CALCULATIONS OF THE GROUND STATE OF ^{16}O

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Steven C. Pieper

Physics Division
Argonne National Laboratory
Argonne, IL 60439-4843

One of the central problems in nuclear physics is the description of nuclei as systems of nucleons interacting via realistic potentials. There are two main aspects of this problem: 1) specification of the Hamiltonian, and 2) calculation of the ground (or excited) states of nuclei with the given interaction. Realistic interactions must contain both two- and three-nucleon potentials and these potentials have a complicated non-central operator structure consisting, for example, of spin, isospin and tensor dependences. This structure results in formidable many-body problems in the computation of the ground states of nuclei.

At present, reliable solutions of the Faddeev equations for the A=3 nuclei with such interactions are routine.[1] Recently, Carlson[2] has made an essentially exact GFMC calculation of the ^{4}He ground state using just a two-nucleon interaction, and there are reliable variational calculations[3] for more complete potential models. Nuclear matter calculations can also be made with reasonable reliability.[4,5] However, there have been very few calculations of nuclei with A>5 using realistic interactions, and none with a modern three-nucleon interaction. In the present paper I present a new technique for variational calculations for such nuclei and apply it to the ground state of ^{16}O. The work reported was done in collaboration with V. R. Pandharipande (University of Illinois, Urbana), and R. B. Wiringa (Argonne National Laboratory).

POTENTIALS AND WAVE FUNCTION

We use the Argonne v_{14} (AV14) two-nucleon potential[6] with the Urbana VII (UVII) three-nucleon potential.[3] Variational wave functions obtained with these interactions give remarkably good agreement with the experimental data for the charge and magnetic form factors of the A=3 and A=4 nuclei.[7] The AV14 contains 13 non-central operator terms and has been fit to the np scattering and bound-state data. The UVII contains the long-range two-pion exchange three-nucleon potential and a phenomenological short-range repulsion. Its coupling constants were adjusted to give a fit to the binding energies of

A=3 and A=4 nuclei and nuclear matter in variational calculations. More recent variational (and Fadeev for ^{3}H) calculations show that these potentials somewhat overbind the light nuclei.[8]

We use the following variational wave function for the ground state of a closed-shell nucleus with N=Z=A/2:

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

where

$$U_{ij}^{(2)} = \sum_{p=2}^{8} u_p(r_{ij}) \, O_{ij}^{(p)} \ , \tag{2}$$

$$u_p(r_{ij}) = f_p(r_{ij})/f_c(r_{ij}) \ , \tag{3}$$

$$U_{ijk}^{(3)} = - \epsilon_1 \tilde{V}_{ijk}^{FM} - \epsilon_2 \tilde{V}_{ijk}^{R} \ , \tag{4}$$

and

$$|\Psi_J\rangle = \prod_{i<j}^{A} f_c(r_i) |\Phi\rangle \ . \tag{5}$$

Here Π designates a symmetrized product and $|\Phi\rangle$ is a completely antisymmetric sum of products of four Slater determinants for spin-up protons, spin-down protons, spin-up neutrons, and spin-down neutrons. The wave functions in the Slater determinants are the solutions of a Woods-Saxon potential well. The sum in Eq. (3) is a sum over the first eight operators (central, $\tau_1 \cdot \tau_2$, $\sigma_1 \cdot \sigma_2$, $\sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2$, S_{12}, $S_{12} \sigma_1 \cdot \sigma_2$, L•S, and L•S$\sigma_1 \cdot \sigma_2$) of the v_{14} interaction. The $f_p(r_{ij})$ and $f_c(r_{ij})$ are the solutions of coupled Euler-Lagrange equations constructed to minimize the two-body cluster energy of nucleon matter at a specific density; see Ref. 5. The $\tilde{V}_{ijk}^{FM}$ and $\tilde{V}_{ijk}^{R}$ are the two-pion and repulsive parts of UVII (see Ref. 3), except that the cut-off parameter, b, is treated as a variational parameter. The wave function Ψ contains as variational parameters: 1) the parameters of the single-particle well used to construct Φ, 2) the nuclear-matter density and the parameters used to find f_c and the f_p, and 3) the b, ϵ_1, and ϵ_2 used in $U_{ijk}^{(3)}$.

