

Gamow shell-model calculations of drip-line oxygen isotopes

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We employ the Gamow shell model (GSM) to describe low-lying states of the oxygen isotopes ^{24}O and ^{25}O . The many-body Schrödinger equation is solved starting from a two-body Hamiltonian defined by a renormalized low-momentum nucleon-nucleon (NN) interaction and a spherical Berggren basis. The Berggren basis treats bound, resonant, and continuum states on an equal footing and is therefore an appropriate representation of loosely bound and unbound nuclear states near threshold. We show that the inclusion of continuum effects has a significant effect on the low-lying 1^+ and 2^+ excited states in ^{24}O . On the other hand, we find that a correct description of binding energy systematics of the ground states is driven by the proper treatment and inclusion of many-body correlation effects. This is supported by the fact that we get ^{25}O unstable with respect to ^{24}O in both oscillator and Berggren representations starting from a ^{22}O core. Furthermore, we show that the structure of these loosely bound or unbound isotopes is strongly influenced by the 1S_0 component of the NN interaction. This has important consequences for our understanding of nuclear stability.

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Introduction. The study of nuclei far from stability is a leading direction in nuclear physics, experimentally and theoretically. It represents a considerable intellectual challenge to our understanding of the stability of matter itself, with potential implications for the synthesis of elements. An important aspect of this research direction is to understand how magic numbers and shells appear and evolve with increasing numbers of neutrons or protons. Except for a qualitative understanding of the neutron and proton dependence of the magic numbers in terms of mean-field models, we lack a quantitative theoretical understanding in terms of the basic constituents of the underlying nuclear many-body Hamiltonian.

For mesoscopic systems like nuclei, the interpretation of the standard magic numbers 2, 8, 20, 28, 50, 82, and 126 is linked to the interplay between the filling up of single-particle (s.p.) orbitals (s.p. picture) and the underlying interactions. Magic numbers lead to so-called shell gaps in the s.p. spectra near the Fermi energy. For various magic numbers, in particular for stable doubly magic nuclei, one can have a large number of stable isotopes (increasing number of neutrons N but fixed number of protons Z) or isotones (increasing number of protons Z and fixed N). Eventually, as one adds more neutrons or protons, *viz.*, moving away from the valley of nuclear stability toward the drip lines, the outermost nucleons literally start to drip off the nuclei, thereby defining the very limits of stable matter.

Nuclei near the drip line are open-quantum many-body systems for which the coupling with the scattering continuum plays an important role and should therefore be explicitly taken into account. Configuration interaction (shell-model) methods, such as the Gamow shell model (GSM) (see Ref. [1] for a recent review of the GSM), the continuum shell model (CSM) [2], or a time-dependent CSM approach [3], have been developed in order to properly include the coupling with the scattering continuum. The inclusion of continuum states complicates the solution of the many-body problem

considerably, as the number of many-body basis states will explode. This has therefore motivated different approaches to the description of loosely bound and unbound nuclear states, such as the density-matrix-renormalization-group (DMRG) [4] and coupled-cluster approaches [5]. Furthermore, complicating the solution strategies of the nuclear many-body problem is the need to include three-nucleon forces (3NFs). Recent results for light nuclei using *ab initio* methods such as the Green's function Monte Carlo (GFMC) [6] and the no-core shell model (NCSM) [7], demonstrate that 3NFs are needed in order to give the correct binding energies and spectroscopy when comparing to experiment. It is still an open research problem as to what the role of 3NFs is in medium-mass and neutron-rich nuclei close to the drip line. This applies also to our understanding of how different parts of the underlying nucleon-nucleon (NN) interaction, such as the spin-orbit force [8,9] and the tensor force [10,11], affect the structure of nuclei close to the drip line.

