Extension of the coupled-cluster method: A variational formalism

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(Received 3 July 2002; published 27 November 2002)

A general quantum many-body theory in configuration space is developed by extending the traditional coupled-cluster method (CCM) to a variational formalism. Two independent sets (destruction and creation sets) of distribution functions are introduced to evaluate the Hamiltonian expectation. An algebraic technique for calculating these distribution functions via two self-consistent set of equations is given. By comparing with the traditional CCM and with Arponen's extension, it is shown that the former is equivalent to a *linear* approximation to one set of distribution functions and the latter is equivalent to a (generalized) random-phase approximation to it. In addition to these two approximations, other higher-order approximation schemes within the formalism are also discussed. As a demonstration, we apply this technique to a quantum antiferromagnetic spin model.

DOI: 10.1103/PhysRevB.66.184427 PACS number(s): 75.10.Jm, 31.15.Dv

I. INTRODUCTION

The main task of a microscopic quantum many-body theory is to study correlations between the constituent particles of a quantum system in a systematic way. The treatment of these many-body correlations is either in real space or in configuration space. A real-space theory usually focuses on the potential part of many-body Hamiltonians; a configuration space theory often starts from the kinetic part of Hamiltonians. One of the most successful real-space quantum many-body theories is the method of correlated basis functions (CBF),[1] in which real-space correlation functions of the ground state are determined variationally. Perhaps, the closest counterpart of configuration-space theories to the real-space CBF is the coupled-cluster method (CCM),[2–4] in which correlation operators are employed to construct the ground state. One key feature of the CCM is that the bra and ket states are not manifestly Hermitian to one another[5].

In this paper, we propose a general variational theory in configuration space by extending the traditional CCM to a variational formalism, in which ket and bra states are Hermitian to one another. The difficult task of evaluating the Hamiltonian expectation can be done by introducing distribution functions, which can then be determined either by a diagrammatic technique or by an algebraic one. The diagrammatic approach developed in this context is quite similar to that of the CBF. In the algebraic approach, one derives two similar sets of self-consistent equations for the distribution functions; these equations can then be tackled by various methods, e.g., iterative method. Easy comparison can be made with the traditional CCM in this approach. We will mainly discuss the algebraic approach in this paper; the diagrammatic approach will be discussed elsewhere.[6] We apply this variational method to a well-known spin model as a demonstration. Some of our preliminary results has been reported in a conference paper[7].

II. THE REPRESENTATION OF A MANY-BODY WAVE FUNCTION

Similar to the method of correlated basis functions (CBF), the coupled-cluster method (CCM) deals directly with the wave functions of a many-body system. We shall take the spin-1/2 antiferromagnetic XXZ model on a bipartite lattice as an example. The model Hamiltonian is given by

$$H=\frac{1}{2}\sum_{l,\rho} H_{l,l+\rho}=\frac{1}{2}\sum_{l,\rho}\left(\Delta s_l^z s_{l+\rho}^z+\frac{1}{2}s_l^+ s_{l+\rho}^-+\frac{1}{2}s_l^- s_{l+\rho}^+\right), \tag{1}$$

where Δ is the anisotropy, the index l runs over all lattice sites, ρ runs over all nearest-neighbor sites, and $s^{\pm}$ are the usual spin raising $(+)$ and lowering $(-)$ operators. The Hamiltonian of Eq. (1) at $\Delta=1$ corresponds to the isotropic Heisenberg model which has been a focus of theoretical study in recent years due to its relevance to high-temperature superconductivity.

In the limit $\Delta\to\infty$, the ground state of Eq. (1) is clearly given by the classical Néel state with alternating spin-up and spin-down sublattices. We shall exclusively use index i for the spin-up sublattice and the index j for the spin-down sublattice. For a finite value of Δ, such as the isotropic point $\Delta=1$, the many-spin correlations in its ground state can then be included by considering the excited states with respect to the uncorrelated Néel model state. These excited states are constructed by applying the so-called configuration creation operators $C_I^\dagger$ to the Néel model state with the nominal index I labelling these operators. In our spin model, the operators $C_I^\dagger$ are given by any combination of the spin-flip operators to the Néel state, namely s_i^- and s_j^+ and the index I in this case corresponds to the collection of the lattice indices (i's and j's). The hermitian conjugate operators of $C_I^\dagger$ are the configuration destruction operator C_I, given by any combination of s_i^+ and s_j^-. For example, the two-spin flip creation operator is given by $C_{ij}^\dagger=s_i^- s_j^+$, and their destruction counterpart, $C_{ij}=s_i^+ s_j^-$.

