Coupled-Cluster and Configuration-Interaction Calculations for Odd-A Heavy Nuclei

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(Received 3 March 2008; published 30 July 2008)

We compare coupled-cluster (CC) and configuration-interaction (CI) results for ^{55}Ni and ^{57}Ni obtained in the pf-shell basis, focusing on the practical equation-of-motion (EOM) CC approximations that can be applied to systems with dozens of correlated fermions. The weight of the reference state and the strength of correlation effects are controlled by the gap between the $f_{7/2}$ orbit and the $f_{5/2}$, $p_{3/2}$, $p_{1/2}$ orbits. Independent of the gap, the CC methods with up to $2p$-$2h$ components in the cluster operator and $3p$-$2h$/$3h$-$2p$ components in the EOMCC excitation operator are more accurate than the computationally more demanding CI approach with up to $3p$-$3h$ excitations and almost as accurate as the even more demanding CI approach truncated at $4p$-$4h$ excitations.

DOI: 10.1103/PhysRevLett.101.052501 PACS numbers: 21.60.Cs, 21.60.Gx, 27.40.+z, 31.15.bw

One of the major challenges in nuclear theory is the development of practical computational approaches to calculate the structure and properties of heavy nuclei. Significant progress has been made in this area, as illustrated, for example, by the recent full configuration-interaction (CI) study of ^{56}Ni in the pf-shell basis, which provided a detailed description of virtually all levels up to about 8 MeV [1]. One would like to perform similar calculations for all heavy nuclei, but the huge dimensionalities of the full CI eigenvalue problem make such calculations often impossible. Indeed, even the pf-shell full CI calculation for ^{56}Ni, which has an M-scheme dimension of $\sim 10^9$ determinants, represents a significant and computationally demanding effort that is near the limit of what is currently possible. Alternative approaches should be considered in order to pave the way to accurate microscopic calculations for heavier nuclei.

A promising approach in this area may be offered by the coupled-cluster (CC) theory [2,3], which is based on the exponential wave function ansatz and is an ideal formalism for performing accurate, size extensive calculations for many-body quantum systems at a relatively low computational cost. Although originally suggested in nuclear physics [2,4], most of the development of CC theory has occurred in quantum chemistry, where CC methods are frequently used to study molecular electronic structure [3,5]. In recent years, CC theory has had a resurgence in the area of nuclear physics with applications to light nuclei in the no-core basis [6–8]. Encouraged by these results, we applied several inexpensive quantum chemistry inspired CC methods to the heavier ^{56}Ni nucleus, as described by the pf-shell basis [9]. This study revealed that the inexpensive CC approach of Ref. [10], in which noniterative corrections due to triply excited clusters are added to the energies obtained with the basic CCSD (CC singles and doubles) [11] and equation-of-motion (EOM) CCSD [12] approximations, produces results that are as accurate as those obtained with the considerably more expensive truncated CI method including up to $4p$-$4h$ (4-particle–4-hole) excitations.

In this Letter, we extend our earlier analysis [9] to the adjacent odd isotopes ^{55}Ni and ^{57}Ni. In particular, we investigate the performance of the particle-removed and particle-attached EOMCC methods [8,13–15], in which the wave functions for ^{55}Ni and ^{57}Ni are built up from the correlated ground state of ^{56}Ni through the suitably defined operators describing the removal or attachment of a nucleon. As in the case of ^{56}Ni, ^{55}Ni and ^{57}Ni are ideal benchmarks for such a study since the effective Hamiltonian for nuclei in this region is well established [1,16] and the full CI calculations, though computationally very demanding, can still be performed, providing the exact solutions for comparison purposes. Furthermore, since these calculations are performed within the pf model space, there are no spurious center-of-mass contaminants that complicate the calculations for light nuclei. Finally, by varying the energy of the $f_{5/2}$, $p_{3/2}$, $p_{1/2}$ orbitals relative to a fixed value of the $f_{7/2}$ orbit, as was done in our ^{56}Ni work [9], we can tune the correlation effects of the system, and study how some of the most practical CC methods perform as the contribution of the reference determinant in the wave function changes.