In this work, we study the ground- and low-lying states of ^{24}O and ^{25}O within the GSM framework. We derive for the first time a realistic effective shell-model interaction that includes the effect of the scattering continuum. The effective interaction is derived using many-body perturbation theory (MBPT) starting with a Hamiltonian that reproduces NN scattering data. The choice of the oxygen isotopes is motivated by several reasons. First, the oxygen isotopes are the heaviest isotopes for which the drip line is well established. There are large experimental campaigns worldwide [12–15] that aim at uncovering the properties of the oxygen isotopes, both at or close to the drip line and beyond. Two out of four stable even-even isotopes exhibit a doubly magic nature, namely, ^{22}O ($Z = 8$, $N = 14$) [16] and ^{24}O ($Z = 8$, $N = 16$) [17,18]. The isotopes $^{25-28}\text{O}$ are all believed to be unstable toward neutron emission, even though ^{28}O is a doubly magic nucleus within the standard shell-model picture. Second, many-body descriptions starting with effective two-body Hamiltonians

defined for a model space comprising the $1s_{1/2}$, $0d_{5/2}$, and $0d_{3/2}$ s.p. orbitals have always defied a proper reproduction of experimental data [19–21]. To remedy this, the two-body shell-model interaction is usually fitted (fully or partially) [2,19,20] to reproduce experimental data for nuclei in the range $16 < A < 40$. Without fitting the two-body Hamiltonians, which are typically derived using MBPT, shell-model calculations of the oxygen isotopes fare reasonably up to ^{20}O , but they yield too compressed spectra in ^{22}O and lead to neutron separation energies that are always positive up to ^{28}O . All isotopes $^{17-28}\text{O}$ that can be reached via this model space result as well bound, in clear contradiction with experiment. Within the above model space, these results pertain to all effective interactions defined via existing two-body NN interactions [19,21]. The ground states and excited states of the odd-even isotopes are also poorly reproduced (see, for example, Refs. [19,20]).

Recent *ab initio* coupled-cluster calculations of the oxygen isotopes [22] showed that chiral NN interactions can produce a rather flat binding energy curve of the oxygen isotopes ranging from ^{24}O to ^{28}O . It was illustrated that the existence of ^{28}O cannot be ruled out from *ab initio* theory starting from modern chiral interactions. It was concluded that 3NFs will eventually decide the matter. Recent shell-model calculations of the oxygen isotopes within the s - d shell showed that inclusion of effective 3NFs gives added repulsion in the heavier oxygen isotopes and results in an unstable ^{28}O [23].

Obviously, the understanding of the evolution of binding energies and the location of the drip line in the oxygen isotopes are still unsolved theoretical problems. As shown in Refs. [22,23], proper treatment of many-body effects are crucial in the oxygen isotopes. However, it is still an open issue as to which role the continuum plays in the evolution of shell structure and in a correct description of binding energy systematics in neutron-rich oxygen isotopes. As discussed in Ref. [24], a proper treatment of the continuum was necessary to explain the parity inversion of the ^{11}Be ground state. It is therefore important to investigate what the role of the continuum is on ground and excited states in neutron-rich oxygen isotopes. It is the aim of this article to throw light on and disentangle the effects coming from many-body correlations and the proximity of the continuum on the evolution of binding energies and shell structure in neutron-rich oxygen isotopes. Further, we will investigate how different components of the NN interaction influence the low-lying resonance states in drip-line oxygen isotopes.

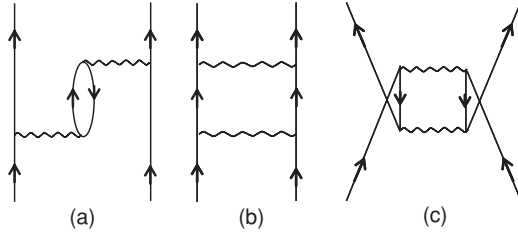
Method, interaction, and model space. In this work we use the GSM to describe the low-lying states in ^{24}O and the ground state of ^{25}O . We construct the effective shell-model interaction starting from ^{22}O as a closed-shell core and use MBPT through second order [21]. The isotope ^{22}O has been found to be a closed-shell nucleus with a considerable shell gap, making it suitable as a starting point for shell-model calculations. With ^{22}O as a closed-shell core, we have at most three valence particles, making effects coming from a proper treatment of the continuum more transparent. So far, the effective interaction has typically been constructed using oscillator states as intermediate particle states. In this work, we investigate for the first time the role of the continuum in

constructing a realistic effective shell-model interaction and in describing the spectra of neutron-rich oxygen isotopes.

