Ground-State and Single-Particle Energies of Nuclei around ^{16}O, ^{40}Ca, and ^{56}Ni from Realistic Nucleon-Nucleon Forces

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We perform *ab initio* calculations for nuclei around ^{16}O, ^{40}Ca, and ^{56}Ni using realistic nucleon-nucleon forces. In particular, ^{56}Ni is computed as the heaviest nucleus in this kind of *ab initio* calculation. Ground-state and single-particle energies including three-body-cluster effects are obtained within the framework of the unitary-model-operator approach. It is shown that the CD-Bonn nucleon-nucleon potential gives quite good results close to the experimental values for all nuclei in the present work.

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One of the most fundamental problems in nuclear physics is to describe and understand nuclear properties from the underlying nuclear forces. To solve this problem, a realistic nucleon-nucleon (NN) interaction [1], which has a strong repulsive core and a complicated spin-isospin structure, has been employed [2]. In addition, to obtain more quantitative results, a three-nucleon (NNN) interaction [3,4] has been used in some cases. Light nuclei with a mass number up to $A \simeq 12$ have been well understood from the *ab initio* calculations employing the realistic NN and NNN interactions with the Green's function Monte Carlo (GFMC) method [4,5] and the no-core shell model (NCSM) [6,7]. While these methods have been successful in the light nuclei, their applications to heavier systems become rather difficult due to the exponential increase in the computer performance needed.

Coupled-cluster (CC) theory or, in other words, the e^S (or e^T) method [8,9] is promising for microscopic calculations of heavy nuclei. Recently, the first calculations for nuclei up to the pf-shell region, ^{48}Ca and ^{48}Ni, have been reported with a CC method including the excitations of the singles and doubles which is referred to as CCSD [10]. Well-converged results in a sufficiently large model space have been obtained using a chiral N^{3}LO NN interaction [11] as one of the realistic NN forces. While the CCSD calculations give results fairly close to the experimental values, there still remain some discrepancies between the results and experiments. One of the reasons for the discrepancies may be attributed to the missing NNN interaction in the calculation. Although the NNN force has been considered to be an indispensable ingredient for a more quantitative description of the nuclear properties, there has been no definite way of using the NNN force directly in the calculation for the heavier nuclei.

Given this situation, it is still worthy to compute nuclear properties using only the realistic NN interaction in a rigorous way and to investigate to what extent nuclei can be described with only the NN force. Such a study could be helpful to evaluate the magnitude of the NNN-force effect in heavier nuclei in future works.

In this Letter, we report the results of calculated ground-state energies and single-particle ones for hole states in nuclei around ^{16}O, ^{40}Ca, and ^{56}Ni with the unitary-model-operator approach (UMOA) [12–14]. The calculation for ^{56}Ni, which is a typical pf-shell nucleus, is performed for the first time within the UMOA framework. Furthermore, ^{56}Ni is the heaviest nucleus for which this kind of *ab initio* calculation has been performed. In the UMOA, a Hermitian effective interaction is derived through a unitary transformation [15,16]. The unitary transformation method has been widely used in other microscopic methods in nuclear physics, such as the NCSM [6,7] and the hyperspherical harmonics effective interaction method (EIHH) [17]. The unitary transformation treats successfully short-range correlations due to the strong repulsive core of the NN force in a *truncated* model space, but the model space should be sufficiently large in the sense of the *ab initio* calculation.

In the UMOA, a unitarily transformed Hamiltonian $\tilde{H}$ of the original many-body Hamiltonian H is given in a cluster-expansion form as $\tilde{H} = e^{-S}He^{S} = \tilde{H}^{(1)} + \tilde{H}^{(2)} + \tilde{H}^{(3)} + \dots$, where S is a two-body anti-Hermitian operator and is determined by solving a decoupling equation between the model space and its compliment [18]. The $\tilde{H}^{(1)}$, $\tilde{H}^{(2)}$, and $\tilde{H}^{(3)}$ are the one-, two-, and three-body cluster (3BC) terms, respectively. The method of the actual calculation and the results of nuclei around ^{16}O including up to the two-body cluster terms using modern NN forces have been given in detail in our previous study [14]. In the present work, we apply this method to the heavier nuclei up to ^{56}Ni and evaluate effects of the 3BC terms systematically. As for the evaluation of the 3BC terms, we follow the prescription given in Refs. [12,13].

