Medium-Mass Nuclei with Normal-Ordered Chiral $NN + 3N$ Interactions

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We study the use of truncated normal-ordered three-nucleon interactions in nuclear structure calculations starting from chiral two- plus three-nucleon Hamiltonians evolved consistently with the similarity renormalization group. We present three key developments: (i) a rigorous benchmark of the normal-ordering approximation in the importance-truncated no-core shell model for ^{4}He, ^{16}O, and ^{40}Ca; (ii) a direct comparison of the importance-truncated no-core shell model results with coupled-cluster calculations at the singles and doubles level for ^{16}O; and (iii) first applications of similarity renormalization group-evolved chiral $NN + 3N$ Hamiltonians in coupled-cluster calculations for medium-mass nuclei ^{16,24}O and ^{40,48}Ca. We show that the normal-ordered two-body approximation works very well beyond the lightest isotopes and opens a path for studies of medium-mass and heavy nuclei with chiral two- plus three-nucleon interactions. At the same time we highlight the predictive power of chiral Hamiltonians.

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Two decades of experience with *ab initio* nuclear structure calculations, including the pioneering work with the Green's Function Monte Carlo approach [1], have shown that three-nucleon ($3N$) interactions play an important role for understanding the structure of nuclei systematically from first principles. Recent advances on nuclear interactions derived within chiral effective field theory (EFT) put additional emphasis on the consistent inclusion of realistic $3N$ interactions in nuclear structure calculations [2–6]. However, for most large-scale many-body approaches, such as the no-core shell model (NCSM) [7] or the coupled-cluster (CC) method [8], the full inclusion of $3N$ interactions increases the computational cost by orders of magnitude and often renders calculations impossible that are routinely performed with two-nucleon (NN) Hamiltonians. In order to resolve this dilemma—the need for $3N$ interactions versus the tremendous computational cost—one might resort to approximate schemes for including the $3N$ interaction, particularly when aiming at a controlled approximation rather than an exact solution of the many-body problem. Density-dependent NN interactions are being used, e.g., in nuclear matter calculations to simulate the effects of $3N$ interactions in a computationally simple approximation (for recent applications see Refs. [9–11]). In the context of the nuclear shell model, effects of $3N$ forces have been included through an effective monopole interaction constructed via normal ordering with respect to the core [12]. In a general context, normal ordering with a nucleus-specific reference state can be used to construct a systematic and improvable lower-rank approximation of the $3N$ interaction for use in a range of different many-body approaches.

In this Letter we present rigorous benchmarks and systematic applications of the normal-ordering approximation for chiral $3N$ interactions. We use the importance-truncated no-core shell model (IT-NCSM) [13,14] for the solution of the many-body problem for ^{4}He, ^{16}O, and ^{40}Ca and compare ground-state energies and expectation values obtained with the full and the truncated normal-ordered $3N$ interaction. We then apply the normal-ordered $3N$ interaction in CC calculations for the ground states of medium-mass nuclei up to ^{48}Ca and discuss the implications for nuclear structure predictions with chiral $NN + 3N$ Hamiltonians.

Normal-ordering approximation.—Transforming the many-body Hamiltonian into a normal-ordered form with respect to a nontrivial vacuum state is a standard technique in quantum many-body physics. Using creation and annihilation operators $a^\dagger_\nu$ and a_ν for a single-particle basis $|\nu\rangle$ defined with respect to a trivial zero-body vacuum state, the operator of a $3N$ interaction formally reads

$$V_{3N} = \frac{1}{36} \sum_{\substack{\nu_1\nu_2\nu_3 \\ \mu_1\mu_2\mu_3}} V^{\nu_1\nu_2\nu_3}_{\mu_1\mu_2\mu_3} A^{\nu_1\nu_2\nu_3}_{\mu_1\mu_2\mu_3}, \tag{1}$$

where $V^{\nu_1\nu_2\nu_3}_{\mu_1\mu_2\mu_3} = \langle\nu_1\nu_2\nu_3|V_{3N}|\mu_1\mu_2\mu_3\rangle$ are antisymmetrized matrix elements, and the operator $A^{\nu_1\nu_2\cdots}_{\mu_1\mu_2\cdots} = a^\dagger_{\nu_1} a^\dagger_{\nu_2} \cdots a_{\mu_2} a_{\mu_1}$ is a shorthand for a normal-ordered product of creation and annihilation operators with respect to the trivial vacuum (vacuum normal-ordering).

