Cluster Expansion Method in Light Nuclei*

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The convergence of the Van Kampen cluster expansion for evaluating the binding energies of light nuclei using a hard-core potential has been studied for different forms of the correlation function f. A Jastrow-type trial function was used with a Slater determinant of harmonic-oscillator wave functions. The variational calculations were performed on H^3 and He^4. For H^3, where all terms in the expansion were included, good convergence was obtained and the binding energy was in good agreement with the results of the Monte Carlo calculation of Tang *et al.*, indicating a good trial function. In the case of He^4, the variation with all terms up to and including three-particle correlation gave a binding energy in agreement with the Monte Carlo results and the same convergence as in H^3. In all the calculations, no subsidiary conditions on the correlation function $f(r)$ were necessary, provided the contribution to the energy from three-particle correlation was included in the variation. Also, the contribution from four-particle correlation was found in all cases to be very small.

I. INTRODUCTION

RECENT Hartree-Fock calculations[1] using the Tabakin potential[2] have given too small a binding energy for the ground state of nuclei, indicating that one may have to go beyond a simple determinantal wave function and introduce correlations into the wave function if one expects to obtain the right binding energy of nuclei starting from a realistic nucleon-nucleon interaction. This is also clear from the fact when the contributions to the energy from second-order perturbation theory[3] were included the results improved appreciably. In the case when the nucleon-nucleon potential is local with short-range repulsion, one has to include two-particle correlation by solving the Bethe-Goldstone equations to obtain an effective interaction which can be used in a Hartree-Fock calculation. This introduces a double self-consistency problem which in general is difficult to solve. In fact, even for nonlocal separable potentials such as that of Tabakin, the difference between the matrix elements of the interaction V and the G matrix is appreciable in nuclear matter,[4] indicating the necessity for obtaining an effective interaction first, and then performing the Hartree-Fock calculation.

An alternative approach, which can both handle the short-range repulsion and at the same time include the correlation in the wave function, is to use a Jastrow-type[5] trial wave function in a variational calculation. This introduces multidimensional integrals which are usually handled by performing a cluster expansion in the energy and retaining the first few terms of the series in the variation. Such a cluster expansion was developed by Iwamoto and Yamada,[6] and used by Yamada and Ohshima[7] in nuclear matter and by Dabrowski[8] in O^{16}. More recently, Clark and Westhaus[9] have generalized the Iwamoto-Yamada expansion and applied the method to Λ-particle binding in nuclear matter[10] and to other systems.[11] In most of the above calculations it was found necessary to put subsidiary conditions on the trial function to guarantee the convergence of the variational calculation. Other cluster expansion have been proposed by Aviles,[12] and by Hartogh and Tolhoek.[13] All the above cluster expansions as well as the one used in this investigation have been recently discussed and compared by Clark and Westhaus.[14]

In the present investigation we study the use of the Van Kampen cluster expansion[15] in calculating the binding energy of light nuclei.[16] In this case, the nth term of the expansion gives the contribution to the binding energy from n-particle correlation. Thus, for a system of A particles, there are A terms in the series for the energy. In using the Van Kampen ex-

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[13] C. D. Hartogh and H. A. Tolhoek, Physica **24**, 721 (1958); **24**, 875 (1958); **24**, 896 (1958).

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[15] N. G. Van Kampen, Physica **27**, 783 (1961).

[16] The Van Kampen cluster expansion was first applied to solid helium by L. H. Nosanow, Phys. Rev. **146**, 120 (1966).

pansion we find that in most cases considered no subsidiary conditions on the trial function are necessary to guarantee convergence in the variation, provided the contributions due to three-particle correlation are included in the variation. Furthermore, by considering systems such as H^3 and He^4, where all the terms in the series can be calculated, we can study the convergence of the series for different forms of the trial function. Such a study can be helpful as a guide in choosing the form of the trial function in going to heavier nuclei.

In Sec. II, we present the formulation of the Van Kampen cluster expansion for finite nuclei,[17] and discuss some of the general properties the wave function has to satisfy. In Sec. III we discuss the results for H^3 and He^4 and study the convergence of the expansion for different forms of the trial wave function. A comparison of the results obtained here with those obtained by Tang *et al.* using a Monte Carlo method[18] will be a test of the convergence of the expansion. Finally, in Sec. IV we present some concluding remarks regarding the choice of the trial function and the convergence of the series. We also discuss the possible extension of the present method to heavier nuclei.

II. FORMULATION

We consider a system of A interacting nucleons of mass m with the Hamiltonian

$$H=-\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2+\sum_{i<j=1}^{A}V(x_i,x_j), \tag{1}$$

where x_i stands for the space coordinate $\mathbf{r}_i$ and the spin isotopic-spin coordinates σ_i and τ_i of the ith nucleon. The potential $V(x_i,x_j)$ is the nucleon-nucleon potential obtained from the two-body data. In the present investigation we restrict ourselves to local potentials which have a hard repulsive core.

