Ground State of ^{16}O

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A variational method is used to study the ground state of ^{16}O. Expectation values are computed with a cluster expansion for the noncentral correlations in the wave function; the central correlation and exchanges are treated to all orders by Monte Carlo integration. The expansion has good convergence. Results are reported for the Argonne v_{14} two-nucleon and Urbana VII three-nucleon potentials.

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One of the most challenging problems in nuclear theory is the calculation of nuclear properties from realistic nuclear forces, which have large two-body tensor and spin-isospin exchange terms, as well as spin- and isospin-dependent three-nucleon interactions. Ground states of ~ 100 particles interacting via spin-independent forces can be calculated fairly accurately with the variational Monte Carlo (VMC) method.[1] Exact results can be obtained for bosons with the Green's-function Monte Carlo (GFMC) method,[2] and very accurate results may be obtained with either GFMC transient estimates[3] or fixed-node methods[4] for fermions.

Exact calculations for nuclei can only be done at present for the trivial $A=2$ deuteron and, by Faddeev methods,[5] for $A=3$. Recently, Carlson[6] has made exact GFMC calculations of the ^{4}He ground state using only two-nucleon interactions, and there are reliable VMC calculations of ^{4}He with complete interaction models including three-body potentials.[7] These, together with variational calculations of nuclear matter using chain summation methods,[8] are used to determine the parameters of the three-nucleon interaction. However, there have been very few calculations of nuclei having $A > 5$ of comparable accuracy using realistic forces, and none with modern three-nucleon interactions. In this paper we present a new technique for such calculations and report results for ^{16}O.

A significant previous effort was made by Kümmel, Lührmann, and Zabolitsky[9] (KLZ), who studied ^{4}He, ^{16}O, and ^{40}Ca with several interaction models by using the coupled-cluster method, retaining all two- and three-body and parts of four-body cluster contributions. In this approximation, called Faddeev-Brueckner-Hartree-Fock-4, they obtained ground-state energies of -6.0 and -5.0 MeV/nucleon for ^{4}He and ^{16}O with the Reid[10] potential. The experimental values are -7.1 and -8.0 MeV/nucleon. Their result for ^{4}He compares well with the exact value of -6.1 MeV/nucleon obtained with GFMC[6] and -6.0 MeV/nucleon from VMC.[11] Including a model three-nucleon interaction lowered these energies to -8.2 and -7.2 MeV/nucleon, but still left ^{16}O unstable by 1 MeV/nucleon with respect to ^{4}He. It thus appears that the relative binding energies of ^{4}He and ^{16}O provide stringent tests of many-body calculations and models of nucleon forces.

The nuclear Hamiltonian can be written as

$$H=\sum\left(-\frac{\hbar^2}{2m}\right)\nabla_i^2+\sum_{i<j}v_{ij}+\sum_{i<j<k}V_{ijk}\,.$$

In the present work, we use the Argonne v_{14} two-nucleon potential[12] with the Urbana VII three-nucleon potential.[7] Argonne v_{14} contains fourteen operators:

$$v_{ij}=\sum_{p=1-14}v^p(r_{ij})O_{ij}^p\,,$$

$$O_{ij}^p=\{1,\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j,\ \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j,\ \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j,$$
$$S_{ij},\ \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_jS_{ij},\ \mathbf{L}\cdot\mathbf{S},\ \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\,\mathbf{L}\cdot\mathbf{S},\ L^2,$$
$$\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_jL^2,\ \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_jL^2,\ \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_jL^2,$$
$$(\mathbf{L}\cdot\mathbf{S})^2,\ \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j(\mathbf{L}\cdot\mathbf{S})^2\}\,.$$

Urbana VII is a sum of a two-pion exchange term, $V_{ijk}^{2\pi}$, and a phenomenological short-range repulsive term, V_{ijk}^R. The V_{ijk}^R is essential for obtaining reasonable nuclear-matter density.