Instead of the trivial vacuum, we can choose a reference state $|\Phi_{\text{ref}}\rangle$ being a Slater-determinant of A single-particle states and reinterpret the creation and annihilation operators as particle or hole creation and annihilation operators with respect to this new vacuum. We have to rearrange the creation and annihilation operators in the particle-hole picture to establish normal-ordering with respect to $|\Phi_{\text{ref}}\rangle$ (reference normal-ordering). Using Wick's theorem and $\tilde{A}^{\nu_1\nu_2\cdots}_{\mu_1\mu_2\cdots}$ as a shorthand for the reference normal-ordered product, we obtain for the $3N$ interaction

$$V_{3N} = W + \sum_{\substack{\nu_1 \\ \mu_1}} W^{\nu_1}_{\mu_1} \tilde{A}^{\nu_1}_{\mu_1} + \frac{1}{4} \sum_{\substack{\nu_1\nu_2 \\ \mu_1\mu_2}} W^{\nu_1\nu_2}_{\mu_1\mu_2} \tilde{A}^{\nu_1\nu_2}_{\mu_1\mu_2} + \frac{1}{36} \sum_{\substack{\nu_1\nu_2\nu_3 \\ \mu_1\mu_2\mu_3}} W^{\nu_1\nu_2\nu_3}_{\mu_1\mu_2\mu_3} \tilde{A}^{\nu_1\nu_2\nu_3}_{\mu_1\mu_2\mu_3}, \quad (2)$$

with matrix elements $W = \frac{1}{6}\sum_{\alpha_1\alpha_2\alpha_3} V^{\alpha_1\alpha_2\alpha_3}_{\alpha_1\alpha_2\alpha_3}$ for the zero-body (0B) term, $W^{\nu_1}_{\mu_1} = \frac{1}{2}\sum_{\alpha_2\alpha_3} V^{\nu_1\alpha_2\alpha_3}_{\mu_1\alpha_2\alpha_3}$ for the one-body (1B) term, $W^{\nu_1\nu_2}_{\mu_1\mu_2} = \sum_{\alpha_3} V^{\nu_1\nu_2\alpha_3}_{\mu_1\mu_2\alpha_3}$ for the two-body (2B) term, and $W^{\nu_1\nu_2\nu_3}_{\mu_1\mu_2\mu_3} = V^{\nu_1\nu_2\nu_3}_{\mu_1\mu_2\mu_3}$ for the residual three-body (3B) term, where α_i labels the occupied single-particle states in $|\Phi_{\text{ref}}\rangle$. The interesting aspect of the reference state as compared to the trivial vacuum is that it contains information about the specific many-body system under consideration—the reference state provides a first approximation to, e.g., the ground state of a closed-shell nucleus. Based on this information, contributions of the $3N$ interaction are demoted to lower-particle ranks. This is the basis of the normal-ordered n-body (NOnB) approximation.