As in our earlier study of ^{56}Ni [9], we use the GXPF1A effective Hamiltonian [16], which was derived from a microscopic calculation based on the renormalized G-matrix theory with the Bonn-C interaction [17], and which was refined by fitting the important linear combinations of two-body matrix elements to low-lying states in nuclei from $A = 47$ to $A = 66$ [16,18]. One aspect of this effective interaction, which is important in this study, is the smooth mass dependence of the two-body matrix elements that scale as $(42/A)^{1/3}$. Additionally, following Ref. [9], we change the shell gap between the single-particle energies, as described above, by an amount ΔG, where $\Delta G = 0$

is the original Hamiltonian used in [1]. We probe the range of ΔG values from -2 MeV, where the contribution of the reference determinant to each wave function of interest is small, to 2 MeV, where each quantum state of interest is dominated by the corresponding reference determinant.

We compare the CC and CI results for the $J^\pi = \frac{7}{2}^-$ ground state of ^{55}Ni and the $\frac{3}{2}^-$ ground state ^{57}Ni, as well as for the low-lying $\frac{5}{2}^-$ and $\frac{1}{2}^-$ excited states of ^{57}Ni. In the CI calculations, the wave function for each state can be built through particle-hole excitations out of a single lowest-energy reference determinant of an appropriate symmetry, $|\Phi_0^{(A)}(j)\rangle$, where A is the mass number of the system and j is the total angular momentum quantum number of the state of interest, provided that the total angular momentum and its projection on the z axis are the same. To obtain the exact solutions for the above states of ^{55}Ni and ^{57}Ni within the pf model space, we performed full CI calculations including all determinants up to $15p$-$15h$ excitations relative $|\Phi_0^{(55)}(\frac{7}{2})\rangle$ in the ^{55}Ni case, and up to $17p$-$17h$ excitations relative to $|\Phi_0^{(57)}(j)\rangle$ ($j = \frac{3}{2}$, $\frac{5}{2}$, or $\frac{1}{2}$) in the ^{57}Ni case. In addition, we considered various approximate CI(np-nh) approaches obtained by truncating the CI wave function expansions at the np-nh excitations, which we represent in this Letter by the particle-hole excitation operators C_n, where $n = 2$, 3, 4, and 6. The largest full CI calculation performed in this work was for the $\frac{1}{2}^-$ state in ^{57}Ni, which has an M-scheme dimension of about 1.4×10^9.

