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Ab initio computation of neutron-rich oxygen isotopes

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We compute the binding energy of neutron-rich oxygen isotopes and employ the coupled-cluster method and chiral nucleon-nucleon interactions at next-to-next-to-next-to-leading order with two different cutoffs. We obtain rather well-converged results in model spaces consisting of up to 21 oscillator shells. For interactions with a momentum cutoff of 500 MeV, we find that ^{28}O is stable with respect to ^{24}O, while calculations with a momentum cutoff of 600 MeV result in a slightly unbound ^{28}O. The theoretical error estimates due to the omission of the three-nucleon forces and the truncation of excitations beyond three-particle–three-hole clusters indicate that the stability of ^{28}O cannot be ruled out from *ab initio* calculations, and that three-nucleon forces and continuum effects play the dominant role in deciding this question.

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Introduction. The neutron drip line marks the limits of stability of neutron-rich isotopes. At present, this line is well established only in the lightest elements, as the cross section for the production of extremely neutron-rich nuclei decreases dramatically as one moves away from nuclei in the valley of β stability (for a recent review, see, for example, Ref. [1]). At present, ^{24}O is the "last" known stable neutron-rich oxygen ($Z = 8$) isotope, and ^{25}O is known to decay under the emission of one neutron [2]. The "next" neutron-rich oxygen isotope ^{26}O has not been observed experimentally [3,4], and systematics for its production cross section suggest that it should have been seen if it were a stable nucleus. Similar estimates suggest that the isotope ^{28}O is unstable [5]. Thus, experiments puts the neutron drip line at ^{24}O. This is remarkable, since ^{31}F is the most neutron-rich fluorine ($Z = 9$) isotope [6]. Thus, the addition of a single proton apparently shifts the drip line by six neutrons.

The theoretical determination of the neutron drip line is a challenging task as well. Near the neutron drip line, small uncertainties in the nuclear interaction are enhanced due to the extreme isospin and the proximity of the continuum. Several theoretical studies have addressed the structure of neutron-rich oxygen and fluorine isotopes. The employed methods and theoretical predictions differ considerably. The *sd* shell model, based on the Brown-Wildenthal USD interaction and the finite-range droplet model, predicts that ^{26}O is stable [7]. Within the *sd-pf* shell model, the present experimental situation of an unstable ^{26}O can be reproduced after a modification of the interaction [8]. Within this model, ^{28}O is unbound by about 1 MeV. Within the same model space, but a different interaction, Poves and Retamosa [9] obtained a stable ^{31}F and a stable ^{28}O. Shell-model descriptions of neutron-rich oxygen isotopes, including the coupling to the continuum, were given in Refs. [10–12]. Within the latter approach [12], two slightly different phenomenological *sd*-shell interactions are employed for oxygen isotopes close to and far away from the valley of β stability. This leads to the result that ^{26}O is unstable with respect to ^{24}O, while ^{28}O is unstable with respect to the emission of two and four neutrons. Clearly, the present theoretical situation does not have the desired predictive power, and calculations suffer from uncertainties in the knowledge of the interaction and from the difficulty to quantify how these uncertainties propagate in the quantum many-body problem. This is an opportunity for *ab initio* calculations to address these challenges.

Ab initio calculations have been very successful in light nuclei [13–18] and have recently also been extended to unbound [19–21] and medium-mass isotopes [22]. In this paper, we present *ab initio* calculations for the neutron-rich oxygen isotopes ^{22,24,28}O, and employ nucleon-nucleon interactions from chiral effective field theory (EFT) [23–27]. These interactions are rooted in QCD and include pion exchange and zero-range forces. The power counting, i.e., the systematic expansion of the interaction in terms of ratios of the probed momentum scale Q over the cutoff Λ_χ, is an important asset. In finite nuclei, Q is about 200 MeV [22], while the cutoffs we employ are $\Lambda_\chi = 500$ and $\Lambda_\chi = 600$ MeV. The variation of our results with the cutoff allows us to quantify uncertainties that are due to the omission of (short-ranged) three-nucleon forces (3NFs). We employ the coupled-cluster method [28–33] for the solution of the quantum many-body problem. This method scales gently with the system size and can accurately compute the binding energies of nuclei with closed subshells. In particular, the possibility to employ large model spaces avoids the need for a secondary renormalization of the chiral interactions from EFT for nuclei such as oxygen and calcium isotopes [22].