Benchmark of the normal-ordering approximation.—To quantify how well such a truncation works, we perform calculations for the ground states of closed-shell nuclei in the IT-NCSM. The IT-NCSM allows us to include the exact $3N$ interaction just as well as any NOnB approximation. The underlying Hamiltonian contains the chiral NN interaction at next-to-next-to-next-to-leading order (N^3LO) of Ref. [15] and the local chiral $3N$ interaction at next-to-next-to-leading order (NNLO) of Ref. [16]. The low-energy constants c_D and c_E are taken from a fit to the ground-state energy and the β-decay half-life of $A = 3$ systems [17]. This initial Hamiltonian is transformed through a similarity renormalization group (SRG) evolution at the two- and three-body level to enhance the convergence behavior of the many-body calculation [18–21]. The SRG evolution represents a continuous unitary transformation parametrized by a flow-parameter α, with $\alpha = 0$ corresponding to the initial Hamiltonian. We will mainly consider two types of SRG-evolved Hamiltonians: The $NN + 3N$-full Hamiltonian starts with the initial chiral $NN + 3N$ Hamiltonian and retains all terms up to the $3N$ level in the SRG-evolution, the $NN + 3N$-induced Hamiltonian omits the chiral $3N$ interaction from the initial Hamiltonian, but keeps all induced $3N$ terms throughout the evolution. The $3N$ terms in both Hamiltonians have quite different characteristics, which makes them useful for benchmarking the normal-ordering approximation. In addition we will employ a range of values of the flow parameter α to generate an even larger set of test cases.

We start with a direct comparison of IT-NCSM calculations for the ground-state energies of ^{4}He and ^{16}O using either the exact $3N$ interaction or the NO2B approximation. The reference state is always the $0\hbar\Omega$ Slater-determinant composed of harmonic-oscillator single-particle states. The IT-NCSM energies as function of the model-space truncation parameter $N_{\max}$ are presented in Fig. 1. We can compare

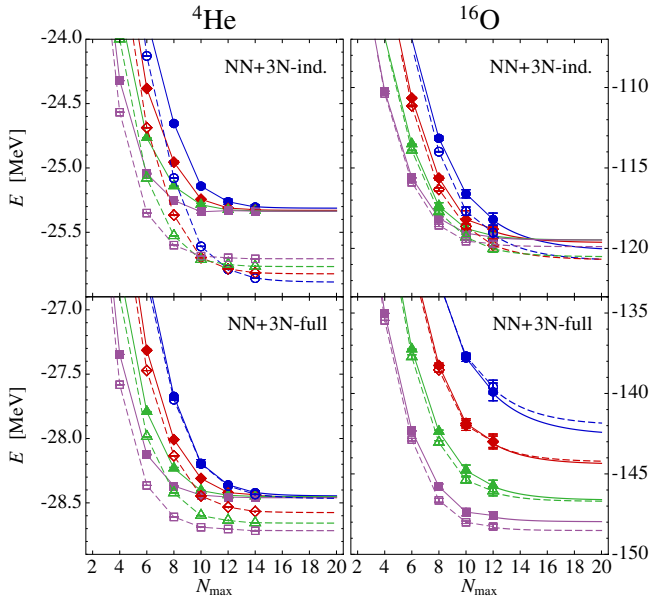

FIG. 1 (color online). IT-NCSM ground-state energies for ^{4}He and ^{16}O as a function of $N_{\max}$ for the $NN + 3N$-induced and the $NN + 3N$-full Hamiltonians for a range of flow parameters: $\alpha = 0.04$ fm^4 (●), 0.05 fm^4 (◆), 0.0625 fm^4 (▲), 0.08 fm^4 (■). Solid symbols correspond to the exact $3N$ interaction, open symbols to the NO2B approximation. Error bars indicate the uncertainties of the threshold extrapolations of the IT-NCSM. Data points are connected by straight lines to guide the eye, beyond the largest $N_{\max}$ an exponential extrapolation fitted to the last four data points is shown.

the converged IT-NCSM ground-state energies for ^{4}He obtained with the exact $NN + 3N$-induced and $NN + 3N$-full Hamiltonians, $-25.33(2)$ and $-28.46(2)$ MeV, respectively, with full NCSM calculations using the same bare chiral Hamiltonians [17], yielding $-25.39(1)$ and $-28.50(2)$ MeV, and with hyperspherical-harmonics calculations using the bare chiral NN interaction [22], yielding -25.38 MeV.