The traditional CCM is based on the Hubbard, Hugenholtz and Coester representation (HHC)[2] for the ground ket state, where the correlations are parametrized by an exponentiated operator as,

$$|\Psi_g\rangle = e^S|\Phi\rangle, \quad S=\sum_I F_I C_I^\dagger . \tag{2}$$

For our spin model, $|\Phi\rangle$ is the Néel state and F_I are the correlation coefficients. The configuration creation operator $C_I^\dagger$ in this case is given by a product of any number of pairs of the spin-flip operators,

$$\sum_I F_I C_I^\dagger = \sum_{n=1}^{N/2} \sum_{i_1\ldots,j_1\ldots} f_{i_1\ldots,j_1\ldots} \frac{s_{i_1}^-\ldots s_{i_n}^- s_{j_1}^+\ldots s_{j_n}^+}{(2s)^n}, \tag{3}$$

where s is the spin quantum number. Although we are mainly interested in $s=1/2$, we keep the factor of $1/2s$ for the purpose of comparison with the large-s expansion. Notice also that in Eq. (3) the spin-flip operators of the i-sublattice always pair with that of the j-sublattice to ensure the total z-component $s^z_{total}=0$. For the bra state, however, the CCM proposes a different, practical form as[3–5],

$$\langle\tilde{\Psi}| = \langle\Phi|\tilde{S}' e^{-S}, \tag{4}$$

where S is as given in the ket state and the *linear* bra state operator $\tilde{S}'$ is constructed by the configuration destruction operators only, namely,

$$\tilde{S}' = 1 + \sum_I \tilde{F}_I \; C_I = 1 + \sum_{n=1}^{N/2} \sum_{i_1\ldots,j_1\ldots} \tilde{f}_{i_1\ldots,j_1\ldots} \frac{s_{i_1}^+\ldots s_{i_n}^+ s_{j_1}^-\ldots s_{j_n}^-}{(2s)^n} . \tag{5}$$

The coefficients $\{F_I,\tilde{F}_I\}=\{f_{i_1\ldots j_1\ldots},\tilde{f}_{i_1\ldots j_1\ldots}\}$ are determined variationally through the Hamiltonian expectation $\langle H\rangle$, noticing the normalization condition $\langle\tilde{\Psi}|\Psi\rangle=1$,

$$\langle\tilde{\Psi}|H|\Psi\rangle = \langle\Phi|\bar{H}|\Phi\rangle, \tag{6}$$

where the similarity-transformed $\bar{H}=e^{-S}He^S$ can be expanded as a series of nested commutators as

$$\bar{H} = H + \frac{1}{1!}[H,S] + \frac{1}{2!}[[H,S],S] + \cdots . \tag{7}$$

In most cases, H contains a finite order of destruction operators. The above series then terminates at a finite order as S contains only the creation operators. Hence, the Hamiltonian expectation value in the CCM is a finite order polynomial function of the coefficients $\{F_I,\tilde{F}_I\}$. More specifically, $\langle H\rangle$ in the CCM is linear in the bra-state coefficients $\tilde{F}_I$ and finite-order polynomial in the ket-state coefficients F_I. Thus, calculations in the CCM in general are quite straightforward; when an approximation scheme is chosen (i.e., a truncation scheme with a finite set of $\{F_I,\tilde{F}_I\}$), no further approximation is necessary in most calculations. However, this CCM parametrization of the ground state is problematic in dealing with long-range correlations as discussed in the context of our spin model calculations in Ref.[8]. More discussion of the problems in this traditional CCM will be given later.

