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# Ab Initio Calculations of Even Oxygen Isotopes with Chiral Two- Plus Three-Nucleon Interactions

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We formulate the In-Medium Similarity Renormalization Group (IM-SRG) for open-shell nuclei using a multi-reference formalism based on a generalized Wick theorem introduced in quantum chemistry. The resulting multi-reference IM-SRG (MR-IM-SRG) is used to perform the first *ab initio* study of all even oxygen isotopes with chiral NN and 3N Hamiltonians, from the proton to the neutron drip lines. We obtain an excellent reproduction of experimental ground-state energies with quantified uncertainties, which is validated by results from the Importance-Truncated No-Core Shell Model and the Coupled Cluster method. The agreement between conceptually different many-body approaches and experiment highlights the predictive power of current chiral two- and three-nucleon interactions, and establishes the MR-IM-SRG as a promising new tool for *ab initio* calculations of medium-mass nuclei far from shell closures.

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*Introduction.* Neutron-rich nuclei are the focus of the experimental program of current and next-generation rare isotope facilities. Emerging phenomena such as halos or neutron skins make these nuclei ideal laboratories to study nuclear interactions in delicately tuned scenarios, and motivate the use of *ab initio* many-body calculations to provide their description from first principles. Such calculations make it possible to confront modern nuclear Hamiltonians from chiral effective field theory (EFT) [1, 2] with a wealth of data beyond few-body systems.

For light nuclei, the *ab initio* No-Core Shell Model (NCSM) [3, 4] provides the capabilities for studies of isotopic chains, but for medium-mass nuclei this approach is not feasible because of its large computational effort. Many-body techniques with more modest computational scaling, such as the Coupled Cluster (CC) [5–7] or Self-Consistent Green’s Function methods [8, 9], can be used to probe nuclei in the vicinity of shell closures, but are not applicable for open-shell nuclei far from shell closures. For such nuclei, a self-consistent Gor’kov formalism was developed recently [10, 11], but this approach is currently limited to second-order terms in the many-body perturbation expansion.

In this Letter, we describe the extension of the In-Medium Similarity Renormalization Group (IM-SRG) framework of Refs. [12, 13] to open-shell nuclei by means of a multi-reference formulation. We use the resulting MR-IM-SRG and two other many-body approaches, the Importance-Truncated No-Core Shell Model (IT-NCSM) and the CC method, to perform the first *ab initio* study of all even oxygen isotopes with chiral NN+3N Hamiltonians.

*Formalism.* The main tools for the derivation of the MR-IM-SRG are the generalized normal-ordering and Wick theorem by Kutzelnigg and Mukherjee [14]. We write a string of creation and annihilation operators in tensorial form,

$$A_{l\dots N}^{1\dots k} \equiv a_1^\dagger \dots a_k^\dagger a_N \dots a_l, \quad (1)$$

and expand it in terms of components that are normal-ordered with respect to an arbitrary reference state  $|\Phi\rangle$  [14–16]. We

obtain

$$A_{l\dots N}^{1\dots k} = :A_{l\dots N}^{1\dots k} : + \lambda_l^1 :A_{mn\dots N}^{23\dots k} : - \lambda_m^1 :A_{ln\dots N}^{23\dots k} : + \dots \\ + (\lambda_l^1 \lambda_m^2 - \lambda_m^1 \lambda_l^2 + \lambda_{lm}^{12}) :A_{n\dots N}^{3\dots k} : + \dots, \quad (2)$$

where  $: \dots :$  indicates normal-ordering, and we have introduced irreducible one- and two-body density matrices  $\lambda^{(1)}$  and  $\lambda^{(2)}$ :

$$\lambda_2^1 \equiv \langle \Phi | A_2^1 | \Phi \rangle, \quad \lambda_{34}^{12} \equiv \langle \Phi | A_{34}^{12} | \Phi \rangle - \lambda_2^1 \lambda_4^3 + \lambda_3^1 \lambda_4^2. \quad (3)$$

The particle rank of the irreducible density matrices is evident from the single-particle indices. Generally, up to  $n$ -body irreducible density matrices  $\lambda^{(n)}$  appear in the expansion of an  $n$ -body operator, which are defined recursively in terms of density matrices of lower rank and encode information about  $n$ -body correlations in the reference state [14]. For an independent-particle state, all matrices except  $\lambda^{(1)}$  vanish.