The comparison of the converged values of the ground-state energy obtained with the NO2B approximation and with the exact $3N$ interaction reveals a multifaceted picture. The largest relative deviation at the level of 2% is observed for ^{4}He with the $NN + 3N$-induced interaction. For both, the $NN + 3N$-induced and the $NN + 3N$-full Hamiltonians, the NO2B approximation leads to an overbinding of up to 0.6 and 0.3 MeV, respectively. Note that the systematics of the deviation as function of the flow parameter α is opposite for both Hamiltonians. For ^{16}O we observe deviations below 1% for the ground-state energy, again with a nontrivial dependence on the Hamiltonian. For $NN + 3N$-induced the NO2B approximation consistently overestimates the binding energy by about 1 MeV, for $NN + 3N$-full the NO2B approximation overbinds by less than 1 MeV for $\alpha = 0.08$ fm^4 and underbinds by less than 1 MeV for $\alpha = 0.04$ fm^4. For ^{40}Ca we have performed IT-NCSM calculations up to $N_{\max} = 8$ again

showing deviations below 1%. For $\alpha = 0.08$ fm^4 the NO2B approximation yields $-310(2)$ MeV and $-472(1)$ MeV as compared to $-309(1)$ MeV and $-468(1)$ MeV for the $N_{\max} = 8$ ground-state energy with the exact $NN + 3N$-induced and $NN + 3N$-full Hamiltonians, respectively.

For a comprehensive picture of its anatomy, we analyze the expectation values of the $3N$ interaction at different levels of the NOnB approximation using IT-NCSM eigenstates obtained with the exact $3N$ interaction for ^{4}He, ^{16}O, and ^{40}Ca for fixed $N_{\max}$. Figure 2 summarizes these expectation values of the $3N$ interaction for a set of $NN + 3N$-induced and $NN + 3N$-full Hamiltonians. For ^{16}O and ^{40}Ca a similar pattern emerges: The NO2B approximation does reproduce the expectation value of the exact $3N$ interaction very well, both for the $NN + 3N$-induced and the $NN + 3N$-full Hamiltonian. The pattern observed for the sequence of NOnB approximations is different for both types of Hamiltonians. For $NN + 3N$-induced the 1B and 2B contributions of the normal-ordered Hamiltonian have opposite sign, with the 1B contribution being significantly larger, whereas for the $NN + 3N$-full Hamiltonian the 1B and 2B contributions are both attractive and of similar size. In all cases the 0B contribution is the largest and overestimates the exact $3N$ expectation value. For ^{4}He the pattern is different. The 0B term does not provide the largest contribution and underestimates the $3N$ expectation value. The signs and relative sizes of the 1B and 2B terms again depend on the Hamiltonian, and the NO2B approximation still shows a sizable deviation from the exact $3N$ expectation value, contrary to the single example presented in Ref. [8].