As already mentioned, the CC methods used in this work are based on the particle-attached and particle-removed EOMCC theories. We focus on the basic methods in this category, which we designate as the EOMCC($2p$-$1h$) and EOMCC($2h$-$1p$) approximations [8,13,14], and the higher-level, yet still inexpensive EOMCC($3p$-$2h$) and EOMCC($3h$-$2p$) schemes [15]. In all of these methods, the ground- and excited-state wave functions for an $(A \pm 1)$-particle system are defined as $|\Psi_\mu^{(A\pm1)}\rangle = R_\mu^{(A\pm1)}|\Psi_0^{(A)}\rangle$, where $|\Psi_0^{(A)}\rangle = \exp(T^{(A)})|\Phi_0^{(A)}(0)\rangle$, with the cluster operator $T^{(A)} = T_1 + T_2$, is the CCSD ground state for the A-particle closed-shell system, and $R_\mu^{(A+1)}$ and $R_\mu^{(A-1)}$ are the particle-attaching and particle-removing operators which generate the $(A+1)$- and $(A-1)$-particle states, respectively, from the A-particle CCSD wave function $|\Psi_0^{(A)}\rangle$. In the EOMCC($2p$-$1h$) approach, the particle-attaching operator $R_\mu^{(A+1)}$ is a sum of the $1p$ (R_{1p}) and $2p$-$1h$ ($R_{2p\text{-}1h}$) components, while in the EOMCC($2h$-$1p$) scheme, the particle-removing operator $R_\mu^{(A-1)}$ consists of the $1h$ (R_{1h}) and $2h$-$1p$ ($R_{2h\text{-}1p}$) components. In addition to the above components, the EOMCC($3p$-$2h$) and EOMCC($3h$-$2p$) methods include the $3p$-$2h$ ($R_{3p\text{-}2h}$) and $3h$-$2p$ ($R_{3h\text{-}2p}$) components in $R_\mu^{(A+1)}$ and $R_\mu^{(A-1)}$, respectively, which are particularly important when the states of interest have significant doubly excited contributions [15]. It is important to note that despite the fact that the above CC methods are based on building the $(A \pm 1)$-particle systems from the related A-particle nucleus, when using the GXPF1A effective Hamiltonian [16] with these schemes one should use the appropriate $A + 1$ or $A - 1$ mass number, and not the mass number A, in scaling the mass dependence of the two-body matrix elements used in the calculation, as described earlier. One of the advantages of using the particle-attached and particle-removed EOMCC methods, as opposed to the standard CC methods that would produce quantum states of the $(A \pm 1)$-particle systems through particle-hole excitations from the appropriate $|\Phi_0^{(A\pm1)}(j)\rangle$ reference states, is that the results are automatically adapted to the angular momentum symmetries. This is a consequence of using the $j = 0$ determinant $|\Phi_0^{(A)}(0)\rangle$ of the closed-shell A-body system as a reference in the EOMCC calculations for the adjacent $(A \pm 1)$-particle systems. The rotational invariance is maintained, since we obtain the $R_\mu^{(A\pm1)}$ operators defining the quantum states $|\Psi_\mu^{(A\pm1)}\rangle$ of the $(A \pm 1)$-particle systems (in our case, eigenstates of ^{55}Ni and ^{57}Ni) by diagonalizing the similarity-transformed Hamiltonian of CC theory, $\exp(-T^{(A)})H\exp(T^{(A)})$, obtained for the $J = 0$ closed-shell ground state of the A-particle reference system (in our case, a CCSD ground state of ^{56}Ni), which is rotationally invariant, in the appropriate configuration spaces corresponding to the many-body components included in $R_\mu^{(A\pm1)}$, as described above.

Table I gives the CC and CI results for the binding energies of ^{55}Ni and ^{57}Ni as functions of the shell gap. As one can see, the EOMCC($3p$-$2h$) and EOMCC($3h$-$2p$) schemes produce highly accurate results for the ground-state energies of both nuclei in the $\Delta G \geq 0$ region. In this region, the EOMCC($3p$-$2h$) and EOMCC($3h$-$2p$) results differ from the exact full CI ground-state energies by about 0.07–0.33 MeV. In the $\Delta G < 0$ region, where the overlap between the full CI ground-state wave functions and the corresponding reference determinants, $S_0^{(A)}(j) = |\langle\Phi_0^{(A)}(j)|\Psi_{0,A}^{\text{full}-\text{CI}}(j)\rangle|$ ($A = 55$ or 57), substantially decreases, the agreement between the CC and full CI results deteriorates, with the errors in the CC results becoming as large as 5.25 MeV. It is important to note though that regardless of the value of ΔG, the EOMCC($3p$-$2h$) and EOMCC($3h$-$2p$) ground-state energies are at least as accurate as, and generally more accurate than, the corresponding CI($3p$-$3h$) energies. Furthermore, although the CI($4p$-$4h$) approximation is somewhat more accurate than the CC schemes studied in this work, there is a reasonably good agreement between the CI($4p$-$4h$) results on the one hand and the EOMCC($3p$-$2h$) and EOMCC($3h$-$2p$) results on the other hand. Even for the smallest value of ΔG, the discrepancies between the ground-state energies obtained in the above two types of CC calculations and the corresponding CI($4p$-$4h$) energies are only about 0.4–0.6 MeV. We should keep in mind that the $\Delta G = -2$ MeV region is so strongly correlated that even the CI($6p$-$6h$) approxima-

TABLE I. Binding energies (in MeV) of ^{55}Ni and ^{57}Ni relative to the corresponding reference energies $\langle\Phi_0^{(A)}(j)|H|\Phi_0^{(A)}(j)\rangle$, $A =$ 55 and 57, respectively, as functions of the shell gap shift ΔG (in MeV). $S_0^{(A)}(j)$ is defined as $|\langle\Phi_0^{(A)}(j)|\Psi_{0,A}^{\text{full}-\text{CI}}(j)\rangle|$.