CLUSTER EXPANSION

For a given set of variational parameters, we must evaluate $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ where the Hamiltonian is

$$H = \sum_{i=1}^{A} \left(-\frac{\hbar^2}{2m}\right) \nabla_i^2 + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} V_{ijk} \ . \tag{6}$$

In addition we will need the expectation value of other operators such as the density. The wave function is a vector in spin-isospin space. Because of the tensor correlations, all 2^A spin components are non-zero. Charge conservation limits the number of isospin components to A!/(Z!(A-Z)!). In the VMC calculations[3] of few-body nuclei this complete vector is used. Each term of the symmetrized product of pair operators contains A(A-1)/2 factors and the sum is sampled instead of being completely evaluated. The U_{ijk} requires some 9A(A-1)(A-2)/6 tensor pair operators. The kinetic energy is computed by differences which requires 6A evaluations of the wave function (additional evaluations are required for the L^2 and $(L\cdot S)^2$ potentials). Table 1 summarizes these numbers and shows the total relative computer effort needed to evaluate the kinetic energy (the dominant part of the calculation) at one configuration of the particles.

Table 1. Effort required to compute the kinetic energy of one configuration of particles using the complete spin-isospin vector.

Nucleus	Vector Length	Pair Operations	Kinetic Energy Evaluations	Total Effort
^{3}He	24	12	18	5.2×10^3
^{4}He	96	42	24	9.7×10^4
^{6}Li	1,280	195	36	9.0×10^6
^{8}He	7,168	532	48	1.8×10^8
^{12}C	3,784,704	2,046	72	5.6×10^{11}
^{16}O	8.4×10^8	5,160	96	4.2×10^{14}
^{40}Ca	1.5×10^{23}	89,700	240	3.3×10^{30}

The few-body method outlined above clearly becomes rapidly impractical for heavier nuclei. Therefore, we use a cluster expansion in terms of the operator being evaluated and the non-central operators in Ψ to compute expectation values. For example, consider the two-body potential:

$$\frac{\langle\Psi|\sum_{i<j} v_{ij}\,|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\sum_{i<j} n_{ij} + \sum_{i<j<k} n_{ijk} + \cdots + n_{12\cdots A}}{1 + \sum_{i<j} d_{ij} + \sum_{i<j<k} d_{ijk} + \cdots + d_{12\cdots A}}\,, \tag{7}$$

$$= \sum_{i<j} e_{ij} + \sum_{i<j<k} e_{ijk} + \cdots + e_{12\cdots A}\,. \tag{8}$$

Here

$$n_{ij} = \int d^3r_1 \ldots d^3r_A \; \Psi_J^\dagger(r_1,\ldots,r_A)(1 + U_{ij}^{(2)})^\dagger \; V_{ij}^{(2)}$$

$$(1 + U_{ij}^{(2)}) \; \Psi_J(r_1,\ldots,r_A) / \int d^3r_1 \ldots d^3r_a |\Psi_J|^2 \; , \tag{9}$$

$$n_{ijk} = \int d^3r_1 \ldots d^3r_A \; \Psi_J^\dagger (1 + U_{ijk}^{(3)})^\dagger \; [S(1 + U_{ij}^{(2)})(1 + U_{ik}^{(2)})(1 + U_{jk}^{(2)})]^\dagger$$

$$[V_{ij}^{(2)} + V_{ik}^{(2)} + V_{jk}^{(2)}] [S(1 + U_{ij}^{(2)})(1 + U_{ik}^{(2)})(1 + U_{jk}^{(2)})](1 + U_{ijk}^{(3)})\Psi_J$$

$$/ \int d^3r_1 \ldots d^3r_A |\Psi_J|^2 - n_{ij} - n_{ik} - n_{jk} \; , \tag{10}$$

and so forth, and S again indicates a symmetrized product. The equations for the d_{ij}, d_{ijk}, ... are similar to those for the n's except there are no potential operators and 1 (corresponding to zero'th order) is subtracted from d_{ij}.

