**Ab-initio computation of the $^{17}\text{F}$ proton-halo state and resonances in $A = 17$ nuclei**

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We perform coupled-cluster calculations of the energies and lifetimes of single-particle states around the doubly magic nucleus $^{16}\text{O}$ based on chiral nucleon-nucleon interactions at next-to-next-to-leading order. To incorporate effects from the scattering continuum, we solve the coupled-cluster equations with a Gamow-Hartree-Fock basis. Our calculations for the $J^\pi = 1/2^+$ proton-halo state in $^{17}\text{F}$ and the $1/2^+$ state in $^{17}\text{O}$ agree well with experiment, while the calculated spin-orbit splitting between $d_{5/2}$ and $d_{3/2}$ states is too small due to the lack of three-nucleon forces. We find that continuum effects yield a significant amount of additional binding energy for the $1/2^+$ and $3/2^+$ states in $^{17}\text{O}$ and $^{17}\text{F}$.

**Introduction.** Halo nuclei [1], i.e. very fragile nuclear systems with a halo consisting of one or more weakly bound nucleons, are fascinating objects. Atomic nuclei with halo ground states exist at the fringes of nuclear existence close to the drip lines. Well-known examples are the two-neutron halo nuclei $^6\text{He}$ and $^{11}\text{Li}$, the proton-halo nucleus $^8\text{B}$, and the two-proton halo nucleus $^{17}\text{Ne}$; see Ref. [2] for a recent review. Halo states can also exist as excited states of nuclei with well-bound ground states. Halo nuclei are difficult to study experimentally due to their feeble nature and the often small production cross sections. They also provide theory with a formidable challenge since the proximity of the continuum introduces a very large number of degrees of freedom. In recent years, several theoretical approaches have been implemented and developed that include continuum effects and enable theorists to describe weakly bound states, nuclear halos, and unbound resonances [3,4,5,6,7,8].

The $A = 17$ neighbors around $^{16}\text{O}$ are particularly interesting and significant nuclei. First, the $3/2^+$ and $1/2^+$ states in $^{17}\text{F}$ are bound by only 600 keV and 105 keV, respectively, making the latter a proton-halo state. This state and astrophysically relevant reactions such as the $^{17}\text{F}(p,\gamma)^{18}\text{Ne}$ reaction [9] have been understood within the shell model embedded in the continuum [3], but an ab-initio description is not yet available. Second, the ground and excited states in $^{17}\text{F}$ and $^{17}\text{O}$ determine the single-particle energies of proton and neutron states with respect to the doubly magic nucleus $^{16}\text{O}$, respectively. These energies are basic ingredients of the nuclear shell model, and they are also key for the understanding of the evolution of shell structure in the fluorine and oxygen isotopes [10]. Recent theoretical efforts aim at ab-initio shell-model calculations with a core for sd-shell nuclei [11]. The ab-initio computation of single-particle energies in $^{17}\text{O}$ and $^{17}\text{F}$ is one necessary ingredient for such an approach. Finally, the ab-initio approach to the proton-halo state in $^{17}\text{F}$ and the $3/2^+$ resonances in $^{17}\text{O}$ and $^{17}\text{F}$ provides us with an ambitious testing ground for the employed method, the high-precision potentials, and the role of three-nucleon forces.

In this Letter, we present an ab-initio calculation of low-lying states of the mirror nuclei $^{17}\text{O}$ and $^{17}\text{F}$. The coupled-cluster method [12] is ideally suited for this endeavor, as it is a most efficient approximation for the computation of ground states of doubly magic nuclei, and the single-particle states in odd-mass neighbors can be computed within the equation-of-motion techniques [13]. For the inclusion of continuum effects, we employ the Berggren [14] single-particle basis of the Gamow shell model [4], i.e. the model space consists of bound-, resonant-, and continuum scattering states. Our calculations employ the chiral nucleon-nucleon interaction at next-to-next-to-next-to-leading order (N³LO) by Machleidt and Entem [15].

