Cluster Expansions for Correlated Wave Functions of Finite Systems

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A theory of correlated wave functions for finite systems is developed which systematically neglects the contribution from three-body cluster terms. The approximation made leads to a derivation of a Bethe-Goldstone equation for finite systems which includes modified occupation probabilities and self-consistent potentials for occupied states. The absence of potentials in unoccupied states follows from the neglect of three-body cluster terms. It is also shown that a careful treatment of the Pauli principle and occupation probabilities allows the application of variational techniques.

Recently, one of us has presented a discussion of the relation between Jastrow theory and the Brueckner-Bethe-Goldstone theories.[1] Simple cluster-expansion methods were developed; however, the results of Ref. 1 were deficient in that the occupation probabilities were only treated in low order and the notation was adapted to the discussion of infinite systems. In this work we remedy these deficiencies by writing the equations of the theory in a general basis appropriate to the treatment of finite systems and presenting a more complete treatment of occupation probabilities.

We consider a Slater determinant,

$$|\Phi\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle , \tag{1}$$

where $|0\rangle$ is the true vacuum state. The letters i, j, k, ... will be used to refer to occupied states and $m, n, p, \ldots$ will be used to refer to unoccupied states. We may introduce a correlated wave function via the relation

$$|\Psi\rangle = e^S |\Phi\rangle , \tag{2}$$

where in general,

$$S = \sum_{n=1}^{N} S^{(n)} , \tag{3}$$

and $S^{(n)}$ is an n-body operator.[2] In this work we investigate the consequences of the approximation,

$$S = S^{(2)} = \tfrac{1}{2} \sum_{nmij} a_n^\dagger a_m^\dagger (nm|f|ij)\, a_j a_i . \tag{4}$$

It is now convenient to define the n-particle uncorrelated states,

$$|i\rangle = a_i^\dagger |0\rangle ,$$
$$|ij\rangle = a_i^\dagger a_j^\dagger |0\rangle , \text{ etc.}, \tag{5}$$

and the *unnormalized*, but correlated states,

$$|\Psi_i\rangle = e^S |i\rangle = |i\rangle ,$$
$$|\Psi_{ij}\rangle = e^S |ij\rangle , \text{ etc.} \tag{6}$$

Further, cluster expansions for the expectation values of operators in the state $|\Psi\rangle$ may be written in terms of the cluster integrals defined as follows:

$$\langle \Psi_{ij} | \Psi_{i'j'} \rangle = \langle ij | i'j' \rangle + \kappa_{ij,\, i'j'}$$
$$= \delta_{ii'}\delta_{jj'} - \delta_{ij'}\delta_{ji'} + \kappa_{ij,\, i'j'} , \tag{7}$$

$$\langle \Psi_{ij} | H | \Psi_{i'j'} \rangle = \langle ij | (t_1 + t_2) | i'j' \rangle + h_{ij,\, i'j'}$$
$$= t_{i,\, i'}\delta_{jj'} + t_{j,\, j'}\delta_{ii'} - t_{i,\, j'}\delta_{ji'}$$
$$- t_{j,\, i'}\delta_{ij'} + h_{ij,\, i'j'} , \tag{8}$$

where in Eq. (8), H is the Hamiltonian of the system and t_n denotes the kinetic energy operator for particle n. We note that the specification of the matrix elements $\langle \Psi_{ijk} | H | \Psi_{i'j'k'} \rangle$ leads to the definition of three-body cluster integrals $h_{ijk,\, i'j'k'}$, etc.

The structure of the cluster expansion may be indicated diagrammatically. In Fig. 1 we indicate a diagrammatic representation for some of the cluster integrals defined above and also the matrix elements of the kinetic energy operator. The rules for constructing the expectation values of operators in the correlated states are given in the work of da Providência.[3] For example, in Fig. 2 we have indicated schematically the cluster expansion for expectation value of the Hamiltonian. These diagrams represent the expression

$$\mathcal{E} = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$$
$$= \sum_i t_{i,\, i} - \sum_{ijk} t_{i,\, j} \kappa_{jk,\, ik} + \sum_{ijkgl} t_{i,\, j} \kappa_{jk,\, gk} \kappa_{gl,\, il} + \cdots$$
$$+ \tfrac{1}{2} \sum_{ij} h_{ij,\, ij} - \sum_{ijkl} h_{ij,\, ik} \kappa_{kl,\, jl} + \cdots . \tag{9}$$

In the representation in which t is diagonal (infinite systems) this expression reduces essentially to that given in the Appendix of Ref. 1.