Products of normal-ordered operators can be expanded by means of a generalized Wick theorem (GWT), e.g.,

$$:A_{56}^{12} : :A_{78}^{34} : = :A_{5678}^{1234} : + \lambda_7^1 :A_{568}^{234} : - \xi_5^3 :A_{678}^{124} : + \dots \\ + (\lambda_7^1 \lambda_8^2 - \lambda_8^1 \lambda_7^2 + \lambda_{78}^{12}) :A_{56}^{34} : - \lambda_{57}^{12} :A_{68}^{34} : + \dots, \quad (4)$$

where  $\xi_2^1 \equiv \lambda_2^1 - \delta_2^1$  [16]. In addition to simple contractions containing  $\lambda^{(1)}$  and  $\xi^{(1)}$  which also occur in the standard Wick theorem, we obtain terms involving  $\lambda^{(2)}, \dots, \lambda^{(n)}$ . Each density matrix must have at least one index from each of the operators in the product — other terms vanish due to the initial normal-ordering (2) [14]. In the following, we work in natural orbitals, i.e., the eigenbasis of  $\lambda^{(1)}$ , where

$$\lambda_2^1 = n_1 \delta_2^1, \quad \xi_2^1 = -\bar{n}_1 \delta_2^1 \equiv -(1 - n_1) \delta_2^1, \quad (5)$$

and the eigenvalues are the occupation numbers  $0 \leq n_a \leq 1$ .

We now consider the IM-SRG operator flow equation

$$\frac{d}{ds} H(s) = [\eta(s), H(s)]. \quad (6)$$

By integrating Eq. (6), we generate a continuous unitary transformation that decouples the ground-state of the Hamiltonian

$H(s)$  from excitations, and solve the many-body problem [12, 13]. Suppressing the flow parameter  $s$  for brevity, we apply the generalized normal-ordering to  $H$  and the generator  $\eta$ , and evaluate the commutator using the GWT to obtain the MR-IM-SRG flow equations:

$$\begin{aligned} \frac{dE}{ds} &= \sum_{ab} (n_a - n_b) (\eta_b^a f_a^b - f_b^a \eta_a^b) \\ &+ \frac{1}{4} \sum_{abcd} (\eta_{cd}^{ab} \Gamma_{ab}^{cd} - \Gamma_{cd}^{ab} \eta_{ab}^{cd}) n_a n_b \bar{n}_c \bar{n}_d \\ &+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd}^{ab}, \end{aligned} \quad (7)$$

$$\begin{aligned} \frac{d}{ds} f_2^1 &= \sum_a \eta_a^1 f_2^a + \sum_{ab} \eta_b^a \Gamma_{a2}^{b1} (n_a - n_b) \\ &+ \frac{1}{2} \sum_{abc} \eta_{bc}^{1a} \Gamma_{2a}^{bc} (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c) \\ &+ \frac{1}{4} \sum_{abcde} \eta_{bc}^{1a} \Gamma_{2a}^{de} \lambda_{bc}^{de} + \sum_{abcde} \eta_{bc}^{1a} \Gamma_{2d}^{be} \lambda_{cd}^{ae} \\ &- \frac{1}{2} \sum_{abcde} (\eta_{2b}^{1a} \Gamma_{ae}^{cd} \lambda_{be}^{cd} - \eta_{2b}^{1a} \Gamma_{de}^{bc} \lambda_{de}^{ac}) - [\eta \leftrightarrow f, \Gamma], \end{aligned} \quad (8)$$

$$\begin{aligned} \frac{d}{ds} \Gamma_{34}^{12} &= \sum_a (\eta_a^1 \Gamma_{34}^{a2} + \eta_a^2 \Gamma_{34}^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{3a}^{12} \\ &\quad - f_a^1 \eta_{34}^{a2} - f_a^2 \eta_{34}^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12}) \\ &+ \frac{1}{2} \sum_{ab} (\eta_{ab}^{12} \Gamma_{34}^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab}) (1 - n_a - n_b) \\ &+ \sum_{ab} (n_a - n_b) ((\eta_{3b}^{1a} \Gamma_{4a}^{2b} - \Gamma_{3b}^{1a} \eta_{4a}^{2b}) - [1 \leftrightarrow 2]), \end{aligned} \quad (9)$$

where  $E = \langle \Phi | H | \Phi \rangle$ , and the one- and two-body parts of  $H$ , denoted by  $f$  and  $\Gamma$ , contain in-medium contributions from the 3N interaction because of the normal ordering [12, 13]. The symbol  $[\eta \leftrightarrow f, \Gamma]$  in Eq. (8) indicates an interchange of the one- and two-body parts of  $\eta$  and  $H$ . To close the system of flow equations (7)–(9), we truncate three-body operators [13] and a term containing  $\lambda^{(3)}$  in the energy flow equation (7). We refer to this truncation as MR-IM-SRG(2).