An upper bound on the ground-state energy of the system is obtained by minimizing the expectation value of the Hamiltonian with respect to a trial function $\Psi(x_1,\cdots,x_A)$. Because of the presence of the hard-core potential in the Hamiltonian, the choice of $\Psi(x_1\cdots x_A)$ must be such that when the distance between two nucleons $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$ is less than the core radius r_c the function $\Psi(x_1\cdots x_A)$ is zero. One such a trial function proposed by Jastrow[5] is of the form

$$\Psi(x_1\cdots x_A)=\Phi(x_1\cdots x_A)\prod_{i<j=1}^{A}f(r_{ij})$$
$$=\Phi(x_1\cdots x_A)F(\mathbf{r}_1\cdots\mathbf{r}_A), \tag{2}$$

where the correlation function $f(r_{ij})$ has the property of being an even function under the exchange of particles i and j and is always positive. Since the correlation function $f(r_{ij})$ was introduced to take care of the hard core in the potential it has to satisfy the following conditions:

$$f(r_{ij})=0, \qquad r_{ij}<r_c$$
$$f(r_{ij})\to 1, \qquad r_{ij}\gg r_c. \tag{3}$$

The wave function $\Phi(x_1\cdots x_A)$ is a model function that possesses all the symmetry properties of the system such as rotational symmetry for finite systems and total antisymmetry in the case of Fermi systems. In the present investigation, we take $\Phi(x_1\cdots x_A)$ to be a determinant of single particle wave functions $\phi_{\gamma i}(x_i)$,[19] i.e.,

$$\Phi(x_1,x_2,\cdots,x_A)=(1/\sqrt{A!})\det[\phi_{\gamma i}(x_1)\cdots\phi_{\gamma A}(x_A)], \tag{4}$$

where the single-particle wave function $\phi_{\gamma i}$ gives a reasonable description of the long-range behavior of the wave function.[20] As we will see, if $\phi_{\gamma i}$ does not have the right asymptotic behavior, then the correlation function $f(r)$ will tend to correct for the discrepancy in ϕ_γ, leading to large contribution from the higher cluster terms. One possible choice for the model function $\Phi(x_1\cdots x_A)$ is the Hartree-Fock wave function for the ground-state of the system.

Using the above trial function, the expectation value of the Hamiltonian is given by

$$E=\frac{\int\Phi^*(x_1\cdots x_A)F(\mathbf{r}_1\cdots\mathbf{r}_A)\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2+\sum_{i<j=1}^{A}V(x_i,x_j)\right]F(\mathbf{r}_1\cdots\mathbf{r}_A)\Phi(x_1\cdots x_A)\prod_{i=1}^{A}dx_i}{\int\Phi^*(x_1\cdots x_A)F^2(\mathbf{r}_1\cdots\mathbf{r}_A)\Phi(x_1\cdots x_A)\prod_{i=1}^{A}dx_i}, \tag{5}$$

where the integral stands for integration over the coordinates and sum over the spin and isospin. Making use

[17] The formalism presented in Sec. II is similar to that presented by J. W. Clark and P. Westhaus (Ref. 14).
[18] Y. C. Tang, E. W. Schmid, and R. C. Herndon, Nucl. Phys. **65**, 203 (1965).
[19] The above choice of $\Phi(x_1\cdots x_A)$ is valid for closed-shell nuclei; for other nuclei it is necessary to take linear combination of determinantal wave functions so that $\Phi(x_1\cdots x_A)$ is an eigenstate of the total angular momentum.
[20] We take ϕ_γ to be normalized single-particle wave functions.

of the identity

$$\Phi^*F\nabla_k^2(F\Phi)+F\Phi\nabla_k^2(F\Phi^*)-2\nabla_k(\Phi^*F)\cdot\nabla_k(\Phi F)$$
$$=[\Phi^*F^2\nabla_k^2\Phi+2\Phi^*F(\nabla_k^2F)\Phi+(\nabla_k^2\Phi^*)F^2\Phi-2F^2\nabla_k\Phi^*\cdot\nabla_k\Phi-2\Phi^*(\nabla_kF\cdot\nabla_kF)\Phi], \quad (6)$$

the kinetic energy in the numerator of Eq. (5) can be written as

$$-\frac{\hbar^2}{2m}\sum_k\int\Phi^*(x_1\cdots x_A)F(\mathbf{r}_1\cdots\mathbf{r}_A)\nabla_k^2F(\mathbf{r}_1\cdots\mathbf{r}_A)\Phi(x_1\cdots x_A)\prod_{i=1}^A dx_i$$
$$=\sum_k\int\Phi^*(x_1\cdots x_A)F^2(\mathbf{r}_1\cdots\mathbf{r}_A)T_k\Phi(x_1\cdots x_A)\prod_{i=1}^A dx_i$$
$$-\frac{\hbar^2}{4m}\sum_k\int\Phi^*(x_1\cdots x_A)F^2(\mathbf{r}_1\cdots\mathbf{r}_A)[\nabla_k^2\ln F(\mathbf{r}_1\cdots\mathbf{r}_A)]\Phi(x_1\cdots x_A)\prod_{i=1}^A dx_i, \quad (7)$$