One may factor out the matrix elements of the kinetic energy operator in Eq. (9). Then by making a selective summation of diagrams we can replace the matrix multiplying $t_{i,\, j}$ by the matrix $\gamma_{j,\, i}$

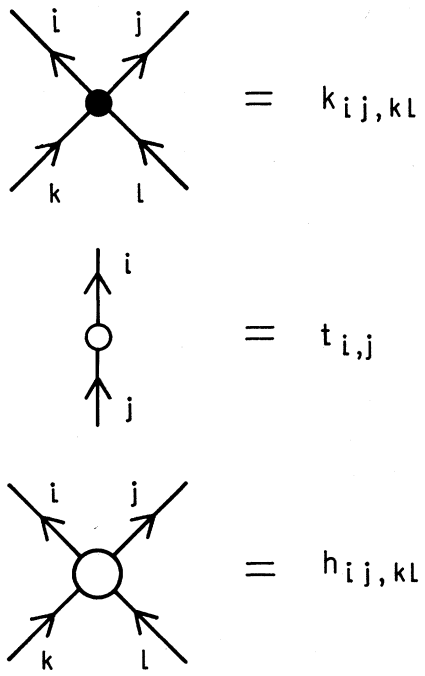

FIG. 1. Diagrammatic representation of the matrix elements of the kinetic energy operator and some two-body cluster integrals. See Eqs. (7) and (8).

indicated diagrammatically in Fig. 3(a). Figure 3(b) gives an algebraic equation for $\gamma_{i,j}$ in our approximation,[4]

$$\gamma_{i,j} = \delta_{ij} - \sum_{glk} \kappa_{ik,gl}\gamma_{g,j}\gamma_{l,k} \,. \tag{10}$$

We may also factor the cluster integrals $h_{ij,kl}$ in Eq. (9). The factor multiplying $h_{ij,kl}$ is $\gamma_{k,i}\gamma_{l,j}$ in a similar approximation to that made above. In making these approximations we neglect terms in the expectation value of H such as that shown in Fig. 4.

Finally in this approximation we obtain the result for $\mathcal{E}$ indicated in Fig. 5, i.e.,

$$\mathcal{E} = \sum_{ij} t_{i,j}\gamma_{j,i} + \tfrac{1}{2}\sum_{ijkl} h_{ij,kl}\gamma_{k,i}\gamma_{l,j} + \cdots \,. \tag{11}$$

This quantity should now be minimized with respect to variations of f and $f^\dagger$, the matrix γ being given by Eq. (10). In order to perform the minimization it is therefore convenient to subtract from $\mathcal{E}$ the quantity [see Eq. (10)]

$$\sum_i \epsilon_{i,i} = \sum_{ij} \epsilon_{i,j}\Big(\gamma_{j,i} + \sum_{gkl} \kappa_{ik,gl}\gamma_{g,j}\gamma_{l,k}\Big) \,,$$

where $\epsilon_{i,j}$ is a Lagrange multiplier. We obtain

$$\mathcal{E} - \sum_i \epsilon_{i,i} = \sum_{ij}(t_{i,j} - \epsilon_{i,j})\gamma_{j,i} + \tfrac{1}{2}\sum_{ijkl}\Big[h_{ij,kl} - \sum_g (\epsilon_{i,g}\kappa_{gj,kl} + \epsilon_{j,g}\kappa_{ig,kl})\Big]\gamma_{k,i}\gamma_{l,j} \,. \tag{12}$$