We could use Eq. (7) as a cluster expansion but it converges very slowly or even diverges. Instead, we define the e_{ij}, e_{ijk}, ... of Eq. (8) by multiplying both sides by the denominator of Eq. (7) and collecting all terms involving ij, ijk, etc. We also observe from Eqs. (7-10) that the n's and d's do not depend on the specific values of i, j, k, ..., so we can write

$$n_{ij} = n_2 \quad , \quad d_{ij} = d_2 \; , \tag{11}$$

$$n_{ijk} = n_3 \quad , \quad d_{ijk} = d_3 \; , \tag{12}$$

etc. We then have

$$e_{ij} = e_2 = n_2/(1 + d_2) \quad , \tag{13}$$

$$e_{ijk} = e_3 = \frac{n_3 - (6d_2 + 3d_3)e_2}{1 + 3d_2 + d_3} \quad , \tag{14}$$

etc. As we will show, the series (8) converges well.

The complete product of central correlations and the complete single-particle part of the wave function appears in each order of our cluster expansion; thus, Eqs. (9-10) define 3A-dimensional integrals. These are evaluated in a Metropolis random walk. Ideally, the random walk would be controlled by $|\Psi_J|^2$, however generating the completely antisymmetric Ψ_J is prohibitive. Instead we compute expectation values with the antisymmetric Ψ_J on the left side and a mixed symmetry Ψ_J that contains just a single product of Slater determinants in Φ on the right side. The symmetrized product of $(1 + U_{ij})$ is also sampled.

Table 2 shows the computer effort required to compute the energy of one configuration at different levels of the cluster expansion. The column labelled "Pair Operations" contains all pair operations required for the wave function and kinetic and potential energy; it is smaller than the product of columns 3 and 4 of Table 1 because of simplifications realized by having U_{ijk} act on a ϕ_J that has just one component. The total of 41,000 for a four-body cluster calculation of ^{16}O can be compared to the value 4.2×10^{14} required for ^{16}O by the few-body method.

Table 2. Effort to compute the energy of one configuration for ^{16}O in the cluster expansion.

Cluster Order	Clusters in Expansion ^4He	^{16}O	^{40}Ca	Average Vector Length	Pair Operations	^{16}O Effort
2	6	120	780	6	9	9
3	4	560	9880	21	88	1350
4	1	1820	91,390	74	236	39,600
5	-	4368	658,008	272	514	711,000

The computer program used for the calculations reported here has been extensively tested by internal checks in which the same quantity is computed in two different ways and by comparisons of calculations of ^4He with the results of our few-nucleon program that does not use a cluster expansion.

RESULTS

Table 3 shows the convergence of the cluster expansion up to the four-body cluster level using our optimal set of variational parameters. The last column shows an estimate by extrapolation from the three- and four-body cluster values of the complete 16-body cluster value. This was obtained as the average of the extrapolations $e_3/(1-x)$ and $e_3\exp(x)$ where $x=e_4/e_3$. Here e_3 and e_4 are respectively the three-body and four-body cluster values of individual components of the kinetic and potential energies. This procedure was tested by extrapolating the two-body and three-body results and comparing them to the four-body term; the extrapolation appears to have less than 25% error.

The first row of Table 3 gives the kinetic energy (with c.m. energy removed). At present we cannot include the L•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 second row shows results for the truncated f_6, v_6 calculation (including the Coulomb potential). The $U^{(3)}$ is included in the three- and four-body cluster results. We see that the expansion converges rapidly for the kinetic and two-body potential energies. The next row shows the expansion of the three-body potential, for which the first contribution is to the three-body cluster. Here the four-body cluster makes a significant contribution and the

extrapolated value is significantly different from the sum of the three- and four-body cluster values. The fourth row shows the two-body cluster value for the combined effect of the p=7 and 8 parts of $U^{(2)}$ and the $7 \le p \le 14$ parts of v_{ij}. This small contribution is not extrapolated.

Table 3. Convergence of the cluster expansion for the ground-state energy of ^{16}O. The entries are in MeV/A.