By integrating Eqs. (7)–(9), we perform a non-perturbative resummation of the Many-Body Perturbation series [12, 13]. The flowing two-body vertex is RG-improved by Eq. (9), e.g., with contributions from generalized ladder (3rd line) and ring diagrams (4th line), which in turn generate corrections to the ground-state energy when  $\Gamma$  is inserted in Eq. (7) [13].

As our default choice for the generator, we use the ansatz of White [13, 17]. The required matrix elements of the Hamiltonian, such as  $\langle \Phi | H : A_{34}^{12} : | \Phi \rangle$ , which couple the reference state to excitations, or  $\langle \Phi | : A_{12}^{34} : H : A_{34}^{12} : | \Phi \rangle$ , which enter

the energy denominators, can be evaluated using the generalized normal ordering. This yields

$$\begin{aligned} \eta_2^1 &= \frac{\bar{n}_1 n_2 f_2^1}{\bar{n}_1 f_1^1 - n_2 f_2^2 + \bar{n}_1 n_2 \Gamma_{12}^{12}} - [1 \leftrightarrow 2] + \dots, \quad (10) \\ \eta_{34}^{12} &= \frac{\bar{n}_1 \bar{n}_2 n_3 n_4 \Gamma_{34}^{12}}{\bar{n}_1 f_1^1 + \bar{n}_2 f_2^2 - n_3 f_3^3 - n_4 f_4^4 + G_{34}^{12}} - [(12) \leftrightarrow (34)] \\ &+ \dots, \quad (11) \end{aligned}$$

where

$$\begin{aligned} G_{34}^{12} &= \bar{n}_1 \bar{n}_2 \Gamma_{12}^{12} + n_3 n_4 \Gamma_{34}^{34} \\ &- (\bar{n}_1 n_3 \Gamma_{13}^{13} + \bar{n}_2 n_4 \Gamma_{24}^{24} + [1 \leftrightarrow 2]). \end{aligned} \quad (12)$$

The dots in Eqs. (10) and (11) indicate terms that are linear in  $\lambda^{(2)}$ . Terms containing  $\lambda^{(n \geq 3)}$  or nonlinear powers of  $\lambda^{(2)}$  are truncated.

In cases where the flow stalls due to small energy denominators, we use Wegner's generator  $\eta = [H, H^{od}]$  as a fallback, defining the one- and two-body parts of the off-diagonal Hamiltonian  $H^{od}$  as

$$\begin{aligned} (f^{od})_2^1 &= \bar{n}_1 n_2 f_2^1 + [1 \leftrightarrow 2], \\ (\Gamma^{od})_{34}^{12} &= \bar{n}_1 \bar{n}_2 n_3 n_4 \Gamma_{34}^{12} + [(12) \leftrightarrow (34)]. \end{aligned} \quad (13)$$

This generator is free of numerical instabilities but less efficient because the flow equations become stiff [12, 13]. In the limit of a single Slater determinant reference state, both generators reduce to the forms used for closed-shell nuclei in [12, 13].

We obtain a reference state for each nucleus by solving the Hartree-Fock-Bogoliubov (HFB) equations, and projecting the resulting state on proton and neutron number,  $|\Phi\rangle = P_N P_Z |\text{HFB}\rangle$  [18]. This choice allows us to enforce spherical symmetry in calculations for even nuclei [19], and greatly increases the single-particle basis sizes we can treat. The natural-orbital basis of  $|\Phi\rangle$  is the usual canonical basis of the HFB vacuum, allowing us to use analytic expressions for the density matrices [20].