Minimizing this quantity with respect to $\gamma_{j,i}$ and with respect to $(ij|f^\dagger|mn)$ we obtain, respectively,

$$\epsilon_{i,j} = t_{i,j} + \sum_{kl}\Big[h_{ik,jl} - \sum_g (\epsilon_{i,g}\kappa_{gk,jl} + \epsilon_{k,g}\kappa_{ig,jl})\Big]\gamma_{l,k} \tag{13}$$

and

$$\sum_{kl}\langle mn|v + t_1 + t_2|\Psi_{kl}\rangle\gamma_{k,i}\gamma_{l,j} - \sum_{ghkl}\langle mn|\Psi_{gh}\rangle \times (\epsilon_{k,i}\delta_{lj} + \epsilon_{l,j}\delta_{ki})\gamma_{g,k}\gamma_{h,l} = 0 \,. \tag{14}$$

The matrix $\epsilon_{i,j}$ is the Brueckner-Hartree-Fock matrix with occupation probabilities for occupied states, and Eq. (14) is essentially the Bethe-Goldstone equation.[5]

If $\epsilon_{i,j}$ and $\gamma_{i,j}$ are diagonal (for instance, in infinite matter), we have, instead of Eqs. (13) and (14),

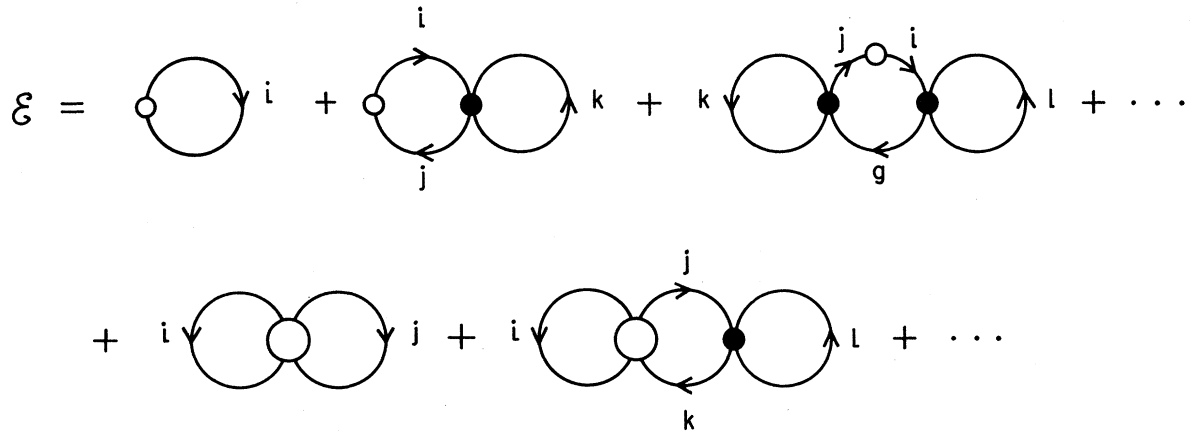

FIG. 2. Diagrammatic representation of the energy in a cluster expansion which neglects three-body (and higher) cluster terms. [See Eq. (10).]

$$\epsilon_i = t_{i,i} + \sum_k [h_{ik,ik} - (\epsilon_i + \epsilon_k)\kappa_{ik,ik}]\gamma_k \,, \tag{13'}$$

$$\langle mn|v + t_1 + t_2|\Psi_{kl}\rangle - \langle mn|\Psi_{kl}\rangle(\epsilon_k + \epsilon_l) = 0 \,. \tag{14'}$$

The last equation leads to

$$\langle mn|\Psi_{kl}\rangle = -\frac{\langle mn|v|\Psi_{kl}\rangle}{t_m + t_n - \epsilon_k - \epsilon_l} \,,$$

because, for infinite matter, t is diagonal. We recover, therefore, the Bethe-Goldstone equation without a self-consistent potential in unoccupied states,

$$|\Psi_{kl}\rangle = |kl\rangle - \sum_{m<n} \frac{|mn\rangle\langle mn|v|\Psi_{kl}\rangle}{t_m + t_n - \epsilon_k - \epsilon_l} \,. \tag{15}$$

