Ab Initio Computation of the ^{17}F Proton Halo State and Resonances in $A = 17$ Nuclei

G. Hagen,[1] T. Papenbrock,[2,1] and M. Hjorth-Jensen[3]

[1]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[3]*Department of Physics and Center of Mathematics for Applications, University of Oslo, N-0316 Oslo, Norway*

(Received 9 March 2010; published 4 May 2010)

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

DOI: 10.1103/PhysRevLett.104.182501 PACS numbers: 21.10.Dr, 21.10.Pc, 21.10.Tg, 21.60.De

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}He, and ^{11}Li, the proton halo nucleus ^{8}B, and the two-proton halo nucleus ^{17}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 [3–7].

The $A = 17$ neighbors around ^{16}O are particularly interesting and significant nuclei. First, the $5/2^+$ and $1/2^+$ states in ^{17}F are bound by only 600 and 105 keV, respectively, making the latter a proton halo state. This state and astrophysically relevant reactions such as the ^{17}F$(p, \gamma)^{18}$Ne reaction [8] 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}F and ^{17}O determine the single-particle energies of proton and neutron states with respect to the doubly magic nucleus ^{16}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 [9]. Recent theoretical efforts aim at *ab initio* shell-model calculations with a core for *sd*-shell nuclei [10]. The *ab initio* computation of single-particle energies in ^{17}O and ^{17}F is one necessary ingredient for such an approach. Finally, the *ab initio* approach to the proton halo state in ^{17}F and the $3/2^+$ resonances in ^{17}O and ^{17}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}O and ^{17}F. The coupled-cluster method [11] is ideally suited for this endeavor. It is a most efficient approximation for the computation of ground states of doubly magic nuclei, and states with dominant single-particle character in odd-mass neighbors can be computed with equation-of-motion techniques [12]. For the inclusion of continuum effects, we employ the Berggren [13] single-particle basis of the Gamow shell model [4]; i.e., the model space consists of bound, resonant, and continuum scattering states. We employ the chiral nucleon-nucleon interaction at next-to-next-to-next-to leading order (N^{3}LO) by Machleidt and Entem [14].

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

$$\hat{H} = \hat{T} - \hat{T}_{\rm cm} + \hat{V} = \sum_{1 \le i < j \le A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \hat{V}. \qquad (1)$$

Here, T and $T_{\rm cm}$ denote the kinetic energy and the kinetic energy of the center-of-mass coordinate, respectively, and V denotes nucleon-nucleon interaction [14] at N^{3}LO. This interaction has a momentum cutoff of $\Lambda_\chi = 500$ MeV ≈ 2.5 fm^{-1}. However, due to the smooth nature of the cutoff we integrate up to 8 fm^{-1} in the computation of matrix elements.

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 [13] 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 nonresonant continuum states are treated on an equal footing. The Berggren ensemble has been successfully used within the Gamow shell model [4] (see Ref. [15] for a recent review), and in *ab initio* coupled-cluster calculations of energies and lifetimes of the helium isotopes [16]. In constructing the single-particle Berggren basis, we follow Ref. [17]. 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 energy spectra in ^{17}O and ^{17}F relative to the ground state of ^{16}O is as follows. First, we employ the intrinsic Hamiltonian (1) and compute the ground-state energy E_0 of ^{16}O. This yields a precise reference value for the computation of energy differences. 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 (1) 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 is the ''single-particle'' energies $E_{\rm sp}^{(\mu)}$, i.e., $E_{\rm sp}^{(\mu)} = \omega_\mu + E_0^* - E_0$.

In coupled-cluster theory [11,18,19], one computes the similarity-transformed Hamiltonian $\bar{H} = e^{-T} H e^T$ for the closed-shell nucleus ^{16}O. Here, $T = \sum_{k=1}^{A} T_k$ is a sum of k-particle k-hole (kp-kh) cluster operators $T_k = (k!)^{-2} \times \prod_{\nu=1}^{k} \sum_{i_\nu a_\nu} t_{i_1 \ldots i_k}^{a_1 \ldots a_k} \hat{a}_{a_1}^\dagger \ldots \hat{a}_{a_k}^\dagger \hat{a}_{i_k} \ldots \hat{a}_{i_1}$, which are defined with respect to the Hartree-Fock reference state $|\phi_0\rangle$. Here and in what follows, the labels $i, j, k, \ldots$ ($a, b, c, \ldots$) denote occupied (unoccupied) single-particle orbitals. The operators $\hat{a}_p$ ($\hat{a}_p^\dagger$) annihilate (create) a fermion in orbital p. In the coupled-cluster singles-doubles (CCSD) approximation, we truncate the cluster expansion by setting $T_a = 0$ for $a > 2$. The triples cluster T_3 can be treated perturbatively by employing the eigenstates of $\bar{H}$. We employ this ΛCCSD(T) technique [20] for our triples approximation. The unknown cluster amplitudes t_i^a and t_{ij}^{ab} are determined from the condition that the similarity-transformed Hamiltonian $\bar{H}$ 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 $\bar{H}$ 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 [21,22] to treat ''bare'' interactions in large model spaces.