In Fig. 1, we first demonstrate $\hbar\Omega$ and ρ_1 dependences of the calculated ground-state energies of ^{16}O including the 3BC effects. Here, $\hbar\Omega$ is the harmonic-oscillator (HO)

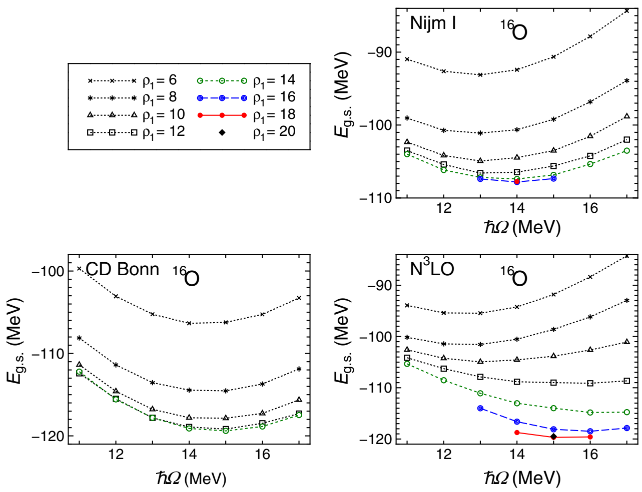

FIG. 1 (color online). The $\hbar\Omega$ and ρ_1 dependences of the calculated ground-state energies $E_{\text{g.s.}}$ of ^{16}O.

energy of the single-particle basis states. The ρ_1 stands for a boundary number defined with a set of the HO quantum numbers $\{n_1, l_1\}$ and $\{n_2, l_2\}$ of the two-body states as $\rho_1 = 2n_1 + l_1 + 2n_2 + l_2$, and specifies the size of the model space of the two-body states. The Nijm-I [19], the CD-Bonn [20], and the chiral N^{3}LO [11] *NN* forces are employed as the realistic *NN* interactions. The Coulomb force is added to the proton-proton channel. It is seen that well-converged results with respect to the boundary number ρ_1 are obtained at $\rho_1 = 18$ and 14 for the Nijm-I and the CD-Bonn interactions, respectively. For the N^{3}LO interaction, the convergence property is rather different from the other two forces. For example, at $\hbar\Omega = 15$ MeV, it is difficult to search for convergence up to $\rho_1 = 14$. However, for the larger values of ρ_1, the results rapidly converge toward the point at $\rho_1 = 20$.

In Table I, we tabulate the energies of the one- and two-body cluster terms $E^{(1+2\text{BC})}$, the 3BC terms $E^{(3\text{BC})}$, and the total ground-state energy $E_{\text{g.s.}}$ of ^{16}O. The binding energy per nucleon BE$/A = -E_{\text{g.s.}}/A$ is also given. The values of $\hbar\Omega = 14$ MeV and $\rho_1 = 18$ for Nijm I, $\hbar\Omega = 15$ MeV and $\rho_1 = 14$ for CD Bonn, and $\hbar\Omega = 15$ MeV and $\rho_1 = 20$ for N^{3}LO are shown as the optimal ones. It is seen that, although the 3BC terms have attractive and sizable contributions to the ground-state energy, the calculated ground-state energies are still less bound than the experimental value. In the present calculation, a genuine *NNN* force is not taken into account. The inclusion of the *NNN* force could compensate for the discrepancies between the theoretical and experimental values, which has been shown in the microscopic studies of light nuclei [4,22]. Note, however, that the energies of 93.6% to the experimental value are attained from only the *NN* force for the CD-Bonn and the N^{3}LO potentials, though 84.4% for the Nijm-I interaction.