An obvious extension of the CCM is to apply the HHC representation to both the ket and bra states. Hence we write

$$|\Psi\rangle = e^S|\Phi\rangle, \quad S=\sum_I F_I C_I^\dagger , \tag{8}$$

$$\langle\tilde{\Psi}| = \langle\Phi|e^{\tilde{S}}, \quad \tilde{S}=\sum_I \tilde{F}_I C_I , \tag{9}$$

where the ket-state and bra-state correlation coefficients F_I and $\tilde{F}_I$ are hermitian conjugate and independent to one another. For our spin model, the model state $|\Phi\rangle$ is the Néel state, and the correlation operators $\Sigma_I F_I C_I^\dagger$ and $\Sigma_I \tilde{F}_I C_I$ are given as in Eqs. (3) and (5). The coefficients $\{F_I,\tilde{F}_I\}$ are then determined by the usual variational equations as

$$\frac{\delta\langle H\rangle}{\delta\tilde{F}_I} = \frac{\delta\langle H\rangle}{\delta F_I} = 0 , \tag{10}$$

where energy expectation is defined in the usual way as

$$\langle H\rangle = \frac{\langle\tilde{\Psi}|H|\Psi\rangle}{\langle\tilde{\Psi}|\Psi\rangle} = \frac{\langle\Phi|e^{\tilde{S}}He^S|\Phi\rangle}{\langle\Phi|e^{\tilde{S}}e^S|\Phi\rangle} . \tag{11}$$

Clearly, the normalization factor $\langle\tilde{\Psi}|\Psi\rangle$ and Hamiltonian expectation $\langle H\rangle$ are highly nontrivial functions of the coefficients F_I and $\tilde{F}_I$. Their calculation in the standard variational approach is in general difficult, contrast to the CCM where the expectation value of the Hamiltonian is a finite-order polynomial of the coefficients, as described earlier. This is perhaps the main reason that little progress has been made in this extension of the CCM except some general discussion and a few attempts[9].

Hence, the key to the extension of the CCM to the standard variational method as described in Eqs. (8)-(11) is to develop a practical and consistent technique to evaluate the normalization factor and the Hamiltonian expectation. It is known in statistical mechanics and real space quantum many-body theory that these evaluations can be done more efficiently by employing distribution functions. One then needs to develop a systematic and consistent scheme to calculate these distribution functions. We have considered two such schemes. One is similar to the traditional technique in statistical mechanics employed by the CBF. In this method, one introduces a generating functional whose functional derivatives are the distribution functions. A diagrammatic technique has been developed to evaluate these distribution functions[6].

The other approach we have considered is an algebraic technique. In this approach, one derives two similar self-consistent sets of equations for the (destruction and creation) distribution functions by taking the advantage of the operator nature in the ground state as given in Eqs. (8)-(9). These self-consistent set of equations can then be tackled by vari-

ous methods such as iteration method. As we shall see, a most simple approximation to one of these two self-consistent sets of equations reproduces the full CCM results, but one can easily go beyond that. We shall mainly discuss the algebraic approach in the followings.

III. DISTRIBUTION FUNCTIONS AND THEIR SELF-CONSISTENT EQUATIONS

We first introduce the so-called bare distribution functions as expectation value of the configuration operators, namely

$$g_I=\langle C_I^\dagger\rangle, \quad \tilde{g}_I=\langle C_I\rangle \quad , \tag{12}$$

where the expectation value is defined in the usual sense as in Eq. (11). In general these bare distribution functions are nontrivial functions of $\{F_J,\tilde{F}_J\}$. Multiplying by the corresponding coefficients, we obtain $F_I g_I$ and $\tilde{F}_I\tilde{g}_I$ which are the the usual full distribution functions useful in the diagrammatic approach[6].

Direct calculation of these functions is certainly not an easy task. Fortunately, by taking the advantage of the properties of the operators, one can derive self-consistent sets of equations which can then be tackled by various methods. In particular, as $C_I^\dagger$ commutes with $S=\Sigma_I F_I C_I^\dagger$ and C_I with $\tilde{S}=\Sigma_I\tilde{F}_I C_I$, one can write

$$g_I=\frac{1}{A}\langle\Phi|e^{\tilde{S}}C_I^\dagger e^S|\Phi\rangle=\frac{1}{A}\langle\Phi|e^{\tilde{S}}e^S C_I^\dagger|\Phi\rangle \quad , \tag{13}$$