This paper is organized as follows. We briefly introduce the interactions and methods we employ and then present the results of our calculations.

Interaction, model space, and coupled-cluster method. We employ the chiral nucleon-nucleon interaction by Entem and Machleidt [26] at next-to-next-to-next-to-leading order (N^{3}LO). This includes terms up to order $(Q/\Lambda_\chi)^4$ in the power counting of the nucleon-nucleon interaction. The interaction has a high-momentum cutoff of $\Lambda_\chi = 500$ MeV,

and a version with cutoff $\Lambda_\chi = 600$ MeV is also available [34]. The low-energy constants of the chiral potentials were determined by fits to the two-nucleon system. We neglect 3NFs that already appear at next-to-next-to-leading order and thereby introduce uncertainties of the order $(Q/\Lambda_\chi)^3$. As physics must be independent of the cutoff (or renormalization scale), any cutoff dependence in our results quantifies the uncertainty due to omitted contributions of short-ranged 3NFs and forces of higher rank. The intrinsic Hamiltonian $\hat{H} = \hat{T} - \hat{T}_{\rm cm} + \hat{V}(\Lambda_\chi)$ is translationally invariant and does not depend on the center-of-mass coordinate. Here $\hat{T}$, $\hat{T}_{\rm c.m.}$, and $\hat{V}(\Lambda_\chi)$ denote the kinetic energy of the A-body system, the kinetic energy of the center-of-mass coordinate, and the chiral nucleon-nucleon interaction with momentum cutoff Λ_χ, respectively. We express the Hamiltonian in a single-particle basis of the spherical harmonic oscillator. Our model-space parameters are the oscillator spacing $\hbar\omega$ of our single-particle basis and the maximal excitation energy $(N + 3/2)\hbar\omega$ of a single-particle state, i.e., the number of major oscillator shell is $N + 1$. As a first step toward the solution of the many-body problem, we solve the spherical Hartree-Fock equations and transform the Hamiltonian to this basis. In drip-line nuclei, the outermost nucleons move in orbitals close to the scattering threshold, making the nuclear wave function exhibit halo-like structures and sometimes even ground states embedded in the continuum. The presence of the scattering continuum in such exotic nuclei makes the use of the oscillator basis not ideal. The unrealistic Gaussian falloff of the oscillator wave functions makes convergence slow for nuclei with dilute matter distributions. However, the Gamow-Hartree-Fock (see, e.g., Ref. [19]) yields occupied single-particle states with nonphysical positive imaginary parts. This difficulty is due to the relatively "hard" interaction we employ. To avoid this problem, we choose to stay within the oscillator basis but employ very large model spaces for an improved description of the tails of the radial wave function.

The nuclear many-body problem is solved with the coupled-cluster method [28–33,35–38]. This approach is based on the similarity transformation of the normal-ordered intrinsic Hamiltonian $\hat{H}_N$,

$$\overline{H} = e^{-\hat{T}} \hat{H}_N e^{\hat{T}}. \tag{1}$$

Here, the Hamiltonian is normal-ordered with respect to a product state $|\psi\rangle$ which serves as a reference. The particle-hole cluster operator

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots + \hat{T}_A \tag{2}$$

is defined with respect to this reference state. It is a sum of the k-particle–k-hole (kp-kh) cluster operators

$$\hat{T}_k = \frac{1}{(k!)^2} \sum_{i_1,\ldots,i_k;a_1,\ldots,a_k} t^{a_1\ldots a_k}_{i_1\ldots i_k} \hat{a}^\dagger_{a_1} \ldots \hat{a}^\dagger_{a_k} \hat{a}_{i_k} \ldots \hat{a}_{i_1}. \tag{3}$$

We use the convention that $i, j, k, \ldots$ label the occupied single-particle orbitals, while $a, b, c, \ldots$ label the unoccupied orbitals. We truncate the cluster operator beyond the $\hat{T}_2$ level and employ ΛCCSD(T) [39,40] as an approximation for the $\hat{T}_3$ clusters. The unknown cluster amplitudes t^a_i and t^{ab}_{ij} in Eq. (2) are determined from the solution of the coupled-cluster equations

$$0 = \langle \psi^a_i | \overline{H} | \psi \rangle, \quad 0 = \langle \psi^{ab}_{ij} | \overline{H} | \psi \rangle. \tag{4}$$