TABLE I. The calculated energies of the one- and two-body cluster terms $E^{(1+2\text{BC})}$, the 3BC terms $E^{(3\text{BC})}$, and the total ground-state energy $E_{\text{g.s.}}$ of ^{16}O. The experimental value is taken from Ref. [21]. All energies are in MeV.

		Nijm I	CD Bonn	N^{3}LO	Expt.
^{16}O	$E^{(1+2\text{BC})}$	−103.72	−115.58	−105.92	
	$E^{(3\text{BC})}$	−4.02	−3.82	−13.57	
	$E_{\text{g.s.}}$	−107.74	−119.39	−119.48	−127.62
	BE$/A$	6.73	7.46	7.47	7.98

The 3BC effect for N^{3}LO is significantly larger than the ones for Nijm I and CD Bonn. A similar tendency is seen in the recent ΛCCSD(T) computation including triples corrections [23]. We have found that the large 3BC contribution also applies to the other nuclei in the present study. Owing to this property, we have not yet obtained the converged results for the other nuclei. For this reason, we do not show the other results for N^{3}LO. One may also notice that the result of $E^{(1+2\text{BC})}$ for N^{3}LO shows a large difference of about 4 MeV from that in our previous study [14]. This is due to strong dependences of $E^{(1+2\text{BC})}$ and $E^{(3\text{BC})}$ on $\hbar\Omega$ and ρ_1 for N^{3}LO.

In Fig. 2, we illustrate the $\hbar\Omega$ and ρ_1 dependences of the total energy $E(= -\text{BE})$ including the 3BC effects of the lowest $1/2^-$ and $3/2^-$ states of the spin-orbit doublet in ^{15}O. These states are representative single-hole states of neutron in ^{15}O. For Nijm I, we take the values of $\hbar\Omega = 14$ and 13 MeV at $\rho_1 = 18$ for the $1/2^-$ and $3/2^-$ states, respectively, as the optimal ones, and for CD Bonn, $\hbar\Omega = 15$ and 14 MeV at $\rho_1 = 14$. These optimal values are tabulated in Table II. The results for the proton-hole states in ^{15}N are also given. The convergence properties for ^{15}N are similar to the case of ^{15}O.

The microscopic description of the spin-orbit splitting in nuclei is a long-standing problem. In Table II, the spin-orbit splitting is denoted by $E_{\text{s.o.}}$ which is the difference of the binding energies between the $1/2^-$ and $3/2^-$ states. Our results show smaller splitting energies than the experimental values for these hole states, which does not contradict previous studies [24,25]. We should note, however, that the magnitude of the lack of the splitting energy

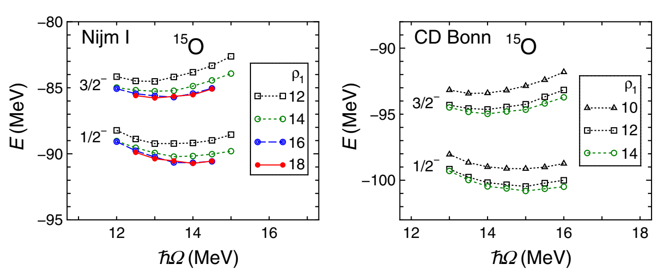

FIG. 2 (color online). The $\hbar\Omega$ and ρ_1 dependences of the calculated energies $E(= -\text{BE})$ of the lowest $1/2^-$ and $3/2^-$ states of the spin-orbit doublet in ^{15}O.

TABLE II. The calculated energies of the one- and two-body cluster terms $E^{(1+2\mathrm{BC})}$, the 3BC terms $E^{(3\mathrm{BC})}$, and the total energy $E(=-\mathrm{BE})$ of the lowest $1/2^-$ and $3/2^-$ states of the spin-orbit doublets in ^{15}O and ^{15}N. The quantity $E_{\mathrm{s.o.}}$ is the spin-orbit splitting energy including the 3BC effects. The energy difference E_{diff} of the ground-state energies between ^{15}O and ^{15}N is also given. All energies are in MeV.