The major advantage of the GSM is that it unifies structure and reaction properties of nuclei, that is, bound and scattering degrees of freedom are treated equally. Nuclei close to the scattering threshold have low-lying states that are in the continuum, and the GSM provides a simple framework for calculating the energy and lifetimes of these states. The starting point of the GSM is the Berggren completeness relation [25]. This s.p. basis treats bound, resonant, and scattering states on an equal footing, and it is the basic idea of the GSM to expand the many-body wave function in Slater determinants built from this basis. The representation of the Hamiltonian will no longer be Hermitian but rather complex symmetric, and a diagonalization will yield bound-state spectra in addition to resonant-state spectra. Hence, the energy and lifetime of the many-body resonant state comes out directly from the approach.

In constructing the s.p. Berggren basis, we start from the one-body Hamiltonian for a spherical Woods-Saxon (WS) potential (see, for example, Ref. [26]). The Berggren basis is obtained by diagonalizing the one-body Hamiltonian in a plane wave basis defined on a deformed contour L^+ in the complex momentum plane (see Ref. [27] for details). This method is also known as the contour-deformation method. There is freedom in choosing the contour L^+ provided the Schrödinger equation can be analytically continued in the complex momentum plane. Fully converged results should be independent of the choice of the contour, and in the following we used two different contours, L_1^+ and L_2^+ , as given in Ref. [27], to check that our results are converged. The parameters of the WS potential are given by $V_0 = 55$ MeV, $V_{so} = 29$ MeV, $R = 3.1$ fm, and $d = 0.45$ fm, where the shorthand V_{so} stands for the spin-orbit term. These parameters are chosen such that the energies of the s.p. orbitals $\nu 0d_{5/2}$, $\nu 1s_{1/2}$, and $\nu 0d_{3/2}$ are close to the experimental values obtained by taking the binding energy differences of ^{21}O - ^{22}O and ^{23}O - ^{22}O . We obtain, in units of MeV, $\epsilon_{\nu 0d_{5/2}} = -6.53(-6.85)$, $\epsilon_{\nu 1s_{1/2}} = -2.73(-2.74)$, and $\epsilon_{\nu d_{3/2}} = 1.43 - 0.01i$ ($1.26 - 0.2i$), where the numbers in parenthesis are experimental values. We refer hereafter to this basis as a WS Gamow basis. In our shell-model study of the oxygen isotopes ^{24}O and ^{25}O , we will use the WS Gamow basis for the neutron partial waves $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$, while for protons and all other partial waves, we use the oscillator representation.

In constructing the effective shell-model interaction for neutron-rich oxygen isotopes, we start from the intrinsic nuclear Hamiltonian $H = t - t_{c.m.} + V$, where t denotes the kinetic energy, and $t_{c.m.}$ is the kinetic energy of the center of mass. For the interaction V , we employ the NN interaction by Entem and Machleidt [28,29] derived from chiral effective field theory (EFT) at next-to-next-to-next-to-leading order ($N^3\text{LO}$) and with a 500 MeV cutoff. This interaction still has considerable high-momentum components, making MBPT nonconvergent. To construct the effective shell-model interaction V_{eff} using MBPT, we use a low-momentum interaction $V = V_{\text{low-}k}$, obtained by integrating out those momentum components above a certain cutoff Λ [30]. Thereafter we generate V in the WS Gamow basis using the procedure

FIG. 1. Second-order contributions to V_{eff} .

outlined in Ref. [27]. It is well known that this renormalization induces forces of higher rank. In a completely renormalized theory, all observables are independent on the cutoff Λ , and therefore the dependence of our results on the cutoff Λ tells us about the missing many-body physics. In this work, we start from a ^{22}O core and limit ourselves to two-body effective shell-model interactions only. Since we have at most three neutrons outside the closed-shell core, it is reasonable to expect that the effect coming from effective three-body forces is small.