ΔG	-2	-1	0	1	2
^{55}Ni					
EOMCC($2h$-$1p$)	-3.649	-2.459	-1.884	-1.542	-1.313
EOMCC($3h$-$2p$)	-3.844	-2.567	-1.951	-1.587	-1.344
CI($2p$-$2h$)	-2.505	-2.013	-1.672	-1.427	-1.244
CI($3p$-$3h$)	-3.295	-2.449	-1.922	-1.580	-1.344
CI($4p$-$4h$)	-4.457	-2.967	-2.150	-1.693	-1.406
CI($6p$-$6h$)	-6.397	-3.519	-2.262	-1.723	-1.417
Full CI	-9.091	-3.920	-2.279	-1.725	-1.417
$S_0^{(55)}(\frac{7}{2})$	0.0362	0.4023	0.8015	0.8919	0.9287
^{57}Ni					
EOMCC($2p$-$1h$)	-3.868	-2.671	-2.080	-1.721	-1.476
EOMCC($3p$-$2h$)	-4.295	-2.871	-2.186	-1.783	-1.516
CI($2p$-$2h$)	-2.692	-2.192	-1.840	-1.584	-1.389
CI($3p$-$3h$)	-3.622	-2.717	-2.146	-1.772	-1.513
CI($4p$-$4h$)	-4.697	-3.217	-2.370	-1.884	-1.575
CI($6p$-$6h$)	-6.534	-3.768	-2.493	-1.918	-1.588
Full CI	-9.391	-4.151	-2.511	-1.921	-1.588
$S_0^{(57)}(\frac{3}{2})$	0.0335	0.4062	0.7802	0.8774	0.9182

TABLE II. Excitation energies (in MeV) of the low-lying states of ^{57}Ni as functions of the shell gap shift ΔG (in MeV). $S_0^{(A)}(j)$ is defined as $|\langle\Phi_0^{(A)}(j)|\Psi_{0,A}^{\text{full}-\text{CI}}(j)\rangle|$.

ΔG	-2	-1	0	1	2
$(5/2)^-$					
EOMCC($2p$-$1h$)	0.658	0.819	0.895	0.937	0.961
EOMCC($3p$-$2h$)	0.625	0.771	0.856	0.908	0.939
CI($2p$-$2h$)	0.812	0.856	0.897	0.927	0.948
CI($3p$-$3h$)	0.781	0.827	0.878	0.917	0.944
CI($4p$-$4h$)	0.692	0.776	0.852	0.904	0.937
CI($6p$-$6h$)	0.360	0.658	0.832	0.900	0.936
Full CI	-0.118	0.402	0.825	0.900	0.936
$S_0^{(57)}(\frac{5}{2})$	0.0193	0.2640	0.7443	0.8596	0.9077
$(1/2)^-$					
EOMCC($2p$-$1h$)	1.259	1.494	1.639	1.739	1.813
EOMCC($3p$-$2h$)	0.669	1.071	1.366	1.562	1.694
CI($2p$-$2h$)	1.279	1.451	1.592	1.699	1.781
CI($3p$-$3h$)	1.009	1.218	1.426	1.588	1.706
CI($4p$-$4h$)	0.763	1.021	1.312	1.530	1.676
CI($6p$-$6h$)	0.395	0.739	1.211	1.499	1.665
Full CI	0.050	0.434	1.184	1.496	1.665
$S_0^{(57)}(\frac{1}{2})$	0.0293	0.2561	0.6577	0.8049	0.8701