	J^π		Nijm I	CD Bonn	Expt.
^{15}O	$3/2^-$	$E^{(1+2\mathrm{BC})}$	−81.17	−90.38	
		$E^{(3\mathrm{BC})}$	−4.61	−4.59	
		E	−85.77	−94.97	−105.78
	$1/2^-$	$E^{(1+2\mathrm{BC})}$	−85.71	−96.24	
		$E^{(3\mathrm{BC})}$	−5.01	−4.58	
		E	−90.72	−100.81	−111.96
		$E_{\mathrm{s.o.}}$	4.95	5.84	6.18
^{15}N	$3/2^-$	$E^{(1+2\mathrm{BC})}$	−84.58	−94.00	
		$E^{(3\mathrm{BC})}$	−4.59	−4.58	
		E	−89.17	−98.58	−109.17
	$1/2^-$	$E^{(1+2\mathrm{BC})}$	−89.14	−99.87	
		$E^{(3\mathrm{BC})}$	−4.99	−4.55	
		E	−94.13	−104.42	−115.49
		$E_{\mathrm{s.o.}}$	4.96	5.84	6.32
		E_{diff}	3.41	3.60	3.54

depends considerably on the interactions employed. For CD Bonn, the differences are only 0.34 and 0.48 MeV for ^{15}O and ^{15}N, respectively. The calculation including the *NNN* force could give a better result as shown in Refs. [24,25].

The energy difference of the ground states between ^{15}O and ^{15}N is denoted by E_{diff} in Table II. Our results are in good agreement with the experiment. Similar tendency has been found in the case of ^{3}He and ^{3}H in our previous work [14]. Since we include the Coulomb force, the small differences between the results and experiment may be attributed to the effects of the charge-independence breaking of the original *NN* forces.

In Fig. 3, we show the $\hbar\Omega$ and ρ_1 dependences of the calculated ground-state energies including the 3BC effects of ^{40}Ca. We take the values of $\hbar\Omega = 13$ MeV and $\rho_1 = 20$ for Nijm I, and $\hbar\Omega = 14$ MeV and $\rho_1 = 18$ for CD Bonn as the optimal values. Since we handle a heavier system ^{40}Ca than ^{16}O, we need a larger model space to obtain the converged results. The optimal values are given in

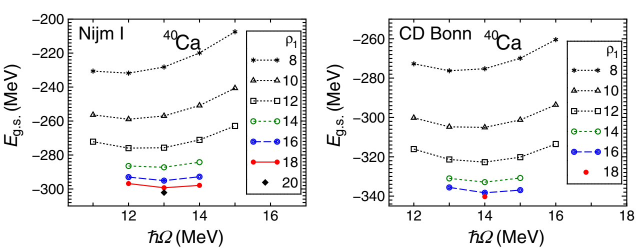

FIG. 3 (color online). Same as Fig. 1, but for ^{40}Ca.

TABLE III. Same as Table I, but for ^{40}Ca.

		Nijm I	CD Bonn	Expt.
^{40}Ca	$E^{(1+2\mathrm{BC})}$	−296.29	−334.34	
	$E^{(3\mathrm{BC})}$	−5.83	−5.92	
	$E_{\mathrm{g.s.}}$	−302.12	−340.27	−342.05
	BE/A	7.55	8.51	8.55

Table III. The results of $E_{\mathrm{g.s.}}$ are less attractive than the experimental value similarly to the case of ^{16}O. However, for CD Bonn, the calculation attains 99.5% of the experimental energy, and the difference between the result and experiment is only 1.78 MeV. This difference is much smaller than that for ^{16}O despite the fact that the absolute value of the ground-state energy of ^{40}Ca is much larger than that of ^{16}O. This fact suggests that the *NNN* force plays a complicated role in the inner (dense) and outer (thin) regions of the nuclei.