To proceed with the construction of the effective shell-model interaction, we need to define a model space for the valence neutrons. Since we will perform our GSM calculations starting with ^{22}O as a closed-shell core, i.e., the $0d_{5/2}$ shell is filled, our many-body states are constructed by letting all valence neutrons act in the model space defined by the s.p. orbitals $1s_{1/2}$ and $id_{3/2}$, where $i = 0, 1, \dots$ denotes the i th discretized continuum state for the $d_{3/2}$ partial wave. The effect of the continuum from the $s_{1/2}$ and $d_{5/2}$ partial waves is taken into account through the construction of the effective interaction. The effective shell-model interaction V_{eff} is then constructed for this model space using MBPT [21],

$$H_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \dots$$

Here $\hat{Q}(\omega)$ is given by diagrams which are valence-linked and irreducible. The argument ω is the starting energy, which is the sum of the unperturbed s.p. energies. The object $\hat{Q}(\omega)$ is defined as

$$\hat{Q}(\omega) = PH_1P + PH_1Q \frac{1}{\omega - QHQ} QH_1P.$$

In this work we take into account diagrams up through second order in perturbation theory in order to construct $\hat{Q}(\omega)$. We list in Fig. 1 the diagrams that contribute up to second order in the effective interaction. The intermediate s.p. states in each diagram can be either resonant states, nonresonant continuum states, or bound states. In our calculations, we neglect the contributions from folded diagrams; see Ref. [21] for further details.

Results. We now turn to the GSM calculations of low-lying states in ^{24}O and ^{25}O . For the case of ^{24}O , we have two neutrons outside the ^{22}O core, and we express the ground state of ^{24}O by filling the $1s_{1/2}$ orbital. This orbital is well bound and with a neutron separation energy of $S_n = 2.7\text{ MeV}$ for ^{23}O [31]. We therefore expect mixing of higher lying states to be small in the ground state of ^{24}O , and we take this effect into account through the construction of the effective interaction using many-body perturbation theory. For the excited states $J = 1$ and $J = 2$ of ^{24}O , we expand the wave function in a set

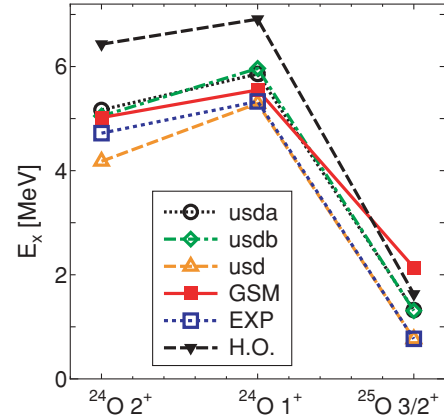


FIG. 2. (Color online) Excitation energies of the $J^\pi = 1^+$ and $J^\pi = 2^+$ states in ^{24}O and the ground-state energy of ^{25}O measured from the ground states in ^{24}O .

of basis states $|iJ^+\rangle = |1s_{1/2} \otimes id_{3/2}; J^+\rangle$. The orbital $id_{3/2}$ denotes the i th discretized s.p. state of the WS Gamow basis, and $i = 1, \dots, n_{\text{Gamow}}$, where n_{Gamow} is typically between 20 and 35. In our calculations, we used $n_{\text{Gamow}} = 30$, and we checked that this was sufficient to reach convergence.