The MR-IM-SRG method can be extended systematically by improving the truncation scheme: One would include 3, ...,  $A$ -body operators when Eq. (6) is expanded in normal-ordered components, as well as additional terms involving irreducible density matrices. While the number of flow equations is the same as in the single-reference case, their complexity grows much more rapidly due to additional terms from the generalized normal ordering [12–14].

*Calculation Details.* Reference states for the MR-IM-SRG calculation are obtained by solving the HFB equations in 15 major harmonic-oscillator (HO) shells, and projecting the resulting state on good proton and neutron numbers [13, 21]. For the 3N interaction, the sum of the HO energy quantum numbers of a 3N basis state is limited by  $e_1 + e_2 + e_3 \leq E_{3\max} = 14$ , as discussed in [13, 22]. Reducing  $E_{3\max}$  from 14 to 12 changes the MR-IM-SRG(2) ground-state energies for oxygen isotopes by less than 1% for the Hamiltonians used

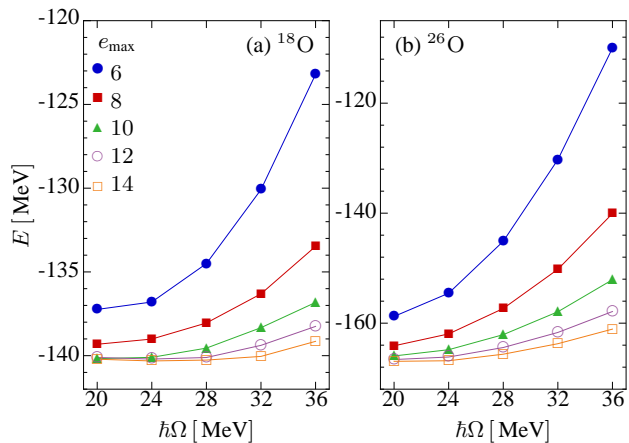


FIG. 1. (Color online) Convergence of the MR-IM-SRG(2) ground-state energies of  $^{18}\text{O}$  and  $^{26}\text{O}$  with respect to the single-particle basis size  $e_{\text{max}}$ , for the NN+3N-full Hamiltonian at  $\lambda_{\text{SRG}} = 2.0 \text{ fm}^{-1}$ .

in this work. The intrinsic NN+3N Hamiltonian is normal-ordered with respect to the reference state, and the residual normal-ordered 3N interaction term is discarded, leading to the normal-ordered two-body approximation (NO2B), which is found to overestimate oxygen binding energies by about 1% [13, 22].

In this Letter, we use the same nuclear Hamiltonians as in our recent IM-SRG and CC studies [13, 22, 23]: The NN interaction is the chiral  $\text{N}^3\text{LO}$  interaction by Entem and Machleidt, with cutoff  $\Lambda_{\text{NN}} = 500 \text{ MeV}/c$  [2, 24]. Our standard three-body Hamiltonian is a local  $\text{N}^2\text{LO}$  3N interaction with initial cutoff  $\Lambda_{3\text{N}} = 400 \text{ MeV}/c$ . The resolution scale of the Hamiltonian is lowered to  $\lambda_{\text{SRG}} = 1.88, \dots, 2.24 \text{ fm}^{-1}$  by means of an SRG evolution in three-body space [25–27]. Hamiltonians which only contain SRG-induced 3N forces are referred to as NN+3N-induced, those also containing an initial 3N interaction as NN+3N-full.

In Fig. 1, we illustrate the convergence of the MR-IM-SRG(2) ground-state energies for  $^{18}\text{O}$  and  $^{26}\text{O}$  with respect to the single-particle basis size. At the optimal  $\hbar\Omega$ , the change in the ground-state energy is 0.1% when we increase the basis from  $e_{\text{max}} = 12$  to 14. This rapid convergence is representative for all Hamiltonians used in this work.