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. The $A = 17$ states that exhibit a dominant single-particle character can be obtained from the ground state of the ''mass-shifted'' ^{16}O by action of the excitation operator

$$R_\mu = \sum_a r^a a_a^\dagger + \frac{1}{2} \sum_{abj} r_j^{ab} a_a^\dagger a_b^\dagger a_j. \qquad (2)$$

Here, μ denotes the parity, spin, and isospin projection of the state we seek to compute, and it is understood that the annihilation and creation operators on the right-hand side of Eq. (2) are coupled to μ. The unknowns r^a and r_j^{ab}, and the excitation energies ω_μ relative to the ground-state energy of the mass-shifted ^{16}O are obtained from solving the eigenvalue problem $[\bar{H}, R_\mu]|\phi_0\rangle = \omega_\mu R_\mu |\phi_0\rangle$; i.e., we seek eigenstates of $\bar{H}$ that are simple excitations (2) of the ^{16}O ground state. This is the particle-attached equation-of-motion method with singles and doubles excitations [19,23].

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 the scattering continuum, we employ a Hartree-Fock basis derived from a harmonic oscillator basis (OHF) and the Gamow-Hartree-Fock (GHF) basis [15] derived from the Woods-Saxon Berggren basis. For well-bound nuclei such as ^{16}O, the coupling to the continuum 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 triples approximation. We find well-converged results for the ground state of ^{16}O in 15 major oscillator shells, and the energy varies by less than 0.5 MeV for 26 MeV $\leq \hbar\omega \leq$ 36 MeV. (See Refs. [21,22] 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 triples approximation.

Figure 1 shows the energies $E_{\rm sp}$ of the $1/2^+$, $3/2^+$, and $5/2^+$ states in ^{17}F relative to the ground state of ^{16}O as a function of $\hbar\omega$. The model space consists of 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 $3/2^+$ and $1/2^+$ states increase with increas-

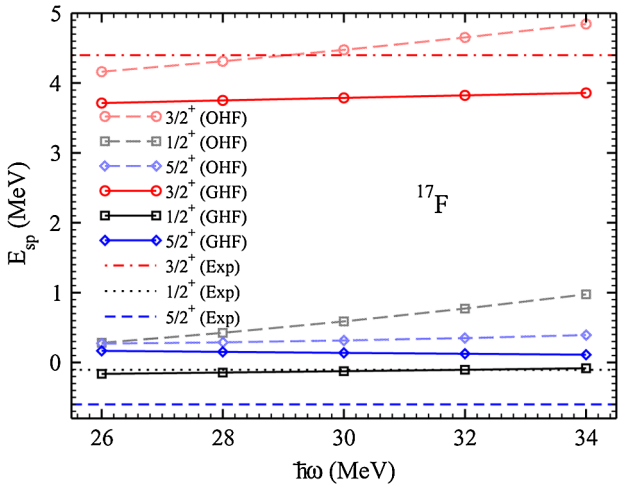

FIG. 1 (color online). Energies of low-lying states in ^{17}F relative to the ^{16}O ground state versus the oscillator frequency $\hbar\omega$, using the nucleon-nucleon potential [14]. Data points with dashed (solid) lines: calculation in oscillator [OHF] (Berggren [GHF]) basis. Horizontal lines: experimental data.

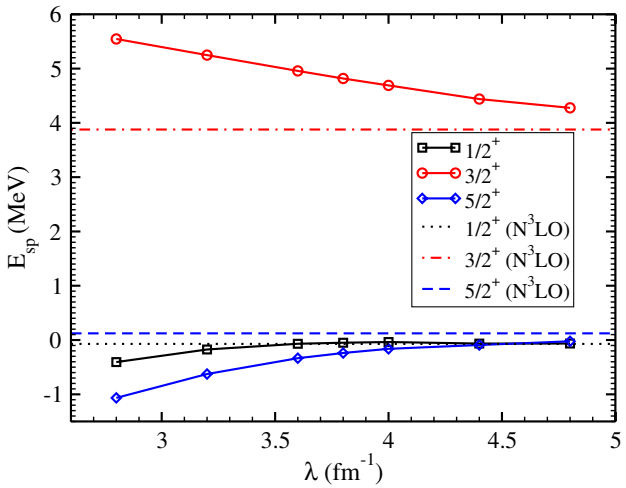

FIG. 2 (color online). Energies of the $1/2^+$, $3/2^+$, and $5/2^+$ states in ^{17}F relative to the ^{16}O ground state (squares, circles, diamonds) versus the momentum cutoff λ. Dotted, dashed, dash-dotted lines: results for a "bare" N^{3}LO potential.