In Fig. 4(a), the $\hbar\Omega$ and ρ_1 dependences of the calculated ground-state energies including the 3BC effects of ^{56}Ni are illustrated for CD Bonn. A converging result is seen at $\hbar\Omega = 14$ MeV and $\rho_1 = 18$. However, the energy difference between the two values for $\rho_1 = 16$ and 18 at the energy minima amounts to 7.38 MeV which is somewhat large compared to the case of ^{40}Ca where the difference is 1.97 MeV. The results for the CD-Bonn potential show a regular pattern of convergence (in contrast to the results for N^{3}LO in Fig. 1). In order to estimate the remaining effect of the larger model space, we perform an extrapolation, as given in Refs. [12,13], using the following formula: $E_{\mathrm{g.s.}}(\rho_1) = E_\infty + Ce^{-\gamma\rho_1^2}$, where E_∞, C, and γ are the coefficients determined in the least-squares fitting procedure. We have found that the data points for $\hbar\Omega = 14$ MeV from $\rho_1 = 8$ to 18 are well fitted with this formula. The curve given by the formula is shown in Fig. 4(b). The optimal values of the coefficients are $E_\infty = -473.17$ MeV, $C = -316.06$ MeV, and $\gamma = 1.3148 \times 10^{-2}$. Therefore, the extrapolated ground-state energy for $\rho_1 \to \infty$ becomes $E_{\mathrm{g.s.}}(\rho_1 \to \infty) = E_\infty = -473.17$ MeV. The difference between the extrapolated value and the result for $\rho_1 = 18$ is 3.82 MeV, and thus the result for $\rho_1 = 18$, is considered to be an almost converged value. The

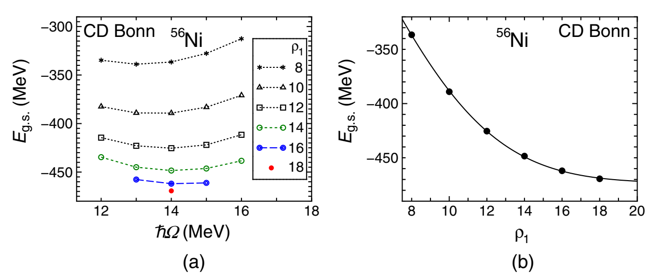

FIG. 4 (color online). (a) Same as Fig. 1, but for ^{56}Ni. (b) The extrapolation curve of $E_{\mathrm{g.s.}}$ of ^{56}Ni. See text for details.

TABLE IV. Same as Table I, but for ^{56}Ni. The results only for the CD-Bonn potential are shown. The extrapolated values for $\rho_1 \to \infty$ are also given.

		$\rho_1 = 18$	$\rho_1 \to \infty$	Expt.
^{56}Ni	$E^{(1+2BC)}$	−452.73	−456.64	
	$E^{(3BC)}$	−16.62	−16.53	
	$E_{g.s.}$	−469.35	−473.17	−483.99
	BE/A	8.38	8.45	8.64

extrapolated value reproduces 97.8% of the experimental ground-state energy.

In Table IV, the optimal value of $\hbar\Omega = 14$ MeV and $\rho_1 = 18$ and the extrapolated one for ^{56}Ni using the CD-Bonn potential are listed. The extrapolation for $E^{(1+2BC)}$ in the same manner has been performed, and its result is also given. It is seen that the 3BC effect of ^{56}Ni is considerably larger than that of ^{40}Ca. This may reflect the difference of the shell closure, namely, $0f_{7/2}$ subshell closed for ^{56}Ni and $1s0d$ major-shell closed for ^{40}Ca.