*Results.* In Fig. 2, we show MR-IM-SRG(2) ground-state energies of the even oxygen isotopes for NN+3N-full Hamiltonians with initial cutoffs  $\Lambda_{3\text{N}} = 350, 400$  and  $450 \text{ MeV}/c$ . For the 3N low-energy constants, we use a fixed  $c_D = -0.2$ , and  $c_E = 0.205, 0.098$ , and  $-0.016$ , respectively, which are fit to the  $^4\text{He}$  binding energy in NCSM calculations [23, 27]. For the NN+3N-full Hamiltonian with  $\Lambda_{3\text{N}} = 400 \text{ MeV}/c$ , we achieve an excellent reproduction of experimental data all the way to the neutron drip line at  $^{24}\text{O}$  [29], with deviations of 1-2%. Recent experiments place the  $^{26}\text{O}$  ground-state resonance at  $E_x \lesssim 150 \text{ keV}$  above the  $^{24}\text{O}$  ground-state energy [30, 31]. We slightly overestimate this energy in our calculation because the HO basis expansion of our single-particle wave functions is ill-suited to the description of resonances

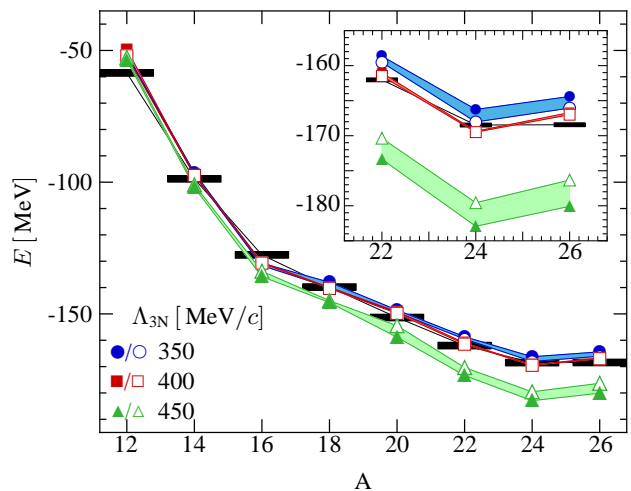


FIG. 2. (Color online) Dependence of the MR-IM-SRG(2) oxygen ground-state energies for the NN+3N-full Hamiltonian on the resolution scale and the initial cutoff  $\Lambda_{3\text{N}}$ . For each  $\Lambda_{3\text{N}}$ , the band is obtained by varying  $\lambda_{\text{SRG}}$  from 2.24 (open symbols) to  $1.88 \text{ fm}^{-1}$  (closed symbols). Experimental values are indicated by black bars [28, 29].

and other continuum states. The inset in Fig. 2 illustrates that the correct drip-line systematics is independent of  $\lambda_{\text{SRG}}$  in the studied range and also robust against variations of the cutoff  $\Lambda_{3\text{N}}$ . This suggests that the long-range part of the two-pion exchange (2PE) 3N interaction, which remains unchanged as we lower  $\Lambda_{3\text{N}}$ , is key to obtaining the proper isotopic trends. The 2PE contribution has significant spin-orbit and tensor terms, and is therefore important for the evolution of the shell structure along the isotopic chain, as also demonstrated in other studies, e.g. [32].

Let us now discuss the effect of varying the resolution scale. As discussed in [13, 22], the  $\lambda_{\text{SRG}}$ -dependence of our energies is the net result of omitted induced 4N interactions, the  $E_{3\text{max}}$  cut, and the MR-IM-SRG(2) truncation of the many-body expansion, while the effect of the NO2B approximation is found to be independent of  $\lambda_{\text{SRG}}$ .

For  $\Lambda_{3\text{N}} = 350 \text{ MeV}/c$  we do not expect significant induced 4N interactions [27]. As  $\lambda_{\text{SRG}}$  is reduced, we capture additional repulsive 3N strength in matrix elements with  $e_1 + e_2 + e_3 \leq E_{3\text{max}}$ . We also speed up the convergence of the many-body expansion and reduce the error due to the MR-IM-SRG(2) truncation, but for the resolution scales considered here, this effect is already saturated. In total, we find a slight artificial increase of the ground-state energies as we lower  $\lambda_{\text{SRG}}$  [13].

For our standard choice  $\Lambda_{3\text{N}} = 400 \text{ MeV}/c$ , effects from omitted 4N interactions, the  $E_{3\text{max}}$  cut, and the many-body truncation cancel, and the  $\lambda_{\text{SRG}}$ -dependence of the energies in Fig. 2 is extremely weak [13]. The omission of 4N interactions becomes the dominant source of uncertainty as we increase  $\Lambda_{3\text{N}}$  to  $450 \text{ MeV}/c$ , resulting in an enhanced  $\lambda_{\text{SRG}}$ -dependence of the ground-state energies of the heavier oxygen isotopes. This is consistent with the even stronger  $\lambda_{\text{SRG}}$ -