where

$$T_k\Phi(x_1\cdots x_A)=-(\hbar^2/2m)[4\Phi^*(x_1\cdots x_A)]^{-1}[\nabla_k^2\mid\Phi(x_1\cdots x_A)\mid^2-4\nabla_k\Phi^*(x_1\cdots x_A)\cdot\nabla_k\Phi(x_1\cdots x_A)] \quad (8)$$

and

$$-\frac{\hbar^2}{4m}\sum_k\nabla_k^2\ln F(\mathbf{r}_1\cdots\mathbf{r}_A)=-\frac{\hbar^2}{2m}\sum_{i<j=1}^A\nabla_i^2\ln f(r_{ij}). \quad (9)$$

In the above, the operator $\sum_kT_k$ gives the contribution to the kinetic energy from the model function Φ, while the expression in Eq. (9) gives the contribution to the kinetic energy from the correlation function $f(r_{ij})$. Since $(-\hbar^2/2m)\nabla_i^2\ln f(r_{ij})$ has the form of a two-body interaction, we can add it to the nucleon-nucleon potential $V(x_i, x_j)$ to get an effective interaction[21] $\tilde{V}(x_i, x_j)$ defined as

$$\tilde{V}(x_i, x_j)=V(x_i, x_j)-(\hbar^2/2m)\nabla_i^2\ln f(r_{ij}). \quad (10)$$

The expectation value of the Hamiltonian can now be written as

$$E=\frac{\int\Phi^*(x_1\cdots x_A)\prod_{i<j=1}^A f^2(r_{ij})\left[\sum_{i=1}^A T_i+\sum_{i<j=1}^A\tilde{V}(x_i, x_j)\right]\Phi(x_1\cdots x_A)\prod_{i=1}^A dx_i}{\int\Phi^*(x_1\cdots x_A)\prod_{i<j=1}^A f^2(r_{ij})\Phi(x_1\cdots x_A)\prod_{i=1}^A dx_i}. \quad (11)$$

If we introduce a normalization integral $I(A,\beta)$ as

$$I(A,\beta)=\int\Phi^*(x_1\cdots x_A)\prod_{i<j=1}^A g(i,j,\beta)$$
$$\times\prod_{i=1}^A h(i,\beta)\Phi(x_1\cdots x_A)\prod_{i=1}^A dx_i, \quad (12)$$

where

$$g(i,j,\beta)=\exp[2\ln f(r_{ij})+\beta\tilde{V}(x_i, x_j)] \quad (13)$$

and

$$h(i,\beta)=\exp[\beta T_i], \quad (14)$$

then the energy can be written in terms of the normalization integral as

$$E=\lim_{\beta\to0}(\partial/\partial\beta)\ln I(A,\beta). \quad (15)$$

Thus the problem of calculating the energy has been reduced to evaluating the normalization integral $I(A,\beta)$. This in general is very difficult, since it involves a $3A$ dimensional integral. Here we perform a cluster expansion in which the terms are ordered according to the number of particles correlated and perform the variation with the first few terms in the series.

Let us write the expectation value of any function of N particles $G(x_1, x_2, \cdots, x_N)$, where $N\leq A$, with respect to the model wave function Φ as

$$\langle G(1,2,\cdots,N)\rangle\equiv\int\Phi^*(x_1\cdots x_A)G(x_1\cdots x_N)$$
$$\times\Phi(x_1\cdots x_A)dx_1\cdots dx_A; \quad (16)$$

[21] The above method for obtaining the effective interaction was first employed by H. W. Jackson and E. Feenberg, Ann. Phys. (N. Y.) **15**, 266 (1961). See also W. J. Mullin, Phys. Rev. **134**, A1249 (1964).

then the normalization integral can be written as

$$I(A,\beta)=\langle \prod_{i<j=1}^{A} g(i,j,\beta) \prod_{k=1}^{A} h(k,\beta)\rangle. \quad (17)$$

As a first approximation to the normalization integral we take all one-particle effects into consideration. This gives

$$I(A,\beta)\simeq I^{(1)}(A,\beta)=\prod_{i=1}^{A}\langle h(i,\beta)\rangle. \quad (18)$$

The contribution to the energy due to one-particle effects is then

$$E^{(1)}=\lim_{\beta\to 0}(\partial/\partial\beta)\,\ln I^{(1)}(A,\beta)=\sum_{i=1}^{A}\langle T_i\rangle. \quad (19)$$

To include the contribution due to two-particle correlation we multiply $I^{(1)}(A,\beta)$ by the correction factor

$$\prod_{i<j=1}^{A}\frac{\langle g(i,j,\beta)h(i,\beta)h(j,\beta)\rangle}{\langle h(i,\beta)\rangle\langle h(j,\beta)\rangle}. \quad (20)$$