**Interaction and model space.** We employ the intrinsic nuclear Hamiltonian

\[
\hat{H} = \hat{T} - \hat{T}_{\text{cm}} + \hat{V} = \sum_{1\leq i < j \leq A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \hat{V}.
\]

Here, $T$ and $T_{\text{cm}}$ denote the kinetic energy and the kinetic energy of the center-of-mass coordinate, respectively, and $V$ denotes the chiral nucleon-nucleon interaction by Entem and Machleidt [15] at N³LO.

As some of the states we seek to compute are resonances or loosely bound halo states, we need to take into account continuum effects. For this purpose we use a Berggren representation [14] for the proton and neutron $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$ partial waves. The Berggren representation is a generalization of the usual completeness relation to the complex energy plane, so that bound-, resonant-, and non-resonant continuum states are treated on an equal footing. The Berggren ensemble has been successfully used within the Gamow shell model [4] (see Ref. [16] for a recent review), and in ab-initio coupled-cluster calculations of energies and lifetimes of the helium isotopes [17]. In constructing the single-particle Berggren basis, we follow the procedure outlined in Ref. [18]. We diagonalize a one-body Hamiltonian with a spherical
Woods-Saxon potential in a spherical-wave basis defined on a discretized contour $L^2$ in the complex momentum plane. We employ a total of 30 Gauss-Legendre mesh points along the contour for each of the $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$ partial waves. Our converged calculations are independent of the choice of contour, and we checked that 30 mesh points is sufficient to reach satisfactory converged results for the calculated energies and lifetimes of the states we consider in this work. For all other partial waves, the basis functions are those of the spherical harmonic oscillator.

**Method.** The computation of the ground and excited states in $^{17}$O and $^{17}$F is a three-step procedure within coupled-cluster theory. First, we employ the intrinsic Hamiltonian $H_0$ and compute the ground-state energy $E_0$ of $^{16}$O. This yields a precise reference value relative to which the single-particle energies will be determined. In the second step, we compute the ground-state energy $E_0^*$ and corresponding cluster amplitudes for a “mass-shifted” nucleus $^{16}$O, where the mass shift $m \rightarrow m' = m(A + 1)/A$ in the intrinsic Hamiltonian $H_0$ ensures that the correct kinetic energy of the center-of-mass is utilized in the third step. In the third step, we act with an effective one-particle creation operator (consisting of superpositions of one-particle and two-particle-one-hole operators) onto the mass-shifted ground state of $^{16}$O. This yields the energies $E_{\mu} = E_{0}^* + \omega_\mu$ of the states with spin and parity $\mu = 1/2^+, 3/2^+, 5/2^+$ in the $A = 17$ nucleus of interest. The difference between these energies and the ground-state energy of $^{16}$O are the single-particle energies $E_{sp}(\mu)$, i.e. $E_{sp}(\mu) = \omega_\mu + E_0^* - E_0$. We briefly describe the three steps in more detail.

In coupled-cluster theory [12, 13, 19], one computes the similarity-transformed Hamiltonian $H = e^{-T}He^{T}$ for the closed-shell nucleus $^{16}$O. Here, $T$ is a sum of particle-hole cluster operators $T = \sum_{k=1}^{A} T_k$. The $k$-particle $k$-hole $(kp-kh)$ cluster operator

$$T_k = \frac{1}{(k!)^2} \left[ a_{1}^{\dagger} \cdots a_{k}^{\dagger} \right] \cdots \left[ a_{i_{A-k}}^{\dagger} \cdots a_{i_{k}}^{\dagger} \right] \left[ a_{i_{A-k}} \cdots a_{i_{1}} \right].$$