ing frequency of the model space in the OHF basis. The $3/2^+$ states in ^{17}O and ^{17}F are well-known resonances, and cannot be described appropriately in an oscillator basis. The $5/2^+$ states exhibit a weaker dependence on $\hbar\omega$ as their localization inside the $l = 2$ centrifugal barrier reduces the coupling to the external scattering continuum.

The coupling to the scattering continuum has a significant effect on the $1/2^+$ and $3/2^+$ states of ^{17}F and ^{17}O. Our calculations in the GHF basis yield an increase of $\sim$1.0 MeV in binding energy for these states compared to our calculations in the OHF basis. The effect is particularly strong for the $1/2^+$ proton halo state in ^{17}F, a state which is not even bound in the OHF basis. Similar continuum coupling effects were found for the $1/2^+$ halo state in ^{11}Be [7] and in the low-lying states of the fluorine and oxygen isotopes [3,24]. The lack of a centrifugal barrier and the very weak binding yield a proton halo (with a root-mean-square radius of $r_{\rm rms} = 5.333$ fm [25]) 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 effective field theory, the leading three-nucleon forces consist of a long-range two-pion exchange, a midrange one-pion exchange, and a short-range three-nucleon contact interaction [26]. Three-nucleon forces are expected to yield additional binding of the order of 0.5 MeV per nucleon [22]. 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 λ. Decreasing the cutoff employed in the construction of the chiral interactions renormalizes the two-nucleon interaction and generates short-ranged three-nucleon forces [27]. We employ the similarity renormalization group (SRG) [28] for the generation of interactions with a cutoff λ, and study the evolution of the excited states in ^{17}F as the cutoff is varied. Figure 2 shows that the spin-orbit splitting between the $3/2^+$ and $5/2^+$ states increases with decreasing cutoff. Interactions with a high momentum cutoff are known to yield a reduced spin-orbit splitting [29], but it is difficult to disentangle continuum and interaction effects [24]. However, the $1/2^+$ 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}F is insensitive to short-range three-nucleon forces.

Let us also comment on the center of mass. Reference [30] demonstrated that the coupled-cluster wave function of the intrinsic Hamiltonian (1) factorizes to a very good approximation into an intrinsic part and a Gaussian for the center of mass. At the cutoff $\lambda = 2.8$ fm^{-1}, we confirmed this behavior for the low-lying states in the $A = 17$ nuclei for a wide range of oscillator frequencies.

TABLE I. Energies of the $1/2^+$ and $5/2^+$ states relative to the ^{16}O ground state, and the spin-orbit splitting $E_{\rm so}(3/2^+ - 5/2^+)$ (in MeV) in ^{17}O and ^{17}F calculated in a Berggren (Gamow) basis (GHF), and the comparison to experiment [31].

	^{17}O			^{17}F		
	$1/2^+$	$5/2^+$	$E_{\rm so}$	$1/2^+$	$5/2^+$	$E_{\rm so}$
GHF	-2.8	-3.2	4.3	-0.082	0.11	3.7
Exp.	-3.272	-4.143	5.084	-0.105	-0.600	5.000

TABLE II. Energies of the $3/2^+$ resonance in ^{17}O and ^{17}F compared to data [31]. $E_{\rm sp} = {\rm Re}[E]$ is the energy relative to the ^{16}O ground state, and the width is $\Gamma = 2{\rm Im}[E]$ (in MeV).

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

Table I summarizes our results for the $1/2^+$, $3/2^+$, and $5/2^+$ states in ^{17}O and ^{17}F, and compares with experiment. The oscillator frequency is $\hbar\omega = 34$ MeV, which corresponds to the energy minimum of the ^{16}O ground state within the CCSD and within the triples approximation. We also show the spin-orbit splitting between the $5/2^+$ and $3/2^+$ states.

Let us also check the consistency of the coupled-cluster method for $A = 17$ nuclei. We compare the one-particle norm $N_1 = |\sum_a r^a r^a|$ to the total norm of the excitation amplitude $N = |\sum_a r^a r^a + \sum_{abj} r_j^{ab} r_j^{ab}|$ and find $N_1/N = 0.87$, $N_1/N = 0.92$, and $N_1/N = 0.87$ for the low-lying $3/2^+$, $1/2^+$, and $5/2^+$ states in ^{17}F, respectively. We find similar ratios for the states in ^{17}O. This shows that these states are dominated by one-particle excitations from the ^{16}O ground state, consistent with the employed method [23].