$$\tilde{g}_I=\frac{1}{A}\langle\Phi|e^{\tilde{S}}C_I e^S|\Phi\rangle=\frac{1}{A}\langle\Phi|C_I e^{\tilde{S}}e^S|\Phi\rangle \quad , \tag{14}$$

where $A=\langle\tilde{\Psi}|\Psi\rangle$ is the normalization constant. In order to find another expression, one inserts the identity $e^{-\tilde{S}}e^{\tilde{S}}$ in the expression of g_I as

$$g_I=\frac{1}{A}\langle\Phi|e^{\tilde{S}}C_I^\dagger e^{-\tilde{S}}e^{\tilde{S}}e^S|\Phi\rangle=\frac{1}{A}\langle\Phi|\underline{C}_I^\dagger e^{\tilde{S}}e^S|\Phi\rangle \quad , \tag{15}$$

where the similarity-transformed operator $\underline{C}_I^\dagger$ can be expanded in the nested commutator series as

$$\underline{C}_I^\dagger=e^{\tilde{S}}C_I^\dagger e^{-\tilde{S}}=C_I^\dagger+\frac{1}{1!}[\tilde{S},C_I^\dagger]+\frac{1}{2!}[\tilde{S},[\tilde{S},C_I^\dagger]+\cdots \quad , \tag{16}$$

and this series is finite as $C_I^\dagger$ is finite and $\tilde{S}$ contains only the destruction operators. By definition, $\langle\Phi|C_I^\dagger=0$, hence $\langle\Phi|\underline{C}_I^\dagger$ can be expressed in a form linear in the destruction operators C_J and finite order polynomial in the coefficients $\tilde{F}_J$. The expectation values of these finite order terms is therefore linear in $\tilde{g}_J$ and finite order polynomial in $\tilde{F}_J$. This yields a linear relation between g_I and $\{\tilde{g}_J\}$. Hence we write

$$g_I=G(\{\tilde{g}_J\},\{\tilde{F}_J\}) \quad , \tag{17}$$

where G is a function linear in $\tilde{g}_J$ and finite order polynomial in $\tilde{F}_J$.

In a similar fashion we write, by inserting identity $e^S e^{-S}$ in the expression for $\tilde{g}_I$,

$$\tilde{g}_I=\frac{1}{A}\langle\Phi|e^{\tilde{S}}e^S\overline{C}_J|\Phi\rangle \quad , \tag{18}$$

with the usual commutation series

$$\overline{C}_I=e^{-S}C_I e^S=C_I+\frac{1}{1!}[C_I,S]+\frac{1}{2!}[C_I,S],S]+\cdots \quad , \tag{19}$$

and we obtain

$$\tilde{g}_I=G(\{g_J\},\{F_J\}) \quad , \tag{20}$$

where G is the same function as in Eq. (17) but now linear in $\{g_J\}$ and finite order polynomial in $\{F_J\}$. As function G is the same in Eqs. (17) and (20), only one calculation is necessary. Notice that from Eqs. (17) and (20), g_I and F_I can be determined as hermitian conjugate to $\tilde{g}_I$ and $\tilde{F}_I$ correspondingly.

The conjugate Eqs. (17) and (20) provide two self-consistent sets of equations for g_I and $\tilde{g}_I$ in terms of the correlation coefficients $\{F_J,\tilde{F}_J\}$. We note that for a particular g_I its equation in general contains a higher-order set $\{\tilde{g}_J\}$, and vice versa, even for a truncated coefficient set $\{F_I,\tilde{F}_I\}$. Therefore, in order to make any practical calculation, one has to make two approximations, a truncation on the number of coefficients $\{F_I,\tilde{F}_I\}$, and a truncation on the number of bare correlation functions $\{g_I,\tilde{g}_I\}$. After these two truncations, one should be able to solve the self-consistent set of equations to obtain g_I and $\tilde{g}_I$ in terms of F_I and $\tilde{F}_I$. This is contrary to the CCM where one needs only one truncation (in $\{F_I,\tilde{F}_I\}$). As we shall see, for a similar truncation in the coefficients $\{F_I,\tilde{F}_I\}$, one of our lowest order truncations in the bare correlation function $\{g_I,\tilde{g}_I\}$ will reproduce the full CCM results. However, it is a simple step to go beyond this approximation by including some higher-order distribution functions g_I which has proved to be essential to obtain the consistent long-range behaviors of the spin correlation functions (and the low-lying excitation energies) as we shall see in our spin model calculation.