Here $|\psi^a_i\rangle = \hat{a}^\dagger_a \hat{a}_i |\phi\rangle$ and $|\psi^{ab}_{ij}\rangle = \hat{a}^\dagger_a \hat{a}^\dagger_b \hat{a}_j \hat{a}_i |\psi\rangle$ are 1p-1h and 2p-2h excitation of the reference state, respectively.

The nonlinear coupled-cluster equations (4) are solved iteratively, and the correlation energy of the ground state is computed from

$$\Delta E_{\rm CCSD} = \langle \psi | \overline{H} | \psi \rangle. \tag{5}$$

We employ a spherical formulation of coupled-cluster theory in which the cluster operator $\hat{T}$ is a scalar under rotations [22]. This formulation reduces considerably the number of unknowns and permits us to explore model spaces exceeding 20 major oscillator shells.

Let us briefly summarize the essential properties of the coupled-cluster method. First, the method fulfills Goldstone's linked cluster theorem and therefore yields size-extensive results; i.e., the error due to the truncation is linear in the mass number A. Size extensivity is an important issue when approximate solutions to all but the lightest nuclei are sought [33,41]. Second, the computational effort scales gently (i.e., polynomial) with the system size. The method has met benchmarks in light nuclei [42,43]. We neglect 3NFs since their application within the coupled-cluster method is presently limited to smaller model spaces [44].

For a more precise computation of the correlation energy, we consider corrections due to triples excitations $\hat{T}_3$ within the ΛCCSD(T) approximation. For this purpose, we solve the left eigenvalue problem

$$\langle \psi | \hat{\Lambda} \overline{H} = E \langle \psi | \hat{\Lambda} \tag{6}$$

of the similarity-transformed Hamiltonian $\overline{H}$. Here, $\hat{\Lambda}$ denotes the deexcitation cluster operator

$$\hat{\Lambda} = 1 + \hat{\Lambda}_1 + \hat{\Lambda}_2, \tag{7}$$

and

$$\hat{\Lambda}_1 = \sum_{i,a} \lambda^i_a \hat{a}_a \hat{a}^\dagger_i, \quad \hat{\Lambda}_2 = \frac{1}{4} \sum_{i,j,a,b} \lambda^{ij}_{ab} \hat{a}_b \hat{a}_a \hat{a}^\dagger_i \hat{a}^\dagger_j. \tag{8}$$

The unknowns λ^i_a and λ^{ij}_{ab} result from the ground-state solution of the left eigenvalue problem (6). They are utilized together with the cluster amplitudes t^a_i and t^{ab}_{ij} to compute the energy correction due to triples clusters as

$$\Delta E_3 = \frac{1}{(3!)^2} \sum_{ijkabc} \langle \psi | \hat{\Lambda} (\hat{F}_{hp} + \hat{V})_N \left| \psi^{abc}_{ijk} \right\rangle \times \frac{1}{\varepsilon^{abc}_{ijk}} \left\langle \psi^{abc}_{ijk} \right| (\hat{V}_N \hat{T}_2)_C | \psi \rangle. \tag{9}$$

Here, $\hat{F}_{hp}$ denotes the part of the normal-ordered one-body Hamiltonian that annihilates particles and creates holes, while $\varepsilon^{abc}_{ijk} \equiv f_{ii} + f_{jj} + f_{kk} - f_{aa} - f_{bb} - f_{cc}$ is expressed in terms of the diagonal matrix elements of the normal-ordered one-body Hamiltonian $\hat{F}$. The subscript C denotes the