We use the following variational wave function:

$$|\Psi\rangle=\left[S\prod_{i<j}(1+U_{ij}^{(2)})\right]\left(1+\sum_{i<j<k}U_{ijk}^{(3)}\right)|\Psi_J\rangle\,,$$

where

$$|\Psi_J\rangle=\prod_{i<j}f^c(r_{ij})\,|\Phi\rangle\,.$$

Here f^c is a central pair correlation, and Φ is an independent-particle antisymmetric wave function determined variationally. The noncentral two-body correlations, induced by the noncentral part of v_{ij}, are essential for obtaining bound nuclei. We use the truncated set

$$U_{ij}^{(2)}=\sum_{p=2-8}u^p(r_{ij})O_{ij}^p\,.$$

The $f^c(r)$ and $u^p(r)$ are determined as for nuclear

matter[8] with the density and other parameters treated variationally. The $U_{ijk}^{(3)}$ represent correlations induced by the V_{ijk} and contain the same operators as V_{ijk}; they reduce the energy by $\sim 7\%$, and their form is discussed elsewhere.[11]

The $U_{ij}^{(2)}$ do not commute with $U_{ik}^{(2)}$, and hence the product of $(1+U_{ij}^{(2)})$ in Ψ is symmetrized. An independent-pair wave function, $\Psi_{\rm IP}$, is obtained when the products of all noncommuting $U_{ij}^{(2)}$ are omitted from Ψ. Carlson and Kalos[13] made a VMC calculation for ^{16}O with $\Psi_{\rm IP}$ by sampling over the $U_{ij}^{(2)}$ in the expectation value. The Monte Carlo sampling errors in their calculation are large, and they worked with semirealistic v_{ij} without V_{ijk} in the Hamiltonian.

The Ψ has $N=2^A\binom{A}{Z}$ spin-isospin components $\psi_n(\mathbf{r}_1,\ldots,\mathbf{r}_A)$, where ψ_n gives the amplitude of the nth spin-isospin state in which each particle has definite σ_z and τ_z. For example, $N=24$, 96, 1280, and 843 448 320 for ^{3}H, ^{4}He, ^{6}Li, and ^{16}O. For central forces one can assign a definite state to each particle and use a single-component $\Psi(r_1,\ldots,r_A)$. However, the strong noncentral components of the nuclear force exchange or flip spins and isospins and thus make such a simplification impossible. The VMC[7] and GFMC[6] calculations of few-body nuclei use all these components and thus are impractical for nuclei having $A>8$.

However, it is possible to evaluate expectation values in Ψ_J of operators having spins and isospins of several particles by using the light-nuclei Monte Carlo methods. Hence, we expand the $\langle H\rangle$ using a cluster expansion[14] only for the $\prod(1+U^{(2)})$ and $(1+\sum U^{(3)})$. The complete product of the central correlations $f^c(r_{ij})$ and the antisymmetry of Ψ are exactly treated in all contributions. In fact, the present n-body contributions contain up to A-body cluster terms of the conventional diagrammatic expansion[14,15] in powers of f^c-1 and the exchanges. This means that each order of the expansion requires the computation of A-body expectation values which are done by Monte Carlo integration. For example, the two-body cluster contribution to $\langle v_{ij}\rangle$ is $n_{ij}/(1+d_{ij})$, where

$$n_{ij}=\langle\Psi_J\,|\,(1+U_{ij}^{(2)})^\dagger v_{ij}(1+U_{ij}^{(2)})\,|\,\Psi_J\rangle\,,$$

and

$$d_{ij}=\langle\Psi_J\,|\,(1+U_{ij}^{(2)})^\dagger(1+U_{ij}^{(2)})\,|\,\Psi_J\rangle-1\,.$$

Table I shows the convergence of the cluster expansion up to the four-body cluster level using our optimal set of variational parameters. The column "sum 1-4" gives the sum of the calculated cluster contributions, while the "sum 1-16" column shows an estimate by extrapolation from the three- and four-body cluster values of the complete sum. This was obtained as the average of the extrapolations $c_3/(1-x)$ and $c_3\exp(x)$, where $x=c_4/c_3$. Here c_3 and c_4 are, respectively, the three- and four-body cluster values of individual components of the kinetic and potential energies. The two methods of extrapolation give total $E/A=-7.11$ and -6.94 MeV, suggesting that the error in the averaged extrapolation is of the order of 0.1 MeV/nucleon. The last column gives the corresponding expectation values for ^{4}He using a similar wave function.[11]

The first row of Table I gives the kinetic energy from which the cm energy is removed by evaluating $\langle(\sum\nabla_i)^2\rangle$. The second row shows the expectation value of the $p=1$-6 terms of v_{ij} and the Coulomb potential. We see that the expansion converges rapidly for the kinetic and two-body potential energies. The next row shows the expansion of $\langle V_{ijk}^{2\pi}\rangle$, for which the first contribution is the three-body cluster. The convergence is not very rapid, and the extrapolated sum is significantly different from the sum of the three- and four-body cluster values. Verifying the convergence of $\langle V_{ijk}^{2\pi}\rangle$ by computing the five-body cluster contribution appears feasible. The convergence is good for $\langle V_{ijk}^{R}\rangle$ shown in the fourth row.