Since Hamiltonian usually contains terms involving both creation operators $C_I^\dagger$ and destruction operators C_I, using the similar argument to the distribution discussed above, it is not difficult to obtain that the expectation value of a general Hamiltonian can be expressed as a function linear in g_I and $\tilde{g}_I$ and a finite order polynomial in F_I or $\tilde{F}_I$,

$$\langle H\rangle=\mathcal{H}(\{g_I\},\{\tilde{g}_I\},\{F_I\})=\mathcal{H}(\{\tilde{g}_I\},\{g_I\},\{\tilde{F}_I\}) \quad . \tag{21}$$

This expression is not unique; using Eqs. (17) or (20), one can express the Hamiltonian expectation as a function linear in g_I and finite-order polynomial in F_I only, or as a function linear in $\tilde{g}_I$ and finite-order polynomial in $\tilde{F}_I$ only,

$$\langle H\rangle = \mathcal{H}'(\{g_I\},\{F_I\}) = \mathcal{H}'(\{\tilde{g}_I\},\{\tilde{F}_I\}) \quad . \tag{22}$$

This expression of the Hamiltonian expectation is useful when we compare with the traditional CCM. Solutions of Eqs. (17) and (20) can be substituted into these equations and we obtain $\langle H\rangle$ as a function of $\{F_I,\tilde{F}_I\}$. Variational calculation in Eq. (10) can then be carried out. In the following, we consider a simple application to the spin model as a demonstration.

IV. TWO-SPIN FLIP APPROXIMATION IN A SPIN MODEL

As a demonstration, we consider a simple truncation approximation in which the correlation operators S and $\tilde{S}$ retain only the two-spin flip correlations as

$$|\Psi_2\rangle = e^{S_2}|\Phi\rangle, \quad \langle\tilde{\Psi}_2| = \langle\Phi|e^{\tilde{S}_2}, \tag{23}$$

where

$$S_2 = \sum_{ij} f_{ij}\frac{s_i^- s_j^+}{2s}, \quad \tilde{S}_2 = \sum_{ij} \tilde{f}_{ij}\frac{s_i^+ s_j^-}{2s}. \tag{24}$$

Using the usual angular momentum commutations

$$[s_l^z, s_{l'}^{\pm}] = \pm s_l^{\pm}\delta_{ll'}, \quad [s_l^+, s_{l'}^-] = 2s_l^z\delta_{ll'}, \tag{25}$$

and the Néel state eigenequations, $s_i^z|\Phi\rangle = s|\Phi\rangle, s_j^z|\Phi\rangle = -s|\Phi\rangle$, it is a straightforward calculation to derive expectation value of various operators with respect to the states of Eqs. (23). In this approximation, for example, the order parameter is derived as

$$M^z = \langle s_i^z\rangle = s - \sum_r n_r, \tag{26}$$

where n_r is the full one-body distribution function given by

$$n_{ij} = f_{ij}g_{ij} = f_{ij}\frac{\langle s_i^- s_j^+\rangle}{2s}, \tag{27}$$

and we have taken the advantage of translational invariance by writing $n_{ij} = n_r$ with $j = i + r$; the usual two-spin correlation function is given by

$$\langle s_i^z s_j^z\rangle = -s^2 + s\left(\sum_{i'} n_{i'j} + \sum_{j'} n_{ij'}\right) - \left(\sum_{i'j'} G_{ij',i'j} + n_{ij}\right), \tag{28}$$

where $G_{ij,i'j'}$ is the full two-body distribution function

$$G_{ij,i'j'} = f_{ij}f_{i'j'}g_{ij,i'j'} = f_{ij}f_{i'j'}\frac{\langle s_i^- s_j^+ s_{i'}^- s_{j'}^+\rangle}{(2s)^2}; \tag{29}$$

and finally, the expectation value of Eq. (1) is then given by

$$\langle H_{ij}\rangle = -\Delta s^2 + s\left(\tilde{g}_{ij} + g_{ij} + \Delta\sum_{i'} n_{i'j} + \Delta\sum_{j'} n_{ij'}\right) - \Delta\left(\sum_{i'j'} G_{ij',i'j} + n_{ij}\right). \tag{30}$$

As can be seen, these physical quantities involve up to two-body distribution functions.