The denominator in Eq. (20) guarantees that when the dynamic correlation is switched off, i.e., $g\to 1$, the correction factor (now including only exchange correlation) does not contribute to the energy. Thus, the contribution to the energy from the correction factor is due to two-particle dynamic correlations. The normalization integral can now be approximated by

$$I(A,\beta)\simeq I^{(2)}(A,\beta)$$

$$=I^{(1)}(A,\beta)\prod_{i<j=1}^{A}\frac{\langle g(i,j,\beta)h(i,\beta)h(j,\beta)\rangle}{\langle h(i,\beta)\rangle\langle h(j,\beta)\rangle}. \quad (21)$$

The corresponding energy is then,

$$E^{(2)}=\lim_{\beta\to 0}(\partial/\partial\beta)\,\ln I^{(2)}(A,\beta)=E_1+E_2, \quad (22)$$

where

$$E_1=E^{(1)}=\sum_{i=1}^{A}\langle T_i\rangle, \quad (23)$$

and

$$E_2=\sum_{i<j=1}^{A}\left(\frac{\langle f^2(i,j)[\tilde{V}(i,j)+T_i+T_j]\rangle}{\langle f^2(i,j)\rangle}-\langle T_i\rangle-\langle T_j\rangle\right) \quad (24)$$

is the contribution to the energy from two-particle correlation. To include the contribution to the energy due to three-particle correlation, we multiply $I^{(2)}(A,\beta)$, by the correction factor

$$\prod_{i<j<k=1}^{A}\frac{\langle g(i,j,\beta)g(i,k,\beta)g(j,k,\beta)h(i,\beta)h(j,\beta)h(k,\beta)\rangle}{I_{i,j,k}{}^{(2)}(A,\beta)}, \quad (25)$$

where

$$I_{i,j,k}{}^{(2)}(A,\beta)=\frac{\langle g(i,j,\beta)h(i,\beta)h(j,\beta)\rangle\langle g(j,k,\beta)h(j,\beta)h(k,\beta)\rangle\langle g(i,k,\beta)h(i,\beta)h(k,\beta)\rangle}{\langle h(i,\beta)\rangle\langle h(j,\beta)\rangle\langle h(k,\beta)\rangle}. \quad (26)$$

Again in this case the denominator in Eq. (25) is such that when $g\to 1$ the contribution to the energy from the correction term is zero. The normalization integral can now be approximated to include one-, two-, and three-body effects, and is written as

$$I(A,\beta)\simeq I^{(3)}(A,\beta)=I^{(2)}(A,\beta)\prod_{i<j<k=1}^{A}\frac{\langle g(i,j,\beta)g(i,k,\beta)g(j,k,\beta)h(i,\beta)h(j,\beta)h(k,\beta)\rangle}{I_{i,j,k}{}^{(2)}(A,\beta)}. \quad (27)$$

The corresponding energy is given by

$$E^{(3)}=\lim_{\beta\to 0}(\partial/\partial\beta)\,\ln I^{(3)}(A,\beta)=E_1+E_2+E_3, \quad (28)$$

where E_1 and E_2 are given by Eqs. (23) and (24), respectively, and E_3 is the contribution to the energy from three-body correlation and is given by

$$E_3=\sum_{i<j<k=1}^{A}\left\{\frac{\langle f^2(i,j)f^2(i,k)f^2(j,k)[\tilde{V}(i,j)+\tilde{V}(i,k)+V(j,k)+T_i+T_j+T_k]\rangle}{\langle f^2(i,j)f^2(i,k)f^2(j,k)\rangle}-\frac{\langle f^2(i,j)[\tilde{V}(i,j)+T_i+T_j]\rangle}{\langle f^2(i,j)\rangle}\right.$$

$$\left.-\frac{\langle f^2(i,k)[\tilde{V}(i,k)+T_i+T_k]\rangle}{\langle f^2(i,k)\rangle}-\frac{\langle f^2(j,k)[\tilde{V}(j,k)+T_j+T_k]\rangle}{\langle f^2(j,k)\rangle}+\langle T_i\rangle+\langle T_j\rangle+\langle T_k\rangle\right\}. \quad (29)$$

TABLE I. Results of the cluster expansion for the energy of H^3 using different trial wave functions compared with the results of Monte Carlo calculation.

n	α_1 (F^{-n})	α_2 (F^{-n})	β (F^{-2})	e (MeV)	r_d (F)	E_1 (MeV)	E_2 (MeV)	E_3 (MeV)	$E=E_1+E_2+E_3$ (MeV)	E(Monte Carlo) (MeV)
1	0.55	5.0	0.16	−9.5	1.3	9.95	−12.92	−4.72	−7.69	−7.78
2	0.3	1.5	0.24	−18.0	1.2	14.93	−19.53	−2.93	−7.53	−7.78

In a similar manner we can correct $I^{(3)}(A,\beta)$ to include the contribution due to four-body correlation and higher many-body correlation. Thus, the series expansion for the energy of a nucleus of A nucleons is

$$E=E_1+E_2+\cdots+E_A, \tag{30}$$

where $E_n(n\leq A)$ is the contribution to the energy from n-particle correlation. If we perform the sum over all the A terms on the right-hand side of equation (30) we obtain the expression for the energy given in Eq. (11). The merit of this expansion and its success, as we will show in the Sec. III, is that the variation can be performed with the first few terms which can be calculated.