(2)

is defined with respect to the Hartree-Fock reference state $|\phi_0\rangle$. Here, and in the following, we sum over repeated indices. The labels $i, j, k, \ldots$ (a, b, c . . .) denote occupied (unoccupied) single-particle orbitals. The operators $a_p$ ($a_p^\dagger$) annihilate (create) a fermion in orbital $p$. In practice, we truncate the cluster expansion by setting $T_a = 0$ for $a > 3$, and treat the triples cluster $T_3$ in the ACCSD(T) approximation [21]. The unknown cluster amplitudes $t_{ia}^{a}$ and $t_{ij}^{ab}$ are determined from the condition that the similarity-transformed Hamiltonian $\overline{H}$ has no 1p-1h excitations and no 2p-2h excitations, respectively, from its Hartree-Fock reference state. The ground-state energy is the expectation value of $\overline{H}$ in the Hartree-Fock reference, with small corrections due to the approximate inclusion of triples added. This approach is used for the computation of the ground-state energies $E_0$ and $E_0^*$ of $^{16}$O and the “mass-shifted” $^{16}$O, respectively. We employ the coupled-cluster method in an angular-momentum coupled scheme [22, 23]. This allows us to obtain well-converged results for “bare” interactions from chiral effective field theory (EFT) in large model spaces consisting of 15-20 oscillator shells.

We wish to study the low-lying states in $^{17}$O and $^{17}$F. These nuclei differ by an additional neutron or proton from the doubly magic $^{16}$O. Excited states (with dominant single-particle character) can be obtained from the ground state of the “mass-shifted” $^{16}$O by action of the excitation operator

$$R_\mu = r^a a^a_{\mu} + \frac{1}{2} t_{ij}^{ab} a^a_{\mu} a^b_\mu .$$

(3)

Here, it is understood that the annihilation and creation operators on the right-hand side of Eq. (3) are coupled to the spin and parity $\mu$ of the excited proton and neutron states that we seek to compute, respectively. This is the particle-attached equation-of-motion coupled-cluster method with singles- and doubles excitations (PA-EOM-CCSD), see e.g. Refs. [20, 24]. The unknowns $r^a$ and $t_{ij}^{ab}$ and the excitation energies $\omega_\mu$ relative to the ground-state energy of the mass-shifted $^{16}$O are obtained from solving the eigenvalue problem

$$[\overline{H}, R_\mu] |\phi_0\rangle = \omega_\mu R_\mu |\phi_0\rangle .$$

(4)

**Results.** We perform a Hartree-Fock (HF) calculation for $^{16}$O and obtain the reference state $|\phi_0\rangle$. In order to assess the role of coupling to the scattering continuum, we present results for the $A = 17$ system, starting from a Hartree-Fock basis derived from a Harmonic Oscillator basis (OHF) and a Woods-Saxon Berggren basis which is the Gamow-Hartree-Fock basis (GHF) [10]. For well-bound nuclei such as $^{16}$O, the coupling to continuum degrees of freedom is negligible. The ground-state energy of $^{16}$O differs by less than 1 keV in the OHF and GHF basis within both the CCSD and the ACCSD(T) approximation. We found well-converged results for the ground state of $^{16}$O in 15 major oscillator shells, and the energy varies by less than 0.5MeV for 26 MeV $\leq \hbar \omega \leq 36$ MeV. (See Refs. [22, 23] for convergence details.) At the energy minimum $\hbar \omega = 34$ MeV, the ground state energy of $^{16}$O is $-107.6$MeV in the CCSD, and $-120.9$MeV in the ACCSD(T) approximation.

Figure 4 shows our PA-EOMCCSD results for the $1/2^+, 3/2^+$, and $5/2^+$ single-particle energies $E_{sp}$ in $^{17}$F as a function of $\hbar \omega$. The data points connected by dashed and solid lines show the coupled-cluster results obtained in the OHF basis and the GHF basis, respectively. The horizontal lines show the experimental single-particle energies. The underlying model space includes 17 major oscillator shells, in addition to 30 Woods-Saxon Berggren states for each of the $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$ partial waves. The results obtained in the GHF basis exhibit a very
weak dependence on the oscillator frequency while this dependence is stronger for the OHF basis. In particular, the energies of the $d_{3/2}$ and $s_{1/2}$ in the OHF basis increase with increasing frequency of the model space. The $3/2^+$ states in $^{17}\text{O}$ and $^{17}\text{F}$ are well-known resonances, and an oscillator basis is clearly not appropriate to describe these states. For the $5/2^+$ states, we find a much weaker effect from the continuum. This is expected since the $l = 2$ centrifugal barrier localizes this state inside the barrier and reduces the coupling with the external scattering continuum.