Term	Cluster Expansion Term				Sum	Extrap.
	1-body	2-body	3-body	4-body		
T	18.2±0.2	13.9±0.2	-1.8±0.2	0.2±0.2	30.5±0.4	30.5
$v_{ij}^{p=1-6, C}$		-41.3±0.3	6.4±0.2	-0.5±0.3	-35.4±0.3	-35.4
V_{ijk}			-2.8±0.1	1.6±0.1	-1.2±0.1	-1.7
$U^{(2)}_{p=7,8}, v_{ij}^{p=7,14}$		-0.3±0.1			-0.3	-0.3
Total	18.2±0.2	-27.8±0.2	1.8±0.2	1.2±0.2	-6.5±0.2	-7.0

Our estimated (by extrapolation) upper bound for the ground-state energy of ^{16}O is -7.0±0.3 MeV/A where the error includes both the Monte Carlo statistical error and an estimate (0.1) of the extrapolation uncertainty. The experimental value is -7.98 MeV/A. This upper bound is the same as our upper bound for the energy of ^4He using the same hamiltonian and a similar wave function; a better wave function gives[8]: -7.47±0.06 MeV/A. Thus in this calculation, we fail to demonstrate that ^{16}O is stable against decay into four alpha particles. It is not clear if this failure is due to inadequacies in the final wave function or in the hamiltonian, however because the wave functions have similar structure, it is reasonable to assume that part of the problem is due to the hamiltonian.

Previous calculations of ^{16}O have also failed to obtain stability against breakup into alpha particles. Kümmel, Lührmann and Zabolitzky[9] used the coupled-cluster method to compute ^4He, ^{16}O, and ^{40}Ca with several interaction models. They retained all two- and three-cluster contributions and some of the four-cluster terms. Their binding energies for the Reid potential are -6.0 and -5.0 MeV/A for ^4He and ^{16}O. More recently, Carlson and Kalos[10] made a VMC calculation for ^{16}O using a truncated Reid potential. Their wave function is of the same form as ours except that only products of commuting $U_{ij}^{(2)}$ are retained (independent-pair wave function) and there is no $U^{(3)}$. They have rather large sampling errors and obtain an E/A consistent with the E/A for ^4He using the same interaction.

Figure 1 shows the cluster expansion of the charge density. This was computed by folding the IJL nucleon form factors[11] (the results are very insensitive to the choice of form factor) with the point nucleon densities computed from the trial wave function (the present wave function has identical proton and neutron distributions). The dash-dot curve is obtained with $|\Psi_J|^2$, and the solid with the complete wave function. The dash-dot and dashed curves show respectively the two- and three-body cluster contributions. Because of large sampling errors, we used the cluster expansion only up to three-body clusters and extrapolated to obtain the higher contributions; this contribution is shown as the dash-dash-dot curve. For $r<1.5$ fm, the sampling errors are $\lesssim 0.05$ fm^{-3}; for larger radii they rapidly decrease. The shaded region is the experimental charge density.[12] Our rms charge radius (computed up to four-body clusters) of 2.62 fm is in reasonable agreement with the experimental average[12] of 2.73 fm.

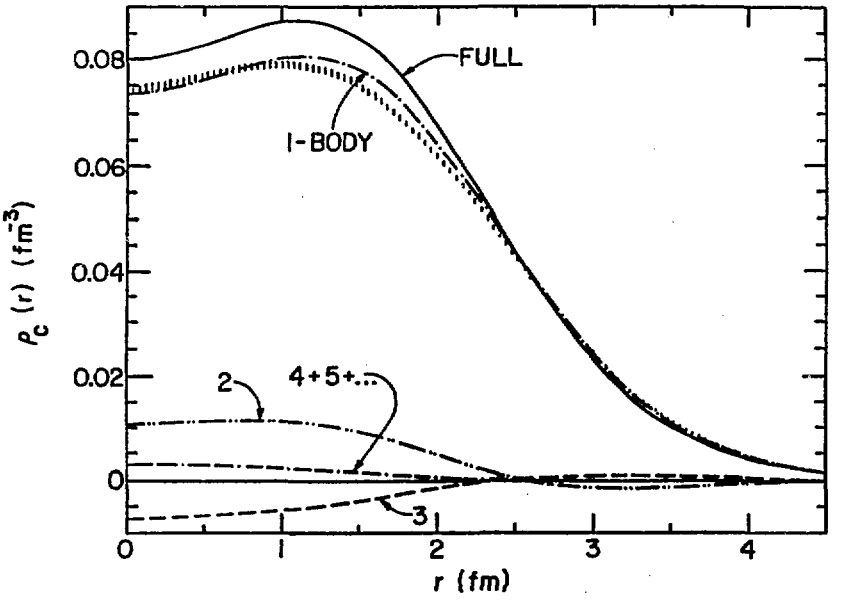

Fig. 1. Charge-density distribution of ^{16}O.