III. CALCULATION

In Sec. II we presented the Van Kampen cluster expansion[14] for the binding energy of a system of A interacting fermions, where the nth term in the series was the contribution to the energy due to n-particle correlation. To study the convergence of the expansion for different choices of the correlation function $f(r)$, we consider the calculation of the binding energy of H^3 and He^4. The reason for choosing these nuclei is that the upper bound on their energy has been obtained, for the same two-body interaction used here, by Tang *et al.*[18] using a Monte Carlo method. This enables us to study the convergence of the cluster expansion by comparing our results with those of Tang *et al.* In the case of H^3 all the terms in the cluster expansion can be calculated. This will not only give the contribution of each term in the cluster expansion to the energy, but also show how good a trial function Ψ we have chosen. On the other hand, for He^4, on the basis of a variation with the first three terms in the series, we can study the effect of neglecting the contribution to the energy from four-particle correlation on the variation. Also, by performing the variation for different forms of the correlation function $f(r)$, we can see how the convergence depends on the choice of $f(r)$.

The two-body interaction is that used by Tang *et al.*[18] in H^3 and He^4, and by Kikuta *et al.*[22] in H^3, and is the form

$$V(x_i,x_j)=\tfrac{1}{2}(1+P_{ij}^{\sigma})V_t(r_{ij})+\tfrac{1}{2}(1-P_{ij}^{\sigma})V_s(r_{ij})+\epsilon_{ij}V_c(r_{ij}), \tag{31}$$

where P_{ij}^{σ} is the usual spin-exchange operator and $V_t(r_{ij})$ and $V_s(r_{ij})$ are the triplet and singlet potentials and have the exponential forms

$$\begin{aligned} V_t(r)&=\infty, && r<r_c\\ &=-V_{0t}\exp[-K_t(r-r_c)], && r>r_c\\ V_s(r)&=\infty, && r<r_c\\ &=-V_{0s}\exp[-K_s(r-r_c)], && r>r_c \end{aligned} \tag{32}$$

where $r_c=0.4$ F, $V_{0t}=475.044$ MeV, $K_t=2.5214$ F^{-1}, $V_{0s}=235.414$ MeV, and $K_s=2.0344$ F^{-1}. The last term in Eq. (31) is the Coulomb interaction, where ϵ_{ij} is taken to be one if i and j label protons, and zero otherwise. For $V_c(r_{ij})$ we use the potential given by Tang *et al.*,[18] i.e.,

$$V_c(r)=(e^2/r)[1-(1+\tfrac{11}{16}\lambda r+\tfrac{3}{16}\lambda^2r^2+\tfrac{1}{48}\lambda^3r^3)e^{-\lambda r}], \tag{33}$$

which is the potential between two protons of exponential charge distribution. The constant λ is related to the rms radius of the proton; for an rms radius of 0.8 F, $\lambda=4.32$ F^{-1}.

Having defined the two-body interaction used here, we proceed to define our trial function Ψ. For the model wave function Φ we take a Slater determinant of harmonic-oscillator wave functions. Since we will be dealing with H^3 and He^4 only, we can write the model function Φ as

$$\Phi(1\cdots A)=\prod_{i=1}^{A}\psi_i(r_i)\chi(\sigma,\tau), \tag{34}$$

where A is three for the triton and four for the α particle. The spin-isospin wave function $\chi(\sigma,\tau)$ is taken to be totally antisymmetric, since we will assume all four particles to be in the $1s$ shell of the harmonic-oscillator states, i.e.,

$$\psi(r)=(\beta/\pi)^{3/4}\exp(-\beta r^2/2), \tag{35}$$

where β is the size parameter of the harmonic oscillator and is taken as a variational parameter. The correlation function $f(r)$ has to be chosen to satisfy the condition stated in Eq. (3). Furthermore, for small r, $f(r)$ should depend primarily on the inter-

[22] T. Kikuta, T. Ohmura, M. Morita, and M. Yamada, Progr. Theoret. Phys. (Kyoto) **15**, 222 (1956); T. Ohmura, *ibid.* **22**, 34 (1959).

action between the two nucleons and comparatively little on the presence of other nucleons in the system. A correlation function that satisfies all the above conditions has in fact been proposed[18,23] and is of the form

$$f(r)=u(r)/r, \qquad r<r_d$$
$$=A+B\exp[-\alpha_1(r^n-r_d{}^n]+C\exp[-\alpha_2(r^n-r_d{}^n)], \qquad r>r_d \quad (36)$$

where $u(r)$ is a solution to the equation

$$-(\hbar^2/m)(d^2u/dr^2)+[V_e(r)-e]u(r)=0 \quad (37)$$

with

$$V_e(r)=\tfrac{1}{2}[V_t(r)+V_s(r)]. \quad (38)$$

It can be shown[24] that V_e is the interaction obtained from Eq. (31) in the absence of the Coulomb interaction after the spin and isospin sums are performed. In Eq. (36) the constants A, B, and C are chosen such that $f(r)$ and its first and second derivative are continuous at r_d and $f(r)\to 1$ for $r\to\infty$. The quantities α_1, α_2, r_d, and e are variational parameters. The calculation will be performed for different values of n to see how the convergence of the cluster expansion and upper bound on the energy depends on n, i.e., on the tail of the correlation function.