The self-consistent set of equations for the bare distribution functions are derived as described in Sec. III. In particular, the equation for the one-body function $\tilde{g}_{ij}$ is

$$\begin{aligned}\tilde{g}_{i_1j_1} = {} & f_{i_1j_1} + \sum_{ij} f_{ij_1}f_{i_1j}g_{ij} \\ & - \frac{2}{2s}f_{i_1j_1}\left(\sum_i f_{ij_1}g_{ij_1} + \sum_j f_{i_1j}g_{i_1j}\right) \\ & + \frac{1}{2s}\sum_{ijj'} f_{ij_1}f_{i_1j}f_{i_1j'}g_{i_1j,ij'} \\ & + \frac{1}{2s}\sum_{ii'j} f_{ij_1}f_{i'j_1}f_{i_1j}g_{ij_1,i'j} \\ & + \frac{2}{(2s)^2}f_{i_1j_1}^2 g_{i_1j_1} + \frac{4}{(2s)^2}f_{i_1j_1}\sum_{ij} f_{ij_1}f_{i_1j}g_{i_1j_1,ij} \\ & + \frac{1}{(2s)^2}\sum_{ii'jj'} f_{ij_1}f_{i'j_1}f_{i_1j}f_{i_1j'}g_{i_1j_1,ij,i'j'}.\end{aligned} \tag{31}$$

The equation for the two-body function $\tilde{g}_{ij,i'j'}$ will contain up to twelve-body functions, etc. The hermitian conjugate of these equations are the self-consistent set of equations for $g_{ij}, g_{ij,i'j'}$, etc. Clearly, we need to make further truncations for any practical calculation.

Consider a simple truncation in which we retain only the first two terms in Eq. (31), noticing that all other terms are higher-order in terms of $1/2s$ expansion,

$$\tilde{g}_{i_1j_1} \approx f_{i_1j_1} + \sum_{ij} f_{ij_1}f_{i_1j}g_{ij}, \tag{32}$$

and similar equation for g_{ij}. Using the Fourier transformation technique and translational symmetry, it is easy to solve the two equations to obtain

$$g_k = \frac{f_k}{1 - f_k\tilde{f}_k}, \quad \tilde{g}_k = \frac{\tilde{f}_k}{1 - f_k\tilde{f}_k}, \tag{33}$$

where g_k and f_k are Fourier transformations of g_{ij} and f_{ij}, etc. To the same order in $1/2s$, the ground-state energy, Eq. (30), is

$$e = \frac{2}{zN}\sum_{i,\rho}\langle H_{i,i+\rho}\rangle = -\Delta s^2 + s(g_1 + \tilde{g}_1) + 2\Delta s\sum_r n_r, \tag{34}$$

where z is the number of nearest-neighbor sites and

$$g_1=\sum_k \frac{\gamma_k f_k}{1-\tilde{f}_k f_k}, \quad \tilde{g}_1=\sum_k \frac{\gamma_k \tilde{f}_k}{1-\tilde{f}_k f_k},$$

$$\sum_r n_r=\sum_k \frac{f_k \tilde{f}_k}{1-\tilde{f}_k f_k}, \tag{35}$$

with

$$\gamma_k=\frac{1}{z}\sum_\rho e^{i\mathbf{k}\cdot\mathbf{r}_\rho}. \tag{36}$$

The variational equations, $\partial e/\partial f_k=\partial e/\partial \tilde{f}_k=0$, reduce to a quadratic equation for f_k and $\tilde{f}_k$. The physical solution to these equations is

$$f_k=\tilde{f}_k=\frac{\Delta}{\gamma_k}(-1+\sqrt{1-\gamma_k^2/\Delta^2}). \tag{37}$$