If we use Eq. (14) we can simplify our expressions for $\mathcal{E}$ and for $\epsilon_{i,j}$. We have

$$\mathcal{E} = \sum_i \epsilon_{i,i} + \sum_{ij} (t_{i,j} - \epsilon_{i,j})\gamma_{j,i} + \tfrac{1}{2}\sum_{ijkl} \langle ij|v|\Psi_{kl}\rangle\gamma_{k,i}\gamma_{l,j} \tag{16}$$

and

$$\epsilon_{i,j} = t_{i,j} + \sum_{kl} \langle \Psi_{ik}|v|jl\rangle\gamma_{l,k} \,. \tag{17}$$

Equations (16) and (17) may be rewritten, using the definition

$$U_{i,j} = \sum_{k,l} \langle \Psi_{ik}|v|jl\rangle\gamma_{l,k} \,: \tag{18}$$

$$\mathcal{E} = \sum_i t_{i,i} + \sum_{ij} U_{i,j}(\delta_{ij} - \gamma_{j,i}) + \tfrac{1}{2}\sum_{ijkl} \langle ij|v|\Psi_{kl}\rangle\gamma_{k,i}\gamma_{l,j} \tag{16'}$$

and

$$\epsilon_{i,j} = t_{i,j} + U_{i,j} \,. \tag{17'}$$

Equations (10), (14), (17), and (16') provide a generalization of Brandow's results for infinite systems.[4,6]

The work reported here is rather closely related to that of Coester and Kümmel,[7] however it differs in our application of the cluster-expansion methods. Thus we are able to study the role of occupation factors and make somewhat closer contact with the conventional Brueckner-Bethe-Goldstone theory.

APPENDIX

In this Appendix we wish to discuss the properties of the matrix $\epsilon_{i,j}$. For this purpose and in