Results for H^3. In the case of H^3, the Van Kampen cluster expansion gives rise to three terms in the series for the energy, i.e.,

$$E=E_1+E_2+E_3, \quad (39)$$

where

$$E_1=3\langle T_1\rangle-E_{\text{c.m.}}=\tfrac{3}{2}(\hbar^2/m)\beta, \quad (40)$$

$$E_2=3[\langle f^2(12)\tilde{V}(12)\rangle/\langle f^2(12)\rangle]=3J, \quad (41)$$

$$E_3=3\frac{\langle f^2(12)f^2(13)f^2(23)\tilde{V}(12)\rangle}{\langle f^2(12)f^2(13)f^2(23)\rangle}-3\frac{\langle f^2(12)\tilde{V}(12)\rangle}{\langle f^2(12)\rangle}=3(Z-J). \quad (42)$$

$E_{\text{c.m.}}$ is the energy due to c.m. motion and should not be included in the energy of the system. Because of our choice of Gaussians for the spacial part of the model wave function Φ, the contribution from the operator T in Eqs. (24) and (29) can be shown to cancel identically. In Eqs. (41) and (42) the quantities J and Z are given by

$$J=\int_0^\infty dr\, r^2 e^{-\beta r^2/2}f^2(r)\tilde{V}(r)\Big/\int_0^\infty dr\, r^2 e^{-\beta r^2/2}f^2(r) \quad (43)$$

and

$$Z=\frac{\int_0^\infty dr_1\int_0^\infty dr_2\int_{|r_1-r_2|}^{|r_1+r_2|} dr_3 r_1r_2r_3 f^2(r_1)f^2(r_2)f^2(r_3)\tilde{V}(r_1)\exp[-\frac{1}{3}\beta(r_1^2+r_2^2+r_3^2)]}{\int_0^\infty dr_1\int_0^\infty dr_2\int_{|r_1-r_2|}^{|r_1+r_2|} dr_3 r_1r_2r_3 f^2(r_1)f^2(r_2)f^2(r_3)\exp[-\frac{1}{3}\beta(r_1^2+r_2^2+r_3^2)]}, \quad (44)$$

where the sum over the spin and isospin has been performed, and $\tilde{V}(r)$ is given by

$$f^2(r)\tilde{V}(r)=f^2(r)V_e(r)+\frac{\hbar^2}{2m}\left[\left(\frac{df}{dr}\right)^2-f(r)\frac{d^2f}{dr^2}-\frac{2}{r}f(r)\frac{df}{dr}\right], \quad (45)$$

where V_e is the effective potential defined in Eq. (38). In Table I we have the results for the upper bound on the energy, with the contribution from each term in the series for both $n=1$ and 2 [n determines the asymptotic behavior of the correlation function; see Eq. (36)], and the results of Tang *et al.*[18] using the Monte Carlo method. On comparing our results with those of the Monte Carlo method, we find that our correlation function with $n=1$ gives a better upper bound than for $n=2$, although both are very good. However, in the case of $n=1$ the convergence of the series is much poorer. In fact, E_3 is 36.5% of E_2 for $n=1$, while for $n=2$ it is only 15.0%. In Fig. 1(a) we have the relative wave function $w(r)$ for $n=1$ and 2 and the Monte Carlo result, where $w(r)$ is defined by the relation

$$\Psi(1,2,\cdots,A)=\prod_{i<j=1}^{A} w(r_{ij})\chi(\sigma,\tau), \quad (46)$$

in which A is 3 for H^3 and 4 for He^4 and the peak of $w(r)$ is normalized to unity in the figure. A comparison of $w(r)$ for the three cases indicates that the wave functions are nearly the same except in the tail ($r>4.0$ F), where $w(r)$ for $n=2$ deviates from the other two because of the Gaussian tail of the correlation function. On the other hand, a comparison of the correlation function $f(r)$ for $n=1$ and 2 in Fig. 2(a) shows that for $n=1$, $f(r)$ has a long tail

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TABLE II. Results of the cluster expansion for the energy of He^4 using different trial wave functions. The quantities in parentheses are upper bound on these quantities.