At present we cannot include the $\mathbf{L}\cdot\mathbf{S}$ parts of $U^{(2)}$ ($p=7,8$), nor the $7\le p\le 14$ parts of v_{ij} in the three- and four-body clusters. Therefore the first four rows show results for just the $u^{p=1\text{-}6}$ and $U^{(3)}$ correlations. The fifth row shows the contributions of terms that contain $p=7$ and 8 parts of $U^{(2)}$ and/or the $7\le p\le 14$ parts of v_{ij} to the two-body cluster. Many-body contributions of this small term are neglected. The various terms have rather similar values for ^{4}He and ^{16}O except the last one. In ^{4}He the main contribution to the $\mathbf{L}\cdot\mathbf{S}$ interactions is from $^3D_1$ states where it is repulsive; in

TABLE I. Convergence of the cluster expansion for the ground-state energy of ^{16}O. The entries are in MeV/nucleon. The numbers and sums have been rounded and hence may not add up.

Term	Cluster contribution: One body	Two body	Three body	Four body	Sum 1-4	Sum 1-16	^{4}He (Ref. 11)
T	18.2 ± 0.2	13.9 ± 0.2	−1.8 ± 0.2	0.2 ± 0.2	30.5 ± 0.4	30.5	27.5
$v_{ij}^{p=1\text{-}6}$ + Coulomb		−41.3 ± 0.3	6.4 ± 0.2	−0.5 ± 0.3	−35.4 ± 0.3	−35.4	−33.0
$V_{ijk}^{2\pi}$			−4.7 ± 0.1	1.9 ± 0.1	−2.8 ± 0.1	−3.2	−3.2
V_{ijk}^{R}			1.9 ± 0.1	−0.4 ± 0.1	1.5 ± 0.1	1.6	1.0
$u^{p=7,8}+v_{ij}^{p=7\text{-}14}$		−0.3 ± 0.1			−0.3	−0.3	0.7
Total	18.2 ± 0.2	−27.8 ± 0.2	1.8 ± 0.2	1.2 ± 0.2	−6.5 ± 0.2	−7.0	−7.0

^{16}O the P waves give attractive $\mathbf{L}\cdot\mathbf{S}$ contributions.

The estimated upper bound for the energy of ^{16}O is -7.0 ± 0.3 MeV/nucleon, considerably above the experimental value of -8.0 MeV/nucleon. VMC calculations of ^{4}He with the present Ψ also give[11] $E/A=-7.0$ MeV. Thus, ^{16}O and ^{4}He are about equally bound in these calculations. It is known[7] that the energy of ^{4}He can be lowered by including three-body terms in $U_{ij}^{(2)}$:

$$u^p(r_{ij})\rightarrow u^p(r_{ij})\prod_{k\neq i,j} f_3^p(r_{ij},r_{ik},r_{ki})\,.$$

Such terms are not considered in the present calculation of ^{16}O. The f_3^p correlations and other improvements result[11] in $E/A=-7.47\pm0.06$ MeV for ^{4}He. Attempts to include such terms in the ^{16}O calculation are in progress. We hope that they have a bigger effect on ^{16}O and help to stabilize it. Note that the present interaction model is not realistic since it overbinds ^{4}He. Thus, it is necessary to improve upon both the interaction model and the wave function to get better results.