tion, which uses up to $6p$-$6h$ excitations in the corresponding wave function expansion, is far from being sufficient. The fact that the EOMCC($3p$-$2h$) and EOMCC($3h$-$2p$) methods, for which the most expensive computational steps scale as $n_o^2 n_u^5$ and $n_o^3 n_u^4$, respectively, produce the results which are better than those obtained with CI($3p$-$3h$) and almost as good as those obtained with CI($4p$-$4h$) is an important finding, since both of these CC methods are significantly less expensive than the CI($3p$-$3h$) and CI($4p$-$4h$) approaches, which require iterative steps that scale as $n_o^3 n_u^5$ and $n_o^4 n_u^6$, respectively (n_o and n_u are the numbers of occupied and unoccupied states in a single-particle basis set, respectively).

Table II, which shows the excitation energies of the $\frac{5}{2}^-$ and $\frac{1}{2}^-$ states of ^{57}Ni, reveals similar accuracy patterns. The EOMCC($3p$-$2h$) approach performs very well up to $\Delta G \approx 0$, but in the much more challenging $\Delta G < 0$ region the method breaks down. However, we again see an excellent agreement between the EOMCC($3p$-$2h$) energies and those of the much more expensive truncated CI results, even in the most challenging $\Delta G < 0$ region. In fact, the discrepancies between the EOMCC($3p$-$2h$) and CI($4p$-$4h$) results for the $\frac{5}{2}^-$ and $\frac{1}{2}^-$ states of ^{57}Ni do not exceed 0.1 MeV, and are usually even smaller, independent of the gap. We conclude that the inexpensive CC approach with up to $3p$-$2h$ components in the EOMCC particle-attaching operator which creates ^{57}Ni from ^{56}Ni, and with one- and two-body components in the cluster operator describing the reference ^{56}Ni nucleus, is capable of producing accuracies similar to those provided by the significantly more expensive CI approach with up to $4p$-$4h$ excitations in the wave function.

We can understand the observed accuracy patterns by comparing the CI and EOMCC wave functions. Indeed, since the reference determinants used to define the CI wave function expansions for ^{55}Ni and ^{57}Ni are related to the reference determinants of the particle-attached and particle-removed EOMCC approaches by a $1p$ or $1h$ excitation, it is straightforward to derive the relationships between the particle conserving CI excitation operators C_n and the many-body components of the particle-nonconserving EOMCC excitation operators $R_\mu^{(A\pm1)}$. In particular, for the ground state of ^{55}Ni, the np-nh excitation operators C_n, $n = 0 - 4$, defining the CI($4p$-$4h$) wave function can be expressed in terms of the np-nh cluster components T_n and $(n+1)h$-np components $R_{(n+1)h\text{-}np}$ defining the particle-removed EOMCC theory as follows: $(C_0 + C_1 + C_2 + C_3 + C_4)|\Phi_0^{(55)}(\frac{7}{2})\rangle = \{R_{1h} + R_{2h\text{-}1p} + R_{3h\text{-}2p} + R_{1h}T_2 + R_{4h\text{-}3p} + R_{2h\text{-}1p}T_2 + R_{1h}T_3 + r_{5h\text{-}4p} + r_{3h\text{-}2p}T_2 + R_{3h\text{-}2p}t_2 + r_{2h\text{-}1p}T_3 + R_{2h\text{-}1p}t_3 + r_{1h}[T_4 + \frac{1}{2}(T_2)^2] + R_{1h}t_4 + R_{1h}t_2T_2\}|\Phi_0^{(56)}(0)\rangle$, where the lowercase letters indicate that only a small subset of the relevant excitations, in which at least one of the unoccupied single-particle indices corresponds to the $1h$ excitation generating the CI reference $|\Phi_0^{(55)}(\frac{7}{2})\rangle$ from the CC reference $|\Phi_0^{(56)}(0)\rangle$, is considered. In arriving at the above relationship, we used the fact that the T_1 cluster component that defines the CCSD wave function of the reference ^{56}Ni nucleus, as described by the pf-shell basis, vanishes due to