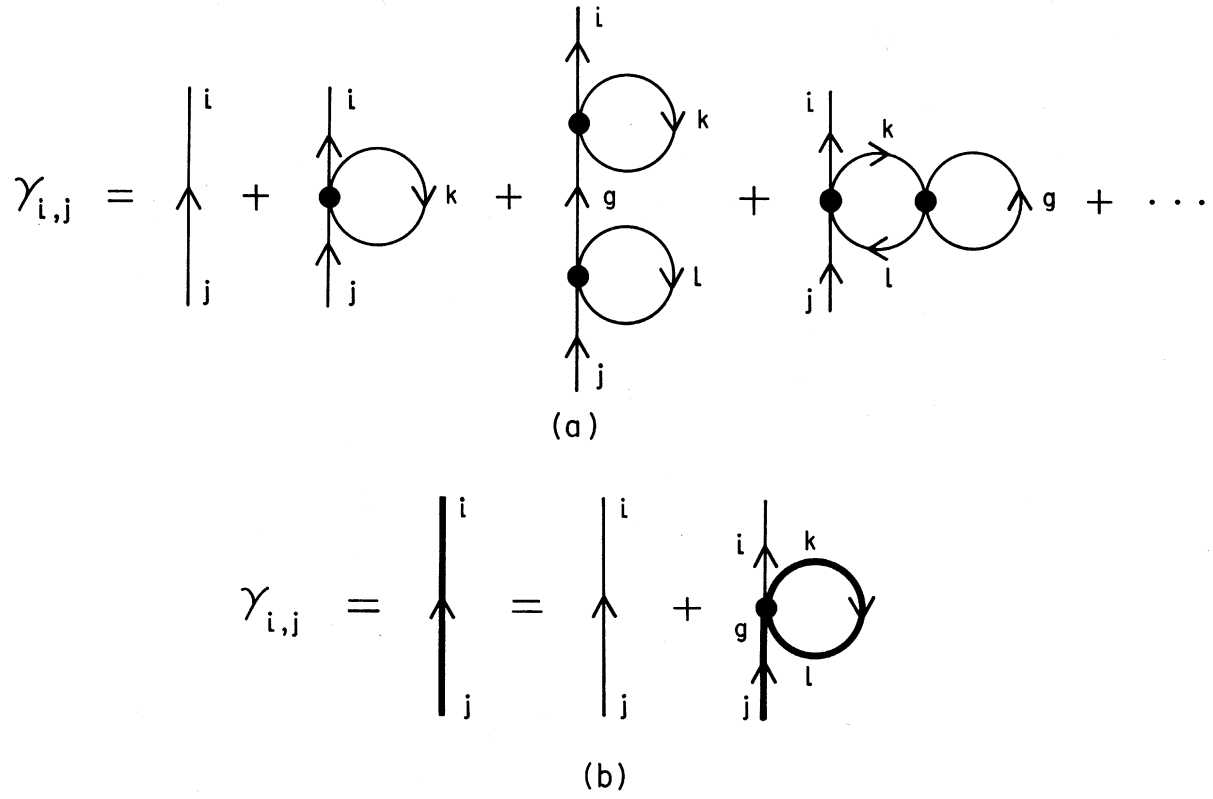

FIG. 3. (a) The quantity $\gamma_{i,j}$ given in terms of cluster integrals, neglecting three-body cluster terms. Indices other than i and j are to be summed over. (b) Diagrammatic representation of an equation for $\gamma_{i,j}$. Indices other than i and j are to be summed over. [See Eq. (10).]

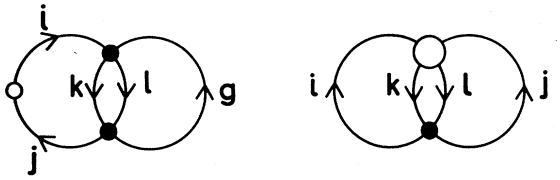

FIG. 4. Two examples of terms neglected in the cluster expansion used here. These terms have the values $-\sum t_{i,j}\kappa_{kl,ig}\kappa_{jg,kl}$ and $\frac{1}{4}\sum h_{kl,ij}\kappa_{ij,kl}$, and are relatively small.

order to avoid a cumbersome notation, it is convenient to represent the matrices $\epsilon_{i,j}$, $t_{i,j}$, $\gamma_{i,j}$, and δ_{ij} by ϵ, t, γ, I or by ϵ_1, t_1, γ_1, I_1 and ϵ_2, t_2, γ_2, I_2 when we wish the matrices to refer to a definite particle (1 or 2). In the same manner we will denote the matrices $h_{ij,kl}$ and $\kappa_{ij,kl}$ by h and κ or h_{12} and κ_{12}. The usual rules for matrix multiplication will be employed. With these conventions we can rewrite Eqs. (10) and (13) in the form

$$\gamma_1 = I_1 - \mathrm{tr}_2\kappa_{12}\gamma_1\gamma_2 , \tag{A1}$$

$$\epsilon_1 = t_1 + \mathrm{tr}_2[h_{12} - (\epsilon_1+\epsilon_2)\kappa_{12}]\gamma_2 , \tag{A2}$$

where tr_2 means that we perform the trace operation with respect to particle 2.

From Eq. (A1) it follows that

$$(I_1 + \mathrm{tr}_2\kappa_{12}\gamma_2)\gamma_1 = I_1 ,$$

so that

$$I_1 + \mathrm{tr}_2\kappa_{12}\gamma_2 = \gamma_1^{-1} . \tag{A3}$$

Since κ is Hermitian it follows that γ is also Hermitian. Now, from Eqs. (A2) and (A3) we obtain

$$\epsilon_1(I_1 + \mathrm{tr}_2\kappa_{12}\gamma_2) = \epsilon_1\gamma_1^{-1} = t_1 + \mathrm{tr}_2 h_{12}\gamma_2 - \mathrm{tr}_2\epsilon_2\kappa_{12}\gamma_2 .$$

Taking the Hermitian adjoint we obtain

$$\gamma_1^{-1}\epsilon_1^\dagger = t_1 + \mathrm{tr}_2\gamma_2 h_{12} - \mathrm{tr}_2(\gamma_2\kappa_{12}\epsilon_2^\dagger) ,$$

which may be rewritten in the form

$$(\gamma_1^{-1}\epsilon_1^\dagger\gamma_1)\gamma_1^{-1} = t_1 + \mathrm{tr}_2 h_{12}\gamma_2 - \mathrm{tr}_2(\gamma_2^{-1}\epsilon_2^\dagger\gamma_2)\kappa_{12}\gamma_2 .$$