Figure 2 shows the longitudinal structure functions, $S_L(k)$, computed as described in Ref. 13. There are several interesting features of our calculation of $S_L(k)$: 1) The structure function obtained with the full wave function (solid curve) is substantially different from the mean-field result (short dashes) which was generated by making a mean-field fit to the computed $\rho(r)$ in Fig. 1. From the size of the experimental ^{12}C error bars, it appears possible to see "dynamic" correlation effects in $S_L(k)$ for $k\lesssim 1$ fm^{-1}. 2) We find that most of these "dynamic" effects are obtained with just the central correlations (Ψ_J); the converged non-central correlations have little total effect on S_L. 3) Contrary to the expectation of Refs. 13 and 14, the S_L for ^{16}O is not an interpolation of those for ^{4}He (dash dot) and nuclear matter (dotted) but is substantially larger for intermediate momentum transfer. We have also demonstrated this for 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.

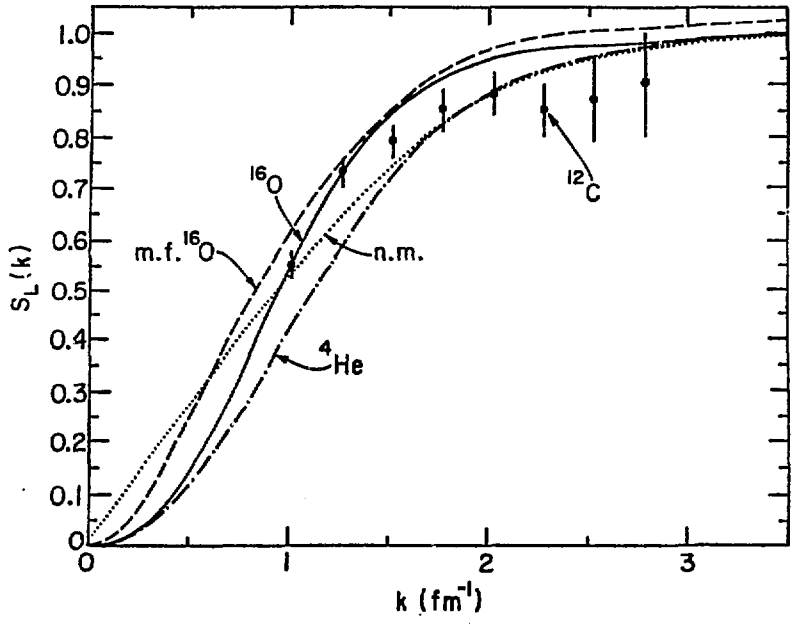

Fig. 2. Longitudinal structure functions. The data[15] are for ^{12}C with a theoretical correction.[14]

CONCLUSION

A cluster expansion in terms of the non-central terms of the wave function is a practical method for computing the ground-state energies of nuclei. The convergence is good, with the four-body clusters really being needed only for the expectation value of the three-body potential. The CPU time need to achieve acceptable statistical errors in reasonable (but not small--the calculation in Table I contains 4,500 samples and took 16.3 CPU hours on a Cray-2S running at an average speed of 125 MFLOPS).

Our upper bound for the ^{16}O ground-state energy fails to show that ^{16}O is stable against decay into four alpha particles. We can assume that further improvements to the form of the wave function will somewhat lower the bound, but it appears that some adjustment of the Urbana VII three-nucleon potential will be necessary to produce accurate ground-state energies for few-body and light nuclei. Work on both of these points is in progress. The longitudinal structure function obtained in this calculation shows significant effects due to dynamical correlations.

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