A calculation without the V_{ijk} requires a separate optimization of the variational parameters and needs no $U_{ijk}^{(3)}$. We find $E/A=-5.8\pm0.3$ MeV for ^{16}O with just the Argonne v_{14} interaction, and so the V_{ijk} increases the binding by 1.2 MeV/nucleon. The corresponding energy for ^{4}He (again with a similar wave function) is -5.6 MeV/nucleon. The KLZ calculation of ^{16}O with the Reid potential results in 0.8 MeV/nucleon less binding than our Argonne v_{14} result. This is consistent with nuclear-matter calculations for the two potentials.[16]

Figure 1 shows the cluster expansion of the charge density. This was computed by folding the Iachello-Jackson-Landé nucleon form factors[17] with the point-nucleon densities computed from the optimum wave function (the results are very insensitive to the choice of the nucleon form factors). Our rms charge radius (computed up to four-body clusters) of 2.62 fm is in reasonable agreement with the experimental average of 2.73 fm.[18]

Figure 2 shows the longitudinal structures functions $S_L(k)$ computed as described in Ref. 19. We note the following: (1) The structure function obtained with the full wave function (solid curve) is substantially different from the mean-field result (dashed curve) which was generated by making a mean-field fit to the computed $\rho(r)$.[19,20] From the size of the experimental ^{12}C error bars,[21] the correlation effects in $S_L(k)$ at small k appear measurable. (2) We find that most of these correlation effects are obtained with just Ψ_J; the noncentral correlations have little net effect on S_L. (3) Contrary to the expectation of Refs. 19 and 22, the S_L for ^{16}O is not an interpolation of those for ^{4}He (dash-dotted curve) and nuclear matter (dotted curve) but is substantially larger for intermediate momentum transfers. We have verified that in mean-field calculations based on experimental density profiles for ^{4}He, ^{16}O, and ^{40}Ca, both the ^{16}O and ^{40}Ca S_L are not interpolations of the results for ^{4}He and Fermi-gas nuclear matter.

In conclusion, a cluster expansion in terms of the noncentral correlations in the wave function appears to be a practical method for computing the ground-state energies of nuclei. The CPU time needed to achieve acceptable statistical errors is reasonable but not small; the calculation in Table I contains 4500 samples and took 16.3 CPU hours on one processor of a Cray-2S running at an average speed of 125 MFLOPS. An order of magnitude more time was spent in variational searches.

Further improvements in the form of the variational wave function and the interaction model are necessary to obtain accurate ground-state energies for few-body and light nuclei. Work on both of these points is in progress. A complete description of this calculation will be published elsewhere.

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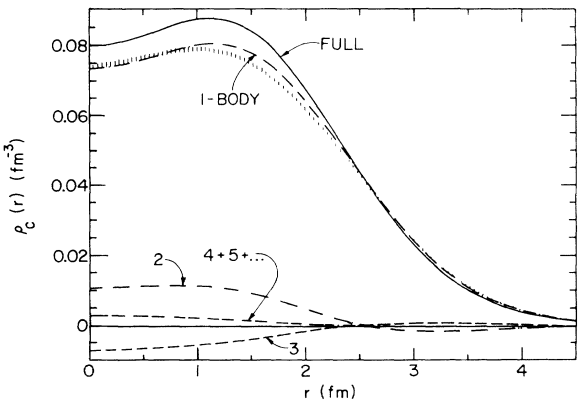

FIG. 1. Charge-density distribution of ^{16}O. The curves show the indicated cluster contribution. The solid curve is the complete result. The shaded area is the experimentally determined density (Fourier-Bessel and sum-of-Gaussians parametrizations as reported in Ref. 18).

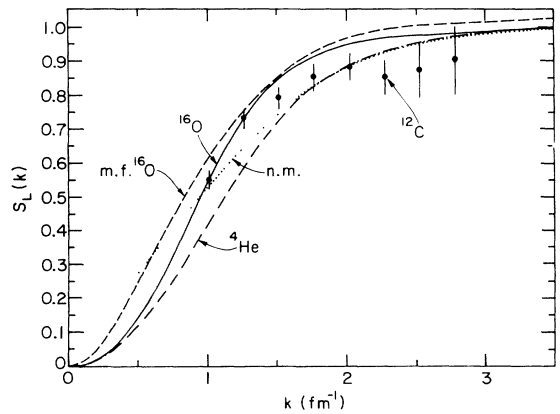

FIG. 2. Longitudinal structure functions. See the text for a description of the curves. The data (Ref. 21) are for ^{12}C with theoretically determined high-energy tail corrections (Ref. 22).

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