Since $\gamma^{-1}\epsilon^\dagger\gamma$ satisfies the same equation as ϵ we see that

$$\epsilon = \gamma^{-1}\epsilon^\dagger\gamma . \tag{A4}$$

The matrix ϵ is not Hermitian, but $\gamma\epsilon$ is:

$$(\gamma\epsilon)^\dagger = \epsilon^\dagger\gamma = \gamma\epsilon\gamma^{-1}\gamma = \gamma\epsilon .$$

This property of ϵ insures that the equation for $|\Psi_{kl}\rangle$, obtained by minimizing $\mathcal{E}$ with respect to $(ij|f^\dagger|mn)$, is the Hermitian adjoint of the equation obtained by minimizing $\mathcal{E}$ with respect to $(mn|f|ij)$, as it should be. Also, $\mathrm{tr}\epsilon$ is real:

$$\mathrm{tr}\epsilon = \mathrm{tr}\,\gamma^{-1}\epsilon^\dagger\gamma = \mathrm{tr}\epsilon^\dagger .$$

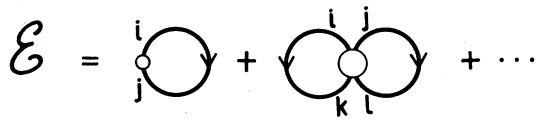

FIG. 5. Diagrammatic representation of the energy of the system [Eq.(12)] (three-body clusters are neglected). The heavy lines represent factors of γ as in Fig. 3.

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[1]C. M. Shakin, Phys. Rev. C 4, 684 (1971).

[2]It is well known that with the appropriate choice of basis states it is not necessary to include $S^{(1)}$ in the theory. Including such a term leads to a generalization of the Hartree-Fock equations.

[3]J. da Providência, Nucl. Phys. 44, 572 (1963).

[4]Equation (10) corresponds to that given in B. H. Brandow [Rev. Mod. Phys. 39, 771 (1967), see pp. 812–813]. In the case of nuclear matter $\gamma_{i,j} = \gamma_i\delta_{ij}$ and $\gamma_i = 1 - \gamma_i \times \sum_k \kappa_{ik}\gamma_k$, where $\kappa_{ik} = \kappa_{ik,ik}$. The quantity $\kappa_i = \sum_k \kappa_{ik}$ is of the order of 0.1 for nuclear matter. If the average value of κ_i is denoted by $\bar{\kappa}$ we have for the average value of γ_i, $\bar{\gamma} = 1 - \bar{\kappa} + 2\bar{\kappa}^2 + \cdots$. This quantity is of the order of 0.9. (The quantity $\bar{\gamma}$ is denoted as $\bar{P}$ by Brandow.)

[5]The analog of the Hartree-Fock equation for correlated systems is obtained by considering the variation of the energy with respect to the parameters of a one-body operator, $S^{(1)}$. More precisely, by requiring that the energy be stationary with respect to the inclusion in S of a small one-body component $S^{(1)}$, one obtains $\langle m|t|i\rangle + \sum_{jk}\langle mj|v_{12}|\Psi_{ik}\rangle\gamma_{k,j} + \sum_{kj}\langle mj|(t_1+t_2)f_{12}|ik\rangle\gamma_{k,j} = 0$ which reduces to the usual Hartree-Fock equation if one neglects $S^{(n)}$, $n \geq 2$ (i.e., $f_{12} = 0$). This equation has also been obtained by H. Kümmel, in *Lectures on the Many-Body Problem*, edited by E. R. Caianiello (Academic, New York, 1962); and to be published.

[6]B. H. Brandow, Phys. Rev. 152, 863 (1966); in *Proceedings of the Lectures in Theoretical Physics*, edited by K. T. Mahanthappa (Gordon and Breach, New York, 1969).

[7]F. Coester, Nucl. Phys. 7, 421 (1958); F. Coester and H. Kümmel, Nucl. Phys. 17, 477 (1960); Kümmel, Ref. 5.