We show in Fig. 2 the excitation energies of the low-lying states in ^{24}O and the ground state in ^{25}O with respect to the ground state of ^{24}O . We used a cutoff $\Lambda = 2.1\text{ fm}^{-1}$ for the $V_{\text{low-}k}$ interaction. We varied the cutoff Λ around 2.1 fm^{-1} and found that our results are nearly independent of the cutoff Λ , meaning that the effect of neglected three- and many-body forces are small and will not change our conclusions. Our GSM calculations give energies for the low-lying states that compare well with the experimental values. The splitting between the 1^+ and the 2^+ states of ^{24}O is close to experiment. The theoretical spacing obtained with our GSM approach is 540 keV, while the corresponding experimental value is 600 keV. Our calculated widths for the 1^+ and 2^+ resonant states are 0.44 and 0.26 MeV, respectively. In Ref. [14], Hoffman *et al.* reported that the widths are $0.03^{+0.12}_{-0.03}\text{ MeV}$ for the 1^+ state and $0.05^{+0.21}_{-0.05}\text{ MeV}$ for the 2^+ state. Our calculations overestimate the width of the 1^+ state compared to experiment. On the other hand, our calculated width of the 2^+ state is within the experimental uncertainties. For the sake of comparison, we show results obtained with other effective interactions. The new universal *sd* Hamiltonians (USDA and USDB), obtained by revising the USD interaction in order to be more suitable for exotic nuclei [20], result in good agreement with experimental data. However, one should note that some effects coming from the continuum and 3NFs are implicitly included in the new USD two-body matrix elements due to the fit made to experimental data. Although the USD interaction reproduces nicely two of the three experimental data points, the 2^+ state in ^{24}O comes out as a bound excited state, a fact that disagrees with recent experiments. We also show results obtained with a pure harmonic oscillator basis. In this case, the discretized continuum is not included in the model space, and we construct the effective interaction using perturbation theory through second order (see Fig. 1) and a model space consisting of neutrons in the orbitals $(1s_{1/2}, 0d_{3/2})$. Using a model space

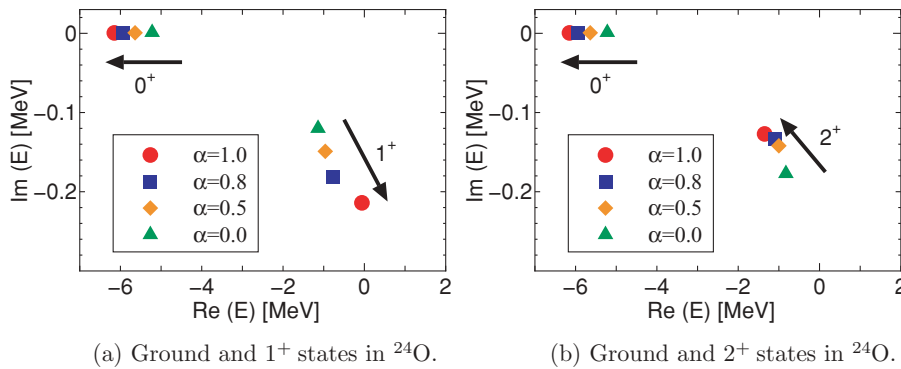


FIG. 3. (Color online) Energies of low-lying resonance states in ^{24}O , as a function of the strength α of the 1S_0 partial wave component of the nucleon-nucleon interaction. See text for further details.

consisting of only bound oscillator orbitals puts the 1^+ and 2^+ states in ^{24}O too high in energy when compared to experiment. With the inclusion of the continuum in the model space, the 1^+ and 2^+ states get lower in energy and also closer to experiment. This clearly shows an effect coming from a proper treatment of the continuum and should therefore be included in a realistic description of low-lying states in ^{24}O . In a recent work by Volya [3], it was also found that the inclusion of the continuum significantly improves the description of these states using the standard USD interaction. Further, the 2^+ state in ^{24}O is a resonant state and cannot be properly described in an oscillator basis.