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The coupling with the scattering continuum has a significant effect on the $1/2^+$ and $3/2^+$ states of $^{17}\text{F}$ and $^{17}\text{O}$. Our calculations using a GHF basis yields $\sim 1.0$ MeV in additional binding energy for these states compared to our calculations with the OHF basis. The effect is particularly strong in the case of the $1/2^+$ proton halo state in $^{17}\text{F}$, which is not even bound in the OHF basis. Similar continuum coupling effects were found for the $1/2^+$ halo state in $^{11}\text{Be}$ and in the low-lying states of the fluorine and oxygen isotopes [23]. The lack of a centrifugal barrier and the very weak binding yield a proton-halo (with a root-mean-square radius of $r_{\text{rms}} = 3.333\text{fm}$ [20]) that is difficult to capture in the oscillator basis. Our calculated binding energy for this state agrees remarkably well with the experimental value of 105 keV. This finding deserves further analysis, and we need to estimate the effects of the omitted three-nucleon forces.

Within chiral EFT, the leading three-nucleon forces consist of a long-range two-pion exchange, a midrange one-pion exchange, and the short-range three-nucleon contact interaction [27]. Three-nucleon forces are expected to yield additional binding of the order of 0.5 MeV per nucleon [23]. The effect of three-nucleon forces on energy differences is more subtle. Within a calculation based on two-nucleon forces we can, however, probe the effect of the three-body contact by a variation of the ultraviolet cutoff $\lambda$. Decreasing the cutoff employed in the construction of the chiral interactions renormalizes the two-nucleon interaction and generates short-ranged three nucleon forces [29]. We employ the similarity renormalization group (SRG) [30] for the generation of interactions with a cutoff $\lambda$, and study the evolution of the excited states in $^{17}\text{F}$ as the cutoff is varied. Figure 2 shows that the spin-orbit splitting between the $d_{3/2}$ and $d_{5/2}$ orbitals increases with decreasing cutoff. However, the $s_{1/2}$ state remains virtually unchanged as the cutoff is lowered to $\lambda \approx 3.2$ fm$^{-1}$. This is not unexpected since the structure of the dilute $1/2^+$ halo state is dominated by long-ranged forces, and the SRG interactions only change the short-range contributions. Thus, our result for the proton-halo state in $^{17}\text{F}$ is insensitive to short-range three-nucleon forces.

Let us also comment on the center-of-mass motion. Ref. [23] demonstrates that the intrinsic Hamiltonian yields a coupled-cluster wave function that factorizes to a very good approximation into an intrinsic part and a Gaussian for the center-of-mass motion. At the cutoff $\lambda = 2.8$ fm$^{-1}$ we checked that this is true for the low-lying states in the $A = 17$ nuclei in a wide range of oscillator frequencies.

![FIG. 1: (Color online) Low-lying single-particle states in $^{17}\text{F}$ relative to the $^{16}\text{O}$ ground-state energy as a function of oscillator frequency $\hbar \omega$. The data points connected by dashed and solid lines employ an oscillator basis (OHF) and a Berggren basis (GHF), respectively. The horizontal lines are experimental data.](image1)

![FIG. 2: (Color online) Single-particle energies of the $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$ states in $^{17}\text{F}$ (squares, circles, and diamonds, respectively) and the results for a “bare” N$^3$LO interaction (dotted, dashed, and dashed-dotted lines, respectively) as a function of the high-momentum cutoff $\lambda$.](image2)
of $^{16}$O. We also show the spin-orbit splitting between the $d_{5/2}$ and $d_{3/2}$ single-particle states.