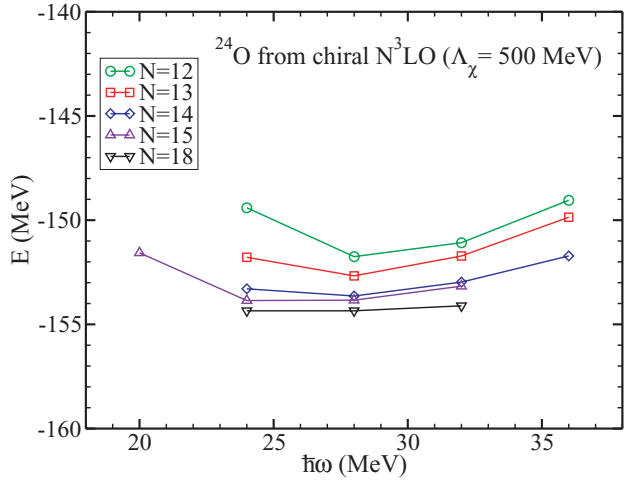

FIG. 1. (Color online) Binding energy [within ΛCCSD(T)] for ^{24}O from a chiral NN potential at order N^{3}LO with high-momentum cutoffs $\Lambda_\chi = 500$ MeV as a function of the oscillator spacing $\hbar\omega$ and the size of the model space.

connected part of the operator, and $|\psi_{ijk}^{abc}\rangle$ is a 3p-3h excitation of the reference state.

Results. We considered the nuclei ^{16,22,24,28}O and computed their ground-state energies within the ΛCCSD(T) approximation for chiral interactions with cutoffs of $\Lambda_\chi = 500$ and $\Lambda_\chi = 600$ MeV. Figures 1 and 2 show the results as a function of the oscillator spacing $\hbar\omega$ of the single-particle basis and parametrized by the number of major oscillator shells $N + 1$ for ^{24}O, and ^{28}O with two chiral cutoffs Λ_χ, respectively. Note that the results are reasonably well converged with respect to the size of the model space. Note also that the "harder" interaction with cutoff $\Lambda_\chi = 600$ MeV requires a larger model space to reach an acceptable convergence. The results for ^{16}O and ^{22}O are of similar quality. Very recently, Hagen, Papenbrock, and Dean demonstrated that the coupled-cluster wave function is approximately a product

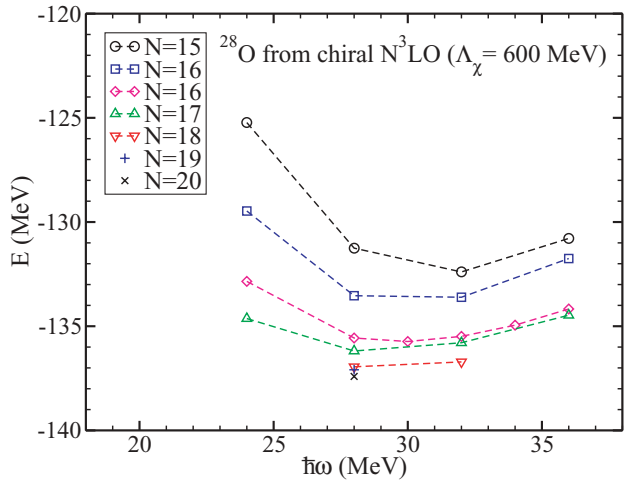

FIG. 2. (Color online) Same as Fig. 1, except for ^{28}O and a chiral cutoff $\Lambda_\chi = 600$ MeV.

TABLE I. Contributions to the binding energy E (in MeV) in neutron-rich oxygen isotopes from chiral interactions with high-momentum cutoff Λ_χ. The contributions E_0, $\Delta E_{\rm CCSD}$, and ΔE_3 denote the Hartree-Fock energy, the correlation energy within the CCSD approximation, and the energy due to the employed triples correction, respectively. For ^{16}O and $\Lambda_\chi = 500$ MeV, the results were taken in 19 major oscillator shells and at the energy minimum $\hbar\omega = 40$ MeV. For all other cases, the results were obtained in the largest model spaces at fixed $\hbar\omega = 28$ MeV.