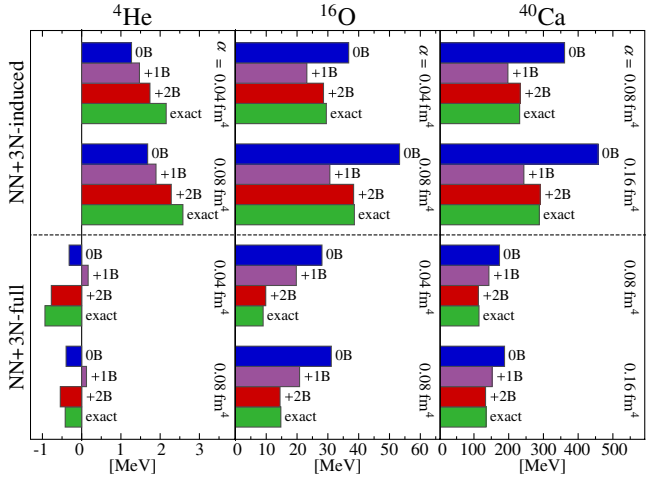

FIG. 2 (color online). Anatomy of the NOnB approximation of the ground-state energies of ^{4}He, ^{16}O, and ^{40}Ca. The bar charts show the expectation values of the $3N$ interaction computed at different levels of the normal-ordering approximation, i.e., NO0B, NO1B, NO2B, and exact $3N$. We employ the $NN + 3N$-induced and $NN + 3N$-full Hamiltonians, each with two values of α (see labels). We use the eigenstates obtained for the exact $3N$ interaction in $N_{\max} = 10$ for ^{4}He and ^{16}O and $N_{\max} = 8$ for ^{40}Ca, all at $\hbar\Omega = 20$ MeV.

This case study shows that there is no universal pattern and no hierarchy in the individual NOnB contributions. The size of the individual terms and also the deviation of the NO2B approximation from the exact $3N$ result depends on the Hamiltonian, the nucleus, and the oscillator frequency. Nonetheless, the $3N$ expectation values in Fig. 2 and the ground-state energies in Fig. 1 demonstrate that the NO2B approximation works very well beyond the lightest nuclei.

Application in coupled-cluster theory.—After validating the NO2B approximation, we are now applying it in ground-state calculations for heavier closed-shell nuclei in the framework of the coupled-cluster method. Coupled-cluster theory is a natural framework since normal-ordering of the Hamiltonian with respect to a reference state is inherent to the formulation of the approach. We have developed an efficient coupled-cluster code using the J-coupled scheme discussed in Ref. [23], which enables us to go to very large model spaces. We limit ourselves to coupled cluster with singles and doubles excitations (CCSD), which has been shown to be a good approximation for soft SRG-evolved interactions [23]. An additional approximation present in the CCSD calculations for technical reasons is a truncation of the $3N$ matrix elements entering the NO2B to harmonic-oscillator principal quantum numbers $e_1 + e_2 + e_3 \leq E_{3\,\max} = 14$.

In a first step, we confront the CCSD results for ^{16}O with the previous IT-NCSM results, both using the NO2B approximation. Figure 3 shows the convergence of the ground-state energies in both methods using the $NN + 3N$-induced and $NN + 3N$-full Hamiltonian. We observe

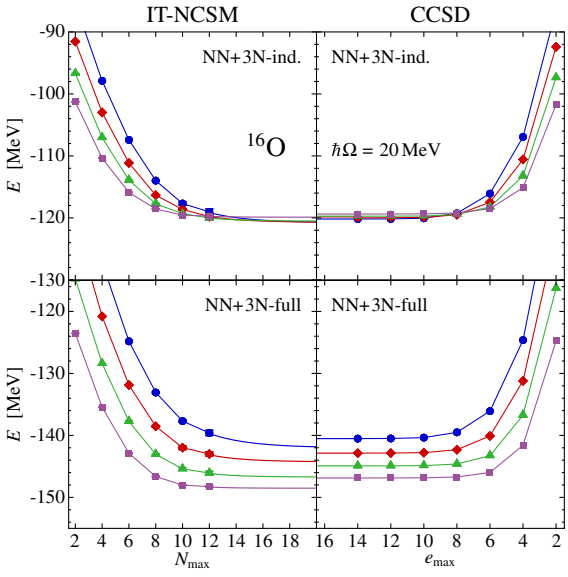

FIG. 3 (color online). Comparison of the ground-state energies of ^{16}O obtained in IT-NCSM and CCSD including $3N$ interactions at the NO2B level for the $NN + 3N$-induced and the $NN + 3N$-full Hamiltonians with $\alpha = 0.04$ fm^4 (●), 0.05 fm^4 (◆), 0.0625 fm^4 (▲), and 0.08 fm^4 (■).