|        | $^{17}$O      | $^{17}$F      |
|--------|--------------|--------------|
| 1/2$^+$ | 5/2$^+$ $E_{sp}$ | 1/2$^+$ 5/2$^+$ $E_{sp}$ |
| GHF    | -2.8        | -3.2        |
| Exp.   | -3.272      | -4.143      |

TABLE I: Single-particle energies of the 1/2$^+$ and 5/2$^+$ states, and the spin-orbit splitting $E_{so}(d_{5/2}-d_{3/2})$ (in units of MeV) in $^{17}$O and $^{17}$F calculated in a Berggren (Gamow) basis (GHF), and the comparison to experiment.[31]

Let us also check the consistency of the PA-EOM-CCSD approximation. By normalizing the excitation amplitudes in Eq. (3) to one, we can compare the norms of the $r^a$ and $r^{ab}$ amplitudes and get a measure of the one-particle structure of the $A = 17$ states. For the low-lying 3/2$^+$, 1/2$^+$, and 5/2$^+$ states in $^{17}$F, we find $|r^a|^2 = 0.87$, $|r^{ab}|^2 = 0.92$, and $|r^{ab}|^2 = 0.87$, respectively. We find similar norms for the states in $^{17}$O. This clearly shows that these states are dominated by one-particle excitations from the $^{16}$O ground state, and the PA-EOM-CCSD approximation is known to perform very well in this case [24].

Within the GHF basis, we obtain a width for the resonance states. Table I shows the calculated energy and width of the $d_{3/2}$ single-particle resonance in $^{17}$O and $^{17}$F in a model space with $\hbar \omega = 34$ MeV. The energy of the $d_{3/2}$ single-particle state in $^{17}$O compares very well with experiment while in $^{17}$F it is within 0.5 MeV. The calculated widths are very reasonable compared to the experimental values, and represent the first ab-initio calculation of resonance in an $A = 17$ nucleus.

|        | $^{17}$O 3/2$^+$ | $^{17}$F 3/2$^+$ |
|--------|-----------------|-----------------|
| $E_{sp}$ | $\Gamma$       | $E_{sp}$       | $\Gamma$       |
| This work | 1.1            | 0.014          | 3.9            | 1.0           |
| Experiment | 0.942          | 0.096          | 4.399          | 1.530         |

TABLE II: Computed 3/2$^+$ single-particle resonance energies in $^{17}$O and $^{17}$F compared to data [51]. The real part $E_{sp} = \text{Re}[E]$, and the width $\Gamma = 2\text{Im}[E]$ are given in units of MeV.

Conclusions. We performed ab-initio coupled-cluster calculations of the energy and lifetimes of the low-lying 1/2$^+$, 3/2$^+$, and 5/2$^+$ states in $^{17}$O and $^{17}$F employing chiral nucleon-nucleon interactions and a Berggren single-particle basis. The single-particle energy of the 1/2$^+$ proton halo state in $^{17}$F agrees well with the experiment, and we checked by cutoff variation that this result is not affected by short-ranged three-nucleon forces. We find a reduced $d_{3/2}-d_{5/2}$ spin-orbit splitting compared to experiment, and confirmed via cutoff variation that this is sensitive to short-ranged three-nucleon forces. The lifetimes of the 3/2$^+$ resonances in $^{17}$F and $^{17}$O agree reasonably well with experimental data. Our calculations also show that the inclusion of continuum effects is necessary for a proper description of the studied single-particle states.

We thank W. Nazarewicz for useful discussions. This work was supported by the U.S. Department of Energy, under Grant No. DE-FG02-96ER40963 (University of Tennessee), and under DE-FC02-07ER41457 (UNEDF SciDAC Collaboration). This research used computational resources of the National Center for Computational Sciences at Oak Ridge National Laboratory.

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