Energies	^{16}O	^{22}O	^{24}O	^{28}O
($\Lambda_\chi = 500$ MeV)				
E_0	25.946	46.52	50.74	63.85
$\Delta E_{\rm CCSD}$	−133.53	−171.31	−185.17	−200.63
ΔE_3	−13.31	−19.61	−19.91	−20.23
E	−120.89	−144.40	−154.34	−157.01
($\Lambda_\chi = 600$ MeV)				
E_0	22.08	46.33	52.94	68.57
$\Delta E_{\rm CCSD}$	−119.04	−156.51	−168.49	−182.42
ΔE_3	−14.95	−20.71	−22.49	−22.86
E	−111.91	−130.89	−138.04	−136.71
Experiment	−127.62	−162.03	−168.38	

of a translationally invariant wave function and a Gaussian for the center-of-mass coordinate [45]. Thus, we do not worry about spurious contributions to the coupled-cluster wave function.

Let us estimate the precision of our results. There are three sources of systematic errors, namely, the truncation level of the coupled-cluster method, the finite size of the model space, and the error due to omitted contributions in the interaction. First, within the ΛCCSD(T) approximation, 3p-3h clusters are treated approximately, and all excitation clusters of higher rank are neglected. Table I shows the different contributions to the binding energy of neutron-rich oxygen isotopes. Comparison of the CCSD correlation energy and the energy due to triples corrections shows that the latter account for 10% (13%) of the former at a cutoff $\Lambda_\chi = 500$ (600) MeV. These ratios are found in similar coupled-cluster calculations of atoms and molecules, and experience in quantum chemistry (see, for example, Ref. [33]) suggests that the truncation of the cluster amplitudes beyond the triples corrections introduces an error of a few percent corresponding to an uncertainty of approximately 5 MeV. Second, we cannot treat an infinite model space, and (as shown in Figs. 1 and 2) the convergence with respect to an increased size of the model space is at the level of a couple of MeV. Thus, the convergence with respect to the size of the model space introduces an error that does not exceed error estimates due to the truncation of the cluster amplitudes. Third, by far the largest uncertainty is due to omissions in the nuclear interaction, as can be seen from a comparison of the results obtained with two different cutoffs. This uncertainty is of the order of 10–20 MeV, and increases with increasing mass number. Note that the deviation from the experimental results is consistent with our error estimates. Overall, we are missing binding energy compared to experiment. Thus, the net effect of the 3NF is expected to be

TABLE II. Root-mean-square point matter radii (in fm) for neutron-rich oxygen isotopes from the chiral interaction with high-momentum cutoff $\Lambda_\chi = 500$ MeV. Oscillator frequencies as in Table I. Experimental data from Ref. [46].

	^{16}O	^{22}O	^{24}O	^{28}O
$\langle r^2\rangle^{1/2}$	2.296	2.405	2.658	2.825
Expt.	2.54(2)	2.88(6)	3.19(13)	

attractive for both cutoffs. Table II gives the rms point matter radii using the chiral interaction with the high-momentum cutoff $\Lambda_\chi = 500$ MeV.

Radii were calculated using the Helmann-Feynman theorem within the ΛCCSD(T) approximation in 19 major oscillator shells. We compare them with the effective point matter radii extracted from interaction cross sections using the Glauber model in the optical limit approximation [46]. Our calculated matter radii are smaller than those extracted from experiment. In our calculated radii, we estimate an uncertainty at the order of ∼0.1 fm from the model-space dependence. The combination of too small radii and underbinding suggests that 3NFs should play a nontrivial role in the structure of these nuclei.

Let us also check whether our error estimates are consistent with the power-counting estimates from chiral EFT. Nogga confirmed that these estimates hold in light nuclei [47]. The omitted 3NFs are of the order $\langle\hat{V}\rangle(Q/\Lambda_\chi)^3$, where Q is the typical momentum scale and $\langle\hat{V}\rangle$ is the expectation value of the two-body interaction. For nuclei in this mass region and a cutoff $\Lambda_\chi = 500$ MeV, we have $Q \approx 200$ MeV and $\langle\hat{V}\rangle \approx 33 \pm 3$ MeV/nucleon (taken from the expectation values of the kinetic and potential energies in Ref. [22], respectively). This puts power-counting estimates from chiral EFT at about 2 MeV/nucleon, and our results are well within this estimate. While the absolute uncertainty on the binding energy is thus considerable, the differences in the binding energies of the considered isotopes (at fixed chiral cutoff Λ_χ) are much closer to the experimental results.