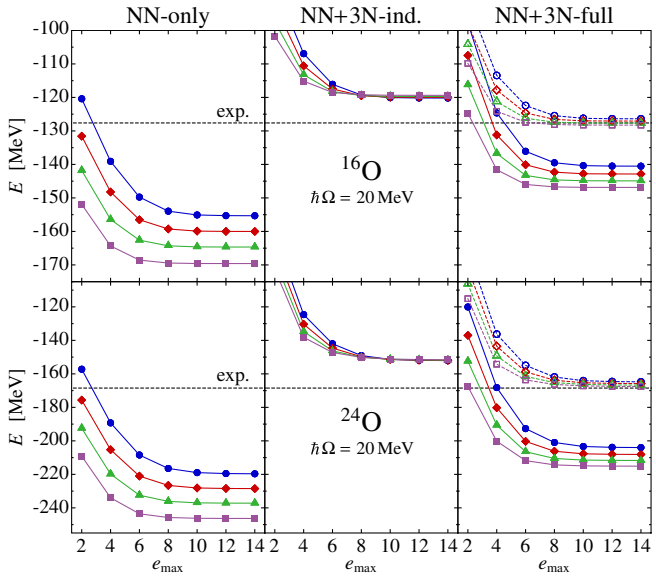

FIG. 4 (color online). CCSD ground-state energies for ^{16}O and ^{24}O as a function of $e_{\max}$ for the three types of Hamiltonians (see column headings) using the NO2B approximation for a range of flow parameters: $\alpha = 0.04$ fm^4 (●), 0.05 fm^4 (◆), 0.0625 fm^4 (▲), and 0.08 fm^4 (■). The filled symbols for the $NN + 3N$-full Hamiltonian are for the standard chiral $3N$ interaction with cutoff 500 MeV, the open symbols for a modified $3N$ interaction with cutoff 400 MeV (see text).

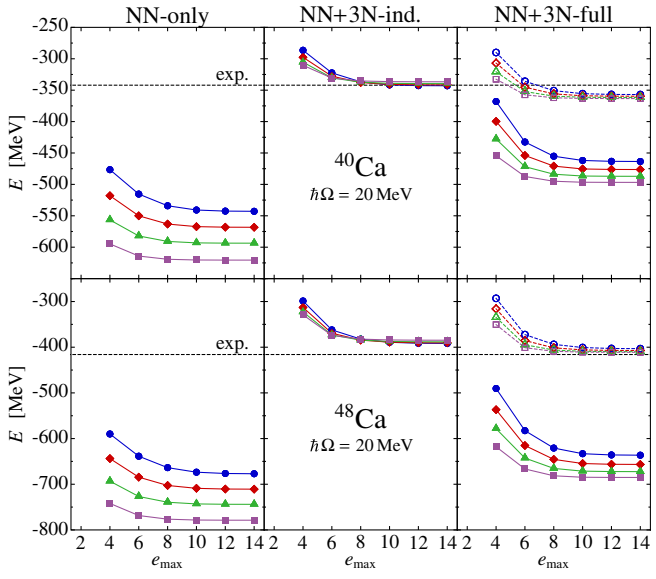

FIG. 5 (color online). Same as Fig. 4 for ^{40}Ca and ^{48}Ca.