n	α_1 (F^{-n})	α_2 (F^{-n})	β (F^{-2})	e (MeV)	r_d (F)	E_1 (MeV)	E_2 (MeV)	E_3 (MeV)	$E=E_1+E_2+E_3$ (MeV)	E_4 (MeV)	r_{rms} (F)
1						(16.8)	(−17.02)	(−31.5)	($E<-33.0$)		
2	0.32	1.6	0.365	−19.0	1.22	34.06	−53.89	−9.53	−29.36	0.34±0.14	1.37
3	0.134	2.5	0.398	−19.2	1.2	37.14	−58.55	−7.83	−29.24	0.34±0.14	1.38
6	0.087	1.5	0.575	−23.5	1.2	53.65	−81.60	0.41	−27.54	0.29±0.15	1.39

while for $n=2$, $f(r)\to 1$ much faster. The reason for the long tail in the case of $n=1$ is that the Slater determinant of harmonic-oscillator wave function does not have the proper asymptotic behavior and the exponential tail of $f(r)$ tries to adjust this asymptotic behavior. In the case of $n=2$ the correlation function itself has a Gaussian tail and this can not improve very much on the asymptotic behavior of the Slater determinant. This long-range behavior of $f(r)$ for $n=1$ leads to a poor convergence of the cluster expansion. This is clear from Eq. (42), since the region of space where both $f(13)$ and $f(23)$ are different from one is larger than in the case of $n=2$; thus, the contribution from E_3 becomes large in magnitude.

From the above results we can conclude, first, that our choice of trial functions even with $n=2$ is good. Second, to guarantee convergence of the cluster expansion we should take $n\geq 2$, i.e., the correlation function should go to one reasonably fast.

Results for He^4. In the case of He^4, the cluster expansion gives rise to a four-term series for the energy. We are going to neglect the contribution to the energy from the four-particle correlation by taking

$$E\simeq E_1+E_2+E_3, \tag{47}$$

where

$$E_1=4\langle T_1\rangle-E_{\text{c.m.}}=\tfrac{9}{4}(\hbar^2/m)\beta, \tag{48}$$

$$E_2=6[\langle f^2(12)\tilde{V}(12)\rangle/\langle f^2(12)\rangle]=6J, \tag{49}$$

$$E_3=12\frac{\langle f^2(12)f^2(13)f^2(23)\tilde{V}(12)\rangle}{\langle f^2(12)f^2(13)f^2(23)\rangle}-12\frac{\langle f^2(12)\tilde{V}(12)\rangle}{\langle f^2(12)\rangle}$$

$$=12(Z-J), \tag{50}$$

where the quantities J and Z are the same as in the case of H^3 and are given in Eq. (43) and (44), with the exception that $\tilde{V}(ij)$ now includes the Coulomb potential when i and j label protons.

In Table II we have the results for the upper bound obtained with the first three terms in the cluster expansion. We have also included the contribution to the energy from four-particle correlation and the rms radius of the system for the optimum value of the parameters obtained from the variation with $E_1+E_2+E_3$. These results should be compared with those obtained from a Monte Carlo calculation,[18] which are

$$E=29.75\pm 0.18 \text{ MeV}, \qquad r_{\text{rms}}=1.40 \text{ F}. \tag{51}$$

In the case of $n=1$, the variation with the first three terms did not yield a minimum; furthermore, the convergence of the series is very poor. This was expected, for we found that in the case of H^3 that for $n=1$, $f(r)$ is long ranged and multiparticle correlation gets to be important. Thus, to attain a minimum in the energy we should perform the variation with all the terms in the expansion and that defeats the purpose of the expansion.

For $n=2$ and 3 the variation with the first three terms yields a minimum in the energy that is in good agreement with the results of the Monte Carlo calculation. This is seen by comparing the results in Table II with those of Eq. (51). Part of the difference between the results in Table II and Eq. (51) is due to the use of a better trial function in the case of Monte Carlo calculations. This is clear from the results for H^3 (Table I) where all terms in the expansion were taken into consideration and the Monte Carlo method gave a slightly better upper bound on the energy than we obtained with our trial function. The difference between the trial function used here and that used in Monte Carlo calculation in H^3 and He^4 is seen in Fig. 1, where the relative wave function $w(r)$ is presented. A comparison of the results for $n=2$ and $n=3$ shows that for $n=3$ the convergence is slightly better since the correlation function $f(r)$ goes to one much faster as shown in Fig. 2(b). On the other hand, the energy is slightly poorer due to the tail of the wave function. If we compare the

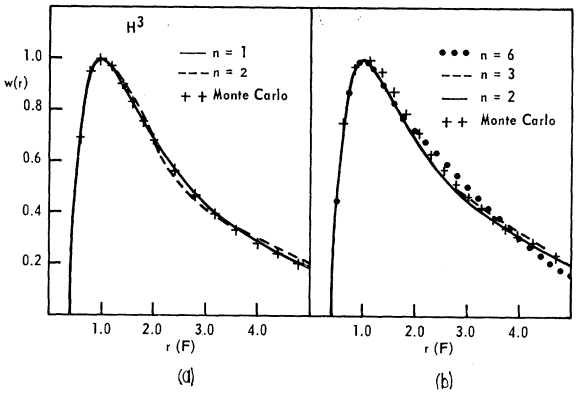

FIG. 1. Comparison of the relative wave function $w(r)$ for different values of n with the corresponding wave function obtained by Monte Carlo method in H^3 and He^4.

convergence of the expansion in H^3 and He^4 for $n=2$ we see that the ratio E_3/E_2 is about the same in these nuclei. This indicates that neglecting the contribution to the energy from four-particle correlation does not effect the variation or the convergence of the series appreciably for $n\geq 2$.