In summary, we have applied the UMOA to the ground states of the closed-shell nuclei ^{16}O, ^{40}Ca, and ^{56}Ni, and the single-hole states in ^{15}O and ^{15}N. The pf-shell nucleus ^{56}Ni is the heaviest one for which this kind of *ab initio* calculation has been performed. The binding energies including the 3BC effects have been obtained using the Nijm I, the CD Bonn, and the chiral N^{3}LO NN interactions. We have found that the chiral N^{3}LO interaction gives rather large 3BC contribution to the ground-state energy of ^{16}O compared to the other two forces. All results lack the binding energies in reproducing the experimental data. However, the magnitude of the missing energy depends considerably on the interactions employed. The CD-Bonn potential gives quite good results close to the experimental values for all nuclei in the present work. The inclusion of the NNN force is expected to make attractive contributions and compensate for the remaining discrepancies between the results and experiments.

One may compare the present results with recent microscopic calculations [10,23,26–28] using realistic NN forces including the ones used here. Although the present and recent methods give similar results, there still remain some discrepancies. It is an important problem to clarify the origins of the discrepancies in order to develop the microscopic many-body methods.

For a deeper understanding of nuclei, the use of more fundamental forces is of great interest. Recently, a novel NN force from a lattice QCD calculation has been reported, and a more elaborate work of nuclear force is in progress [29]. We will pursue studies using forces based upon the lattice QCD.

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[1] R. Machleidt, Adv. Nucl. Phys. **19**, 189 (1989).
[2] H. Kamada *et al.*, Phys. Rev. C **64**, 044001 (2001).
[3] J. Fujita and H. Miyazawa, Prog. Theor. Phys. **17**, 360 (1957).
[4] S. C. Pieper *et al.*, Phys. Rev. C **64**, 014001 (2001).
[5] S. C. Pieper and R. B. Wiringa, Annu. Rev. Nucl. Part. Sci. **51**, 53 (2001).
[6] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).
[7] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000).
[8] F. Coester, Nucl. Phys. **7**, 421 (1958).
[9] R. J. Bartlett and M. Musiał, Rev. Mod. Phys. **79**, 291 (2007).
[10] G. Hagen *et al.*, Phys. Rev. Lett. **101**, 092502 (2008).
[11] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001 (R) (2003).
[12] K. Suzuki, R. Okamoto, and H. Kumagai, Phys. Rev. C **36**, 804 (1987).
[13] K. Suzuki and R. Okamoto, Prog. Theor. Phys. **92**, 1045 (1994).
[14] S. Fujii, R. Okamoto, and K. Suzuki, Phys. Rev. C **69**, 034328 (2004).
[15] S. Ōkubo, Prog. Theor. Phys. **12**, 603 (1954).
[16] K. Suzuki, Prog. Theor. Phys. **68**, 246 (1982).
[17] N. Barnea, W. Leidemann, and G. Orlandini, Phys. Rev. C **61**, 054001 (2000).
[18] K. Suzuki and S. Y. Lee, Prog. Theor. Phys. **64**, 2091 (1980).
[19] V. G. J. Stoks *et al.*, Phys. Rev. C **49**, 2950 (1994).
[20] R. Machleidt, F. Sammarruca, and Y. Song, Phys. Rev. C **53**, R1483 (1996).
[21] G. Audi and A. H. Wapstra, Nucl. Phys. A **565**, 1 (1993).
[22] P. Navrátil *et al.*, Phys. Rev. Lett. **99**, 042501 (2007).
[23] G. Hagen *et al.*, Phys. Rev. C **80**, 021306(R) (2009).
[24] K. Andō and H. Bandō, Prog. Theor. Phys. **66**, 227 (1981).
[25] S. C. Pieper and V. R. Pandharipande, Phys. Rev. Lett. **70**, 2541 (1993).
[26] L. Coraggio *et al.*, Phys. Rev. C **73**, 014304 (2006).
[27] C. Barbieri, Phys. Lett. B **643**, 268 (2006).
[28] J. R. Gour *et al.*, Phys. Rev. C **74**, 024310 (2006).
[29] N. Ishii, S. Aoki, and T. Hatsuda, Phys. Rev. Lett. **99**, 022001 (2007); N. Ishii, S. Aoki, and T. Hatsuda (private communication).