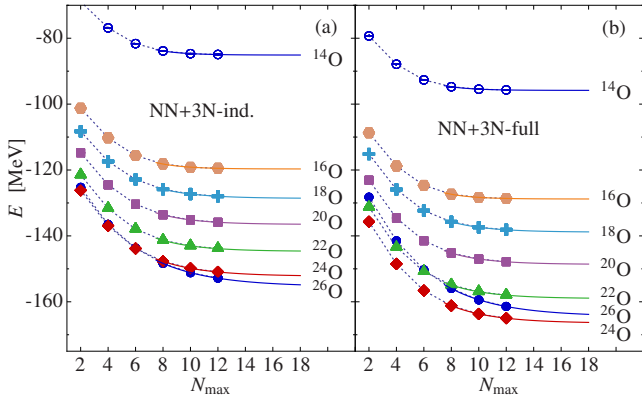


FIG. 3. (Color online) IT-NCSM ground-state energies of the even oxygen isotopes for the NN+3N-induced (a) and NN+3N-full Hamiltonians (b) at  $\lambda_{\text{SRG}} = 1.88 \text{ fm}^{-1}$ . Solid lines indicate the energy extrapolation based on  $N_{\text{max}} = 8 - 12$  data, dotted lines guide the eye for smaller  $N_{\text{max}}$ . Uncertainties due to the importance truncation are smaller than the symbols used to represent the data. All energies are obtained at optimal  $\hbar\Omega$ .

dependence for  $\Lambda_{3\text{N}} = 500 \text{ MeV}/c$  observed in Refs. [23, 26, 27].

To assess the quality of our MR-IM-SRG(2) ground-state energies, we compare them to results from the IT-NCSM, which yields the exact NCSM results within quantified uncertainties from the importance truncation [26, 33]. In the IT-NCSM calculations, we use the full 3N interaction without NO2B approximation, and the  $E_{3\text{max}}$  cut is naturally compatible with the IT-NCSM model space truncation [13]. In Fig. 3 we show the convergence of the oxygen ground-state energies for the NN+3N-induced and NN+3N-full Hamiltonians as a function of  $N_{\text{max}}$ , along with exponential fits which extrapolate  $N_{\text{max}} \rightarrow \infty$  [26, 33, 34]. With the exception of  $^{26}\text{O}$ , all isotopes converge well, and the uncertainties of the threshold and model spaces truncations of the IT-NCSM results are typically about 1 MeV. For  $^{26}\text{O}$ , the rate of convergence is significantly worse, which is expected due to the resonance nature of this ground state.

The neutron-rich oxygen isotopes are the heaviest nuclei studied so far in the IT-NCSM with full 3N interactions. For  $^{26}\text{O}$ , the computation of the complete  $N_{\text{max}}$  sequence shown in Fig. 3 requires about 200,000 CPU hours. In contrast, a corresponding sequence of single-particle basis sizes in the MR-IM-SRG requires only about 3,000 CPU hours on a comparable system. Overall, the method scales polynomially with  $\mathcal{O}(N^6)$  to larger basis sizes  $N$ , which makes it ideally suited for the description of medium- and heavy-mass nuclei.

In Fig. 4, we compare the MR-IM-SRG(2) and IT-NCSM ground-state energies of the oxygen isotopes, for the NN+3N-induced and NN+3N-full Hamiltonians with  $\lambda_{\text{SRG}} = 1.88 \text{ fm}^{-1}$  to experiment. For the latter, the overall agreement between the two very different many-body approaches and experiment is striking: Except for slightly larger deviations in  $^{12}\text{O}$  and  $^{26}\text{O}$ , we reproduce experimental binding energies within 2-3 MeV. This is a remarkable demonstration of the