a very good agreement of the converged ground-state energies, with the IT-NCSM giving 1 to 2 MeV more binding. This difference is consistent with the contributions expected from triples corrections and the missing $3N$ matrix elements with $E_{3\max} > 14$. The latter point has been confirmed by comparing to lower $E_{3\max}$ cuts. Altogether, the CCSD calculations for ^{16}O with soft SRG-evolved $NN + 3N$ Hamiltonians in NO2B approximation provide a ground-state energy within 1% to 2% of the IT-NCSM results with the exact $3N$ interaction. Using CCSD with the NO2B approximation we can now study the systematics of ground-state energies with SRG-evolved chiral $NN + 3N$ Hamiltonians beyond ^{16}O. Following the analysis of Ref. [18] we discuss the α dependence observed with the NN-only, the $NN + 3N$-induced, and the $NN + 3N$-full Hamiltonians for ^{16}O and ^{24}O, shown in Fig. 4, and for ^{40}Ca and ^{48}Ca, shown in Fig. 5. For all nuclei we observe the same pattern: The NN-only Hamiltonian exhibits strong α dependence of the converged ground-state energies hinting at induced $3N$ interactions. Their inclusion at the $NN + 3N$-induced level eliminates the α dependence, thus providing a strong indication that induced $4N$ contributions originating from the initial NN are irrelevant for ground-state energies. The converged energies, therefore, correspond to the solutions for the initial chiral NN interaction. We obtain $-120.2(+0.8)$ MeV for ^{16}O ground-state energy, $-152.1(+0.5)$ MeV for ^{24}O, $-343(+6)$ MeV for ^{40}Ca, and $-392(+7)$ MeV for ^{48}Ca using the $NN + 3N$-induced Hamiltonian at $\alpha = 0.04$ fm^4 for $e_{\max} = 14$. The numbers in parenthesis give the change when going to $\alpha = 0.08$ fm^4 as a measure for the residual α dependence. These results are in very good agreement with the CC results reported in Refs [23,24] for the bare chiral NN interaction.

When including the initial $3N$ interaction, i.e., when using the $NN + 3N$-full Hamiltonian, the α dependence reemerges, indicating that $4N$ terms induced by the initial $3N$ interaction become sizable. These CCSD results confirm the findings of Ref. [18] and extend the systematics to heavier nuclei.

In addition to the standard chiral $3N$ interaction [17] with cutoff momentum of 500 MeV, we also employ a chiral $3N$ interaction with a modified cutoff of 400 MeV and $c_E = 0.098$ refitted to reproduce the ^{4}He binding energy. We keep the value $c_D = -0.2$ as in the standard $3N$ interaction. Based on the findings of Ref. [17] a selective change of the $3N$ cutoff or of c_E will not affect the triton lifetime. Effectively the lower cutoff reduces the strength of the two-pion terms of the $3N$ interaction and limits them to lower momenta. As a result the α dependence and thus the induced $4N$ contributions are reduced significantly. This allows for a quantitative comparison of the $NN + 3N$-full predictions with experimental binding energies. We obtain ground-state energies of $-126.4(-1.9)$ MeV for ^{16}O, $-164.8(-2.8)$ MeV for ^{24}O, $-357(-6)$ MeV for ^{40}Ca, and $-403(-8)$ MeV for ^{48}Ca using $\alpha = 0.04$ fm^4 with the change when going to $\alpha = 0.08$ fm^4 given in parenthesis. The agreement with experiment is remarkable. For ^{16}O and ^{24}O the predictions based on the chiral $NN + 3N$ Hamiltonian reproduce the experimental energies within the theoretical uncertainties.

Even for ^{40}Ca and ^{48}Ca the agreement with experiment is surprisingly good, given the fact that no information beyond ^{4}He was used to fix the Hamiltonian. This is evidence that this chiral $NN + 3N$ Hamiltonian, although not fully consistent regarding the chiral order and the cutoff choice in NN and $3N$ terms, contains all the relevant physics for nuclear structure predictions over a large mass range.

Conclusions.—We have demonstrated that the NO2B approximation allows for accurate nuclear structure calculations using SRG-evolved chiral $NN + 3N$ Hamiltonians in cases where the inclusion of the exact $3N$ interaction is computationally too demanding. For many-body methods that can handle $3N$ interactions exactly, normal ordering is an option for including chiral $4N$ interactions. Therefore, it provides a valuable tool to exploit the full physics potential of chiral Hamiltonians. In this context we have shown that a chiral $3N$ interaction with reduced cutoff can yield binding energy systematics consistent with experiment—ongoing investigations of the spectroscopy of p- and sd-shell nuclei confirm the quality and universality of this Hamiltonian. A generalization of the normal-ordering approximation to open-shell systems and excited states using multi-determinantal reference states [25] is the subject of present research.

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