Turning to the case of the ground state of ^{25}O , our GSM calculations correctly predict that it is particle unstable but put it at a higher energy ($E = 2.1$, $\Gamma = 0.5$ MeV) compared with recent experimental data ($E = 0.77$, $\Gamma = 0.17$ MeV). To get a better description of this state, configurations such as $\nu(1s_{1/2})(id_{3/2})^2$ should be included, since the GSM is currently solved in a filling configuration. We compare again our GSM result for ^{25}O with a shell-model calculation where only the bound oscillator orbitals $(1s_{1/2}, 0d_{3/2})$ define the model space. An important point to note is that ^{25}O comes out higher in energy than ^{24}O , reflecting that it is unstable toward neutron emission. Even though the oscillator basis cannot provide us with a width or a lifetime for the ground state of ^{25}O , it predicts ^{25}O as particle unstable and illustrates that the continuum coupling is not a dominant mechanism in explaining the position of the drip line of the oxygen isotopes. Thus, irrespective of whether we use a complex Gamow s.p. basis that defines a model space consisting of the $(1s_{1/2}, id_{3/2})$ states (with $i = 0, \dots, n_{\text{Gamow}}$), or a harmonic oscillator basis with the $(1s_{1/2}, 0d_{3/2})$ states only, ^{25}O is unstable against particle emission as long as we use ^{22}O as a closed-shell core. This has important consequences for our theoretical understanding of the stability of matter. As pointed out in a recent calculation by Hagen *et al.* [22], many-body forces such as three-body interactions are crucial to explaining the correct position of the drip lines. The fact that a calculation of ^{25}O with ^{22}O as a closed-shell core gives the correct qualitative description of the ground state of ^{25}O , hints at the fact that with three valence neutrons only, missing many-body physics does not play a central role. This should be contrasted to realistic calculations that utilize ^{16}O as a closed core. With nine valence neutrons, ^{25}O is strongly overbound using the standard model space comprising the oscillator orbitals $(1s_{1/2}, 0d_{5/2}, 0d_{3/2})$ and a two-body effective interaction derived using MBPT.

However, the location of the excited states in ^{24}O and the width of the ground state of ^{25}O depend crucially on the choice of basis, and we have shown that a GSM basis is needed to explain these states.

We conclude this work with an investigation of which parts of the NN interaction may play an important role in our understanding of the above excited states in ^{24}O . To achieve this, we single out the 1S_0 partial wave component of the NN interaction and vary its strength. This partial wave is particularly important to our understanding of pairing correlations in nuclei. To investigate the importance of this partial wave on the low-lying resonance states in ^{24}O , we vary the strength as $\tilde{V}(\alpha) = \alpha \times \langle S = 0, L = 0; J = 0 | V | S = 0, L = 0; J = 0 \rangle$, $\alpha \in [0, 1]$ in a bare NN potential. Clearly, $\alpha = 0$ corresponds to a NN interaction with no contribution from this partial wave, while $\alpha = 1$ corresponds to the original interaction. The low-lying resonance states are calculated for each $\tilde{V}(\alpha)$, and the results are shown in Fig. 3. One can clearly see how the 1S_0 partial wave in the NN interaction influences the many-body resonances in ^{24}O . The ground state gains additional binding when α increases, since the ground state can be well described by the $\nu(1s_{1/2})^2$ configuration. At $\alpha = 0$, the position of 1^+ and 2^+ are interchanged with respect to experiment, and they are degenerate if one analyzes the real part of the resonance energies. When α increases to the full interaction strength, the $1^+ - 2^+$ splitting increases to 530 keV, a result close to experiment. The 1S_0 partial wave, a central contribution to pairing in nuclei, is thus crucial to explaining correctly the low-lying resonant states in ^{24}O .

Conclusions. We have described the low-lying states in the oxygen isotopes ^{24}O and ^{25}O within the framework of the GSM and effective interactions derived through many-body perturbation theory. We have shown that there is a fine interplay between many-body effects and the proximity of the continuum, and we demonstrated that the inclusion of the continuum has significant effect on the excited states of ^{24}O . To predict the location of the drip line, we found that a proper inclusion of many-body forces and correlation effects are the deciding factors. Furthermore, the 1S_0 partial wave component of the NN interaction, an important contribution to strong pairing correlations in nuclei, plays an important role in explaining the correct value of these states. We conclude that the location of the drip line and excited states in the oxygen isotopes can only be determined by proper inclusion of both many-body correlations and the coupling with continuum degrees of freedom.

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