. We computed the potential energy V via the Hellman-Feynman theorem. The fourth column shows the energy deviation $\Delta E \equiv E - E_{\mathrm{exp}}$ from the experimental binding energy E_{exp} for the considered nuclei. This difference is mainly due to the omitted 3NFs and the missing triples correction. Note that ^{40}Ca is particularly tightly bound when compared to the other nuclei. The isotopes ^{16}O, ^{48}Ca, and ^{48}Ni all lack about $\Delta E/A \approx 1.2$ MeV of binding energy when compared to experiment, while this difference is considerably smaller for ^{40}Ca. This result is somewhat surprising since ^{48}Ca is thought to be a better example of a doubly magic nucleus than ^{40}Ca. There seems to be a cancellation between triples corrections and contributions of 3NFs in ^{40}Ca. In other words, the isospin dependence and/or mass dependence of the 3NF is expected to be nontrivial. The charge radii R are corrected according to Ref. [34] to account for the finite charge radii of the nucleons. They are computed from the leading approximation of the center-of-mass corrected intrinsic density [25]. Note that the radii change about 0.1–0.25 fm as the oscillator spacing $\hbar\omega$ is varied in the range that is shown in the previous figures, and they decrease with increasing values of $\hbar\omega$.

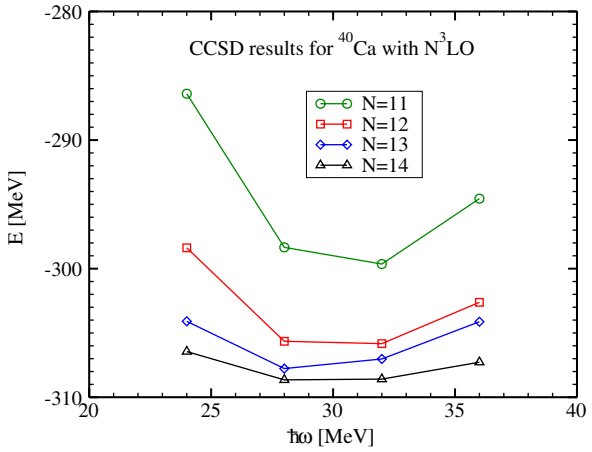

FIG. 3 (color online). Same as Fig. 1 but for ^{40}Ca.

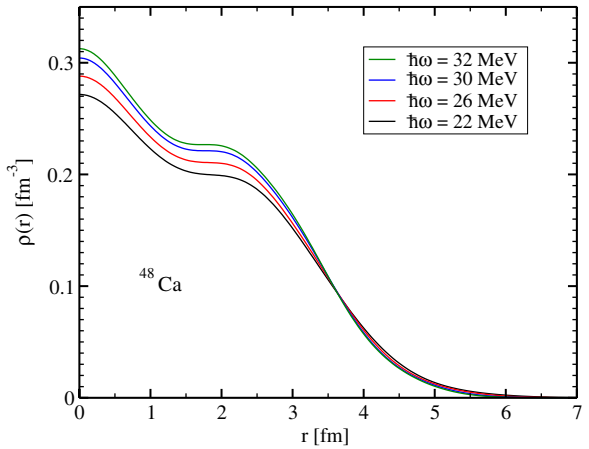

FIG. 5 (color online). Densities for ^{48}Ca from a chiral NN potential at order NNNLO for different oscillator spacings.

TABLE I. CCSD results for various nuclei from a chiral nucleon-nucleon potential at order NNNLO. E/A and V/A: ground-state and potential energy per nucleon, respectively. $\Delta E/A$: difference to the experimental ground-state energy (theoretical mass table evaluations for ^{48}Ni). R and R_{exp} are the computed and measured charge radius.

Nucleus	E/A [MeV]	V/A [MeV]	$\Delta E/A$ [MeV]	R [fm]	R_{exp} [fm]
^{4}He	−5.99	−22.75	1.08	1.86	1.64
^{16}O	−6.72	−30.69	1.25	2.71	2.74
^{40}Ca	−7.72	−36.40	0.84	3.24	3.48
^{48}Ca	−7.40	−37.97	1.27	3.22	3.47
^{48}Ni	−6.02	−36.04	1.21	3.50	

We also compute the one-body density matrices $\rho_{pq} = \langle \hat{a}_p^\dagger \hat{a}_q \rangle$ of the ground states within the equation-of-motion CCSD [35]. The diagonalization of this matrix yields natural orbitals and the corresponding occupations. These model-dependent quantities are, of course, not observables but rather tied to the specific interaction we employed. The dominant occupation probabilities are larger than 0.95, and this indicates that the considered nuclei are indeed doubly magic. This result is nontrivial. Note that the Hartree-Fock approximation does not even yield bound nuclei. Yet the CCSD correlations imprinted onto the Hartree-Fock state yield a rather simple state. To our knowledge, this is the first time the phenomenological shell-model picture of independent nucleon motion arises within an *ab initio* approach.

Summary.—We have studied the saturation properties of chiral NN interactions at the order NNNLO in medium-mass nuclei within the CCSD approximation of coupled-cluster theory. Our results exhibit a very satisfactory convergence with respect to the size of the model space and are only weakly dependent on the oscillator parameter. We find that the employed bare chiral NN potential underbinds nuclei by about 1 MeV per nucleon. The comparison of ^{40}Ca with ^{48}Ca and ^{48}Ni hints at an isospin dependence of the 3NF in medium-mass nuclei. Within the CCSD approximation, the proton-rich nucleus ^{48}Ni is less tightly bound by 1.38 MeV per nucleon than its mirror nucleus ^{48}Ca, and this result is in good agreement with theoretical mass table evaluations. These calculations pave the way to probing chiral interactions in even heavier nuclei and link the phenomenological shell model to *ab initio* calculations. The inclusion of triples corrections and 3NFs is underway.

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