symmetry. Although formally all of the above components of the $R_\mu^{(55)}$ and $T^{(56)}$ operators must be included in order to fully describe the CI($4p$-$4h$) wave function, we know from our previous study of ^{56}Ni [9] that the T_4 clusters play a very small role in describing the CC ground state of ^{56}Ni (which is the starting point for the particle-removed EOMCC calculations for ^{55}Ni). Furthermore, based on the relatively small differences between the EOMCC($2h$-$1p$) and EOMCC($3h$-$2p$) results, as seen in Table I, along with our experiences with the analogous valence systems in quantum chemistry, we can anticipate that the role of higher than $3h$-$2p$ excitations, such as $R_{4h\text{-}3p}$ and $r_{5h\text{-}4p}$, is minimal. This means that the EOMCC($3h$-$2p$) method incorporates all of the important correlations present in ^{55}Ni that are included in the CI($4p$-$4h$) wave function except for those related to the T_3 clusters (the $R_{1h}T_3$, $r_{2h\text{-}1p}T_3$, and $R_{2h\text{-}1p}t_3$ terms in the above relationship). This explains why the EOMCC($3h$-$2p$) approach improves the CI($3p$-$3h$) results. The latter method does not include the $4p$-$4h$ excitations C_4, which in the EOMCC($3h$-$2p$) calculations are represented by the product terms, such as $R_{3h\text{-}2p}T_2$ or $\frac{1}{2}R_{1h}(T_2)^2$. The above analysis also suggests that if T_3 clusters are small then the EOMCC($3h$-$2p$) and CI($4p$-$4h$) results should be similar. This is exactly what we observe in our calculations. As shown in our earlier work on ^{56}Ni [9], the T_3 clusters are small in the $\Delta G \geq 0$ region, while becoming increasingly important when the shell gap decreases. This explains the similarity of the EOMCC($3h$-$2p$) and CI($4p$-$4h$) results when $\Delta G \geq 0$ and the growing deviation between these results in the $\Delta G < 0$ region. The above analysis indicates that it would be worthwhile to incorporate T_3 clusters in the EOMCC framework, as discussed in the context of quantum chemistry in [15,19], to improve the description of the $\Delta G < 0$ region. Similar analyses and conclusions can be made for the ground and excited states of ^{57}Ni.

In summary, we compared the CC and CI results for ^{55}Ni and ^{57}Ni obtained in the pf-shell basis. By varying the energy gap between the $f_{7/2}$ orbit and the $f_{5/2}$, $p_{3/2}$, $p_{1/2}$ orbits we tested the performance of the most practical CC methods, based on the concept of attaching a particle to or removing a particle from the related closed-shell nucleus, as a function of the weight of the reference determinant in the wave function. We showed that for situations where the reference determinant provides a reasonable representation of the ground- or excited-state wave function (i.e., the overlap between the reference determinant and the exact wave function is on the order of 0.9 or greater), the CC schemes with up to $3p$-$2h$ and $3h$-$2p$ components in the particle-attaching and particle-removing operators that produce the $(A \pm 1)$-body systems out of the A-body nucleus yield highly accurate results for the binding and excitation energies, very close to full CI. For the remaining situations, where the shell gap in the reference nucleus is small, the analogous CC binding and excitation energies are often as good as the results of the much more expensive CI diagonalization involving up to $4p$-$4h$ determinants in the wave function. Mathematical analysis suggests that the CC results reported in this Letter could be further improved by including the effects of T_3 clusters in the description of the reference ^{56}Ni nucleus, particularly in the small-shell-gap region, where the absence of these clusters appears to be the main reason for the observed discrepancies between the CC and full CI energies.

Supported by the National Science Foundation and the U.S. Department of Energy. We thank Morten Hjorth-Jensen for help with the matrix elements of the GXPF1A Hamiltonian. We also thank Morten Hjorth-Jensen, David Dean, and Thomas Papenbrock for discussions.

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