Within the GHF basis, we obtain a width for the resonance states. Table II shows the calculated energy and width of the $3/2^+$ resonant states in ^{17}O and ^{17}F relative to the ^{16}O ground state for $\hbar\omega = 34$ MeV. The real part of the energy of the $3/2^+$ 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 a resonance in an $A = 17$ nucleus.

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 $3/2^+$-$5/2^+$ 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 states.

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

[1] I. Tanihata *et al.*, Phys. Rev. Lett. **55**, 2676 (1985).
[2] B. Jonson, Phys. Rep. **389**, 1 (2004).
[3] K. Bennaceur *et al.*, Phys. Lett. B **488**, 75 (2000).
[4] N. Michel *et al.*, Phys. Rev. Lett. **89**, 042502 (2002); R. Id Betan *et al.*, Phys. Rev. Lett. **89**, 042501 (2002).
[5] A. Volya and V. Zelevinsky, Phys. Rev. Lett. **94**, 052501 (2005); N. Michel, W. Nazarewicz, and M. Ploszajczak, Phys. Rev. C **75**, 031301(R) (2007).
[6] K. M. Nollet *et al.*, Phys. Rev. Lett. **99**, 022502 (2007).
[7] S. Quaglioni and P. Navrátil, Phys. Rev. Lett. **101**, 092501 (2008).
[8] D. W. Bardayan *et al.*, Phys. Rev. Lett. **83**, 45 (1999).
[9] O. Sorlin and M. G. Porquet, Prog. Part. Nucl. Phys. **61**, 602 (2008).
[10] A. F. Lisetskiy *et al.*, Phys. Rev. C **78**, 044302 (2008).
[11] F. Coester, Nucl. Phys. **7**, 421 (1958); F. Coester and H. Kümmel, Nucl. Phys. **17**, 477 (1960); J. Čížek, J. Chem. Phys. **45**, 4256 (1966); J. Čížek, Adv. Chem. Phys. **14**, 35 (1969); H. Kümmel, K. H. Lührmann, and J. G. Zabolitzky, Phys. Rep. **36**, 1 (1978).
[12] J. R. Gour *et al.*, Phys. Rev. C **74**, 024310 (2006).
[13] T. Berggren, Nucl. Phys. **A109**, 265 (1968).
[14] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001 (R) (2003).
[15] N. Michel *et al.*, J. Phys. G **36**, 013101 (2009).
[16] G. Hagen *et al.*, Phys. Lett. B **656**, 169 (2007).
[17] G. Hagen, M. Hjorth-Jensen, and N. Michel, Phys. Rev. C **73**, 064307 (2006).
[18] D. J. Dean and M. Hjorth-Jensen, Phys. Rev. C **69**, 054320 (2004).
[19] R. J. Bartlett and M. Musiał, Rev. Mod. Phys. **79**, 291 (2007).
[20] S. A. Kucharski and R. J. Bartlett, J. Chem. Phys. **108**, 5243 (1998); A. D. Taube and R. J. Bartlett, J. Chem. Phys. **128**, 044110 (2008).
[21] G. Hagen *et al.*, Phys. Rev. Lett. **101**, 092502 (2008).
[22] G. Hagen *et al.*, Phys. Rev. C **80**, 021306(R) (2009).
[23] S. Hirata, M. Nooijen, and R. J. Bartlett, Chem. Phys. Lett. **328**, 459 (2000).
[24] N. Michel *et al.*, arXiv:1002.0770; N. Michel *et al.*, Nucl. Phys. **A752**, 335 (2005).
[25] R. Morlock *et al.*, Phys. Rev. Lett. **79**, 3837 (1997).
[26] E. Epelbaum *et al.*, Phys. Rev. C **66**, 064001 (2002).
[27] A. Nogga, S. K. Bogner, and A. Schwenk, Phys. Rev. C **70**, 061002(R) (2004); E. D. Jurgenson, P. Navrátil, and R. J. Furnstahl, Phys. Rev. Lett. **103**, 082501 (2009).
[28] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C **75**, 061001(R) (2007).
[29] S. C. Pieper and V. R. Pandharipande, Phys. Rev. Lett. **70**, 2541 (1993).
[30] G. Hagen, T. Papenbrock, and D. J. Dean, Phys. Rev. Lett. **103**, 062503 (2009).
[31] D. R. Tilley, H. R. Weller, and C. M. Cheves, Nucl. Phys. **A564**, 1 (1993).