Let us focus on the binding energy of ^{28}O with respect to ^{24}O. While it would certainly be interesting to include ^{26}O in this comparison, we cannot address this nucleus within the spherical coupled-cluster method because of its open-shell character. Recall, however, the experimental evidence [3,4] against the stability of ^{26}O. This makes the comparison of ^{28}O and the last known stable isotope ^{24}O particularly interesting. Figure 3 shows that the ground-state energies relative to ^{22}O change little as one goes from ^{24}O to ^{28}O. This is a remarkable result of our *ab initio* calculations. In shell-model calculations with an ^{16}O core, the ground-state energies typically increase strongly (in absolute value) as more neutrons are added, and an adjustment of the interaction is necessary [12]. We study this phenomenon further by employing a similarity renormalization group (SRG) transformation [48] of the Hamiltonian with cutoff $\Lambda_\chi = 500$ MeV. As we lower the smooth SRG momentum cutoff from 4.1 to 3.5 fm^{-1}, we find

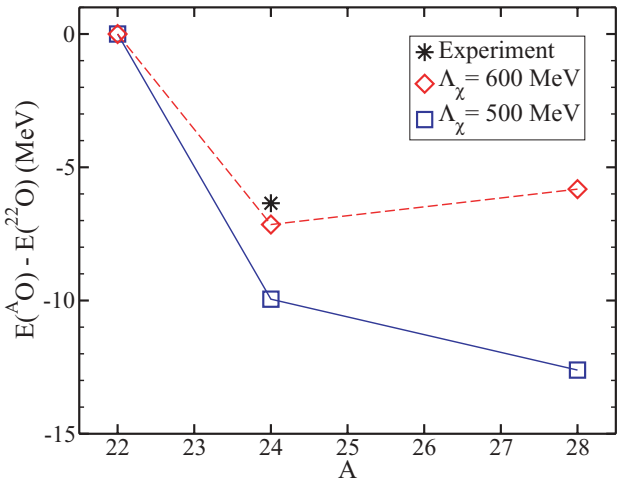

FIG. 3. (Color online) Ground-state energies of neutron-rich oxygen isotopes ^{A}O relative to ^{22}O for chiral interactions with two different cutoffs Λ_χ.

that the ground-state energy of ^{28}O decreases farther relative to ^{24}O. Thus, a softening of the nucleon-nucleon interaction has to be compensated for by 3NFs that yield less attraction (or even repulsion) in ^{28}O than in ^{24}O. There is no cutoff in this range that simultaneously would reproduce the experimental binding of ^{22}O and ^{24}O. Note also that the expected contributions of 3NFs become repulsive for very low cutoffs to compensate for the overbinding of the soft nucleon-nucleon interactions.

At a cutoff $\Lambda_\chi = 500$ MeV, we find that ^{28}O is bound by about 2.7 MeV with respect to ^{24}O. However, the situation is reversed at the higher cutoff $\Lambda_\chi = 600$ MeV, and the difference is about -1.3 MeV. Given the uncertainties of our calculation as discussed in the preceding paragraph, it is presently not possible to reach a conclusion regarding the existence of ^{28}O. However, the preceding discussion also makes it clear that—within interactions from chiral EFT—the stability of ^{28}O depends mainly on the contributions of the three-nucleon force, and that even small contributions can tip the balance in either direction. This is the main result of this paper. Our *ab initio* calculations also suggest that the recent results from phenomenological shell-model approaches regarding the unbound character of ^{28}O might be viewed with caution. The combination of 3NFs, the proximity of the continuum, and the isospin dependence pose a challenge for reliable theoretical predictions.

In summary, we performed *ab initio* calculations for neutron-rich oxygen isotopes employing chiral nucleon-nucleon interactions at order N^{3}LO. We probed the effects of missing physics (such as three-nucleon forces) by studying the cutoff dependence of our results, and we estimated the uncertainties due to the finite size of the model space and the truncation of the cluster operator. Our results show that the absolute binding energies have considerable uncertainties. However, the differences in binding energies are much closer to experiment. We find a small difference in the binding energies of ^{24}O and ^{28}O. Thus, our results cannot rule out a stable ^{28}O

with respect to ^{24}O. The cutoff dependence of the results shows that three-nucleon forces are the dominant contributions that tip the balance.

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