We have also calculated E_4 and the rms radius using a Monte Carlo method for the optimum values of the parameters from a variation with the first three terms. We find that E_4 is small and almost independent of n, provided a minimum in the energy is obtained. Also, the rms radius obtained here is in good agreement with the results of the Monte Carlo calculation of Tang *et al.* and independent of n. All this seems to indicate that if $n\geq 2$ the Van Kampen cluster expansion converges with the first three terms in the series and the results for the upper bound on the energy and rms radius are in good agreement with those obtained using the Monte Carlo method of Ref. 18. Furthermore, since E_4 is small and E_3/E_2 is about the same in H^3 and He^4, we expect the cluster expansion to give good results in heavier nuclei for $n\geq 2$.

Upon going from $n=1$ to $n=2$ we were able to perform the variation with only the first three terms, neglecting the contribution from four-particle correlation. The question is, can n be taken large enough so as to neglect the contribution from three-particle correlation and yet obtain a good result for the energy? To test this possibility we have performed the variation for $n=6$ taking the first three terms in the expansion. From the results in Table II we observe that the convergence of the series is very good, and in fact the contribution to the energy from E_3 and E_4 is small. Also, from Fig. 2(b) we see that the correlation function $f(r)$ for $n=6$ is of much shorter range than in the case of $n=2$ or 3, which is the reason for the faster convergence in this case. However, as expected, the energy obtained is off by ~ 2 MeV because of the Gaussian tail of the wave function. When the variation for $n=6$ was performed with the first two terms only, i.e., no three-particle correlation included, no minimum for the energy was obtained, and in this case the correlation function $f(r)$ was still of short range. From the above results for $n=6$ we can conclude that E_3 is necessary for obtaining a minimum in the energy, even though the asymptotic for of f was explicitly chosen with the idea of suppressing $|E_3|$. Therefore, to perform a variational calculation using the cluster expansion and with no subsidiary conditions on the given family of correlation function $f(r)$ other than $n\geq 2$, one has to include the contribution from three-particle correlation in the variation.

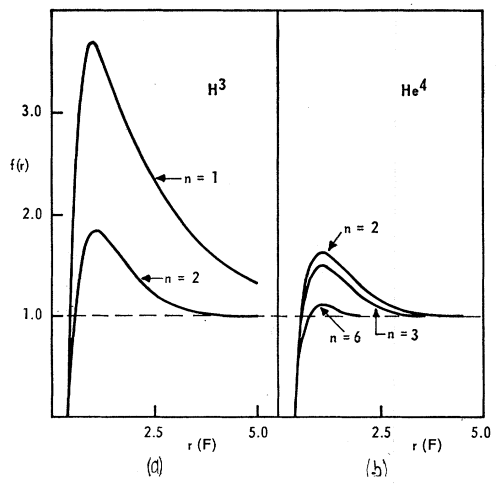

FIG. 2. Comparison of the correlation function $f(r)$ for different values of n in H^3 and He^4.

IV. CONCLUSION

From the results of the above investigation we can draw the following conclusions: First, a comparison of the upper bound on the energy and wave function of H^3 obtained here with those of Monte Carlo calculations indicates that our choice of trial function is good, i.e., we obtain the upper bound to within 0.5 MeV of the Monte Carlo result. Second, in He^4, with $n\geq 2$, the variation with the first three terms converges and the upper bound is in good agreement with the result of Monte Carlo calculation. At the same time in all cases where a minimum in the energy was obtained with the first three terms, E_4 was less than 0.5 MeV. Third, in both H^3 and He^4 the ratio E_3/E_2 is about the same for $n=2$, which indicates that this convergence will hold for heavier nuclei like O^{16}. Also, since the average separation between nucleons in He^4 is about the same as in heavier nuclei, we expect the cluster expansion to have the same convergence in heavier nuclei. Fourth, the results for $n=6$ indicate that the contribution E_3 from three-particle correlation should be included in the variation to obtain a minimum, if we require that no subsidiary conditions be placed on the class of correlation function $f(r)$ other than $n\geq 2$. Finally, we have seen in H^3 and He^4 that for $n=1$ the correlation functions becomes long ranged because of the poor asymptotic behavior of the model function Φ used here. Thus, if one uses a Hartree-Fock wave function which has the proper asymptotic behavior or Woods-Saxon single-particle wave function, one might be able to remove the restriction on n. However, in that case the calculational procedure becomes more difficult.

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