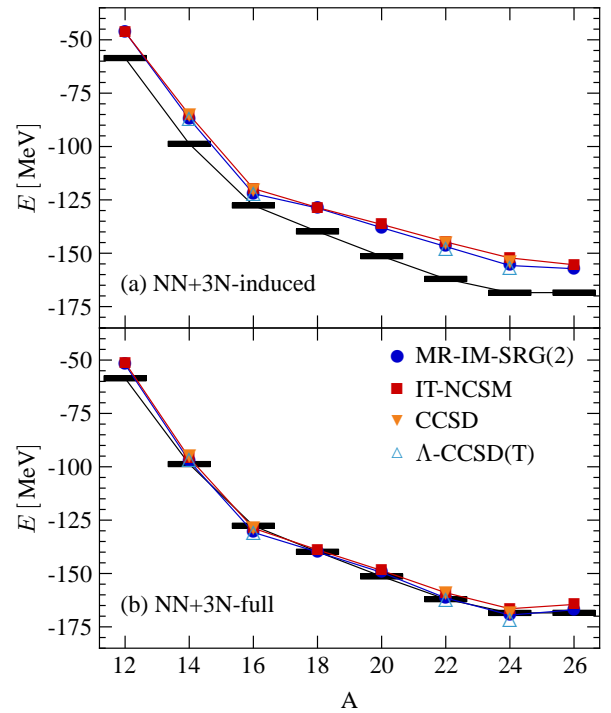


FIG. 4. (Color online) Oxygen ground-state energies for the NN+3N-induced (top) and NN+3N-full (bottom) Hamiltonian with  $\Lambda_{3\text{N}} = 400 \text{ MeV}/c$ . MR-IM-SRG(2), CCSD, and  $\Lambda$ -CCSD(T) results are obtained at optimal  $\hbar\Omega$ , using 15 major oscillator shells and  $E_{3\text{max}} = 14$ . The IT-NCSM energies are extrapolated to infinite model space. Experimental values are indicated by black bars [28, 29].

predictive power of current chiral NN+3N Hamiltonians, at least for ground-state energies. For further confirmation, we perform CC calculations with singles and doubles (CCSD), as well as perturbative triples ( $\Lambda$ -CCSD(T)) [15, 22, 35, 36] for oxygen isotopes with sub-shell closures. Using the same Hamiltonians in NO2B approximation, the MR-IM-SRG energies are bracketed by the CC results, and similar to the  $\Lambda$ -CCSD(T) values, consistent with the closed-shell results discussed in [13].

For the NN+3N-induced calculation, which should be compared to calculations with the bare chiral NN interaction [6], the reproduction of experimental trends fails, and the neutron drip line is predicted at the wrong mass, because  $^{26}\text{O}$  is bound with respect to  $^{24}\text{O}$ . This illustrates the crucial importance of the chiral 3N interaction for a proper description of the structure of neutron-rich nuclei [32].

Let us now address the uncertainties of our results. The MR-IM-SRG(2) energies lie 1.5–2% below the IT-NCSM results. About 1% of this deviation is caused by the NO2B approximation. The uncertainty due to the  $E_{3\text{max}}$  cut is less than 1% at low  $\lambda_{\text{SRG}}$ . While these uncertainties exhaust the greater part of the 1.5–2% deviation between MR-IM-SRG(2) and IT-NCSM, and suggest a very small uncertainty due to the many-body truncation, we assume a more conservative many-body truncation error of 1–1.5%, and an overall uncertainty of our oxygen energies at the level of 3–3.5%, consistent with

our closed-shell IM-SRG calculations [13]. Because all irreducible many-body density matrices vanish in closed-shell nuclei, our findings indicate that the truncation of terms containing  $\lambda^{(n \geq 3)}$  and non-linear powers of  $\lambda^{(2)}$  is negligible compared to the truncation of induced three-body operators. A more detailed analysis of the MR-IM-SRG truncation scheme will be presented in a future publication.

*Conclusions.* We have generalized the IM-SRG approach to multi-reference states, and used the resulting MR-IM-SRG method to perform the first *ab initio* study of all even oxygen isotopes with chiral NN+3N Hamiltonians, along with the IT-NCSM and the CC method. The MR-IM-SRG results are in excellent agreement with those from the other methods, confirming its reliability, and the method's modest computational demands make it ideally suited for the description of medium- and heavy-mass open-shell nuclei far from shell closures.

Our calculated oxygen ground-state energies agree remarkably well with experimental binding energies within theoretical uncertainties of 3%. This is achieved without any readjustment of the interaction to experimental data beyond  ${}^4\text{He}$ , and therefore constitutes an impressive demonstration of the predictive power of chiral NN+3N Hamiltonians. The present work also highlights the importance of the 3N interaction for the nuclear structure of neutron-rich nuclei, as demonstrated by the robust reproduction of the oxygen drip line.

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