The ground-state energy and order parameter are then obtained as

$$e=-\Delta s^2+s\Delta\sum_k (-1+\sqrt{1-\gamma_k^2/\Delta^2}) \tag{38}$$

and

$$M^z=s-\frac{1}{2}\sum_k \left(\frac{1}{\sqrt{1-\gamma_k^2/\Delta^2}}-1\right). \tag{39}$$

On the surface, one may conclude the energy from Eq. (38) becomes a complex number as $\Delta<1$. But as $\Delta<1$, different solutions to Eq. (37) may be used and the corresponding energy from Eq. (34) remains real. We leave further discussion and its possible implication of a quantum phase transition to somewhere else.

It is not difficult to include the contribution of higher-order many-body distribution functions within our variational formalism. Consider the two-spin correlation function of Eq. (28), which contain the important full two-body distribution function. The bare two-body distribution functions $g_{ij,i'j'}$ and $\tilde{g}_{ij,i'j'}$ can be calculated through their self-consistent set of equations by keeping the same order terms in the $(1/2s)$ expansion as we have done for the one-body distribution function in Eqs. (31)-(32). Without going into details of derivation, to the same approximation, we obtain the following results

$$g_{ij,i'j'}\approx g_{ij}g_{i'j'}+g_{ij'}g_{i'j} \tag{40}$$

which, in fact, is usually referred as random-phase approximation. A simpler way to obtain the same results for the two-body functions is to employ the following sequential equation

$$\frac{\partial}{\partial f_{i'j'}}g_{ij}=g_{ij,i'j'}-g_{ij}g_{i'j'}, \tag{41}$$

to g_{ij} and $\tilde{g}_{ij}$ in Eq. (32) and its hermitian conjugate.

Hence, the normalized two-spin correlation function becomes

$$c_r=\langle s_i^z s_{i+r}^z\rangle-\langle s_i^z\rangle\langle s_{i+r}^z\rangle=-g_r\tilde{g}_r=-g_r^2. \tag{42}$$

In fact, our above results of the ground-state energy, order parameter and the correlation function are the same as that of the spin-wave theory[10,11]. In particular, the long-range behavior of the correlation function $c_r\propto 1/r^2$ as $r\to\infty$ for a square lattice system at $\Delta=1$ can not be obtained without the contribution of the two-body distribution function. Using iteration method for solving the equations of g_{ij} and $\tilde{g}_{ij}$, it is straightforward to include higher-order contribution for other physical quantities. But we refrain ourselves from more detailed calculation in this article as our main purpose here is to introduce the new variational formalism and its comparison with the traditional CCM.

V. COMPARISON WITH THE CCM

In order to make a more detailed comparison with the traditional CCM, we first summarize our variational extension. We apply the HHC representation of Eqs. (8)-(9) for the ground state wave function of a quantum many-body system to *both* the ket and bra states with two independent, hermitian conjugate correlation coefficients $\{F_I,\tilde{F}_I\}$ which are determined by the variational equations as

$$\frac{\partial\langle H\rangle}{\partial F_I}=\frac{\partial\langle H\rangle}{\partial \tilde{F}_I}=0.$$

The difficult task of expressing the Hamiltonian expectation $\langle H\rangle=\mathcal{H}(\{F_I,\tilde{F}_I\})$ can be done by introducing the bare distribution functions $g_I=\langle C_I^\dagger\rangle$ and $\tilde{g}_I=\langle C_I\rangle$ and solving their self-consistency equations

$$g_I=G(\{\tilde{g}_J\},\{\tilde{F}_J\}), \quad \tilde{g}_I=G(\{g_J\},\{F_J\}).$$

Using the expression of Eq. (22) for the Hamiltonian expectation

$$\langle H\rangle=\mathcal{H}'(\{g_I\},\{F_I\}),$$

we see that the traditional CCM is equivalent to the *linear approximation* in the self-consistensy equation for g_I, namely

$$g_I\approx\tilde{F}_I, \tag{43}$$

for all possible values of I; the Hamiltonian expectation is then reduced to a simple form

$$\langle H\rangle\approx\mathcal{H}_{\mathrm{CCM}}(\{\tilde{F}_I\};\{F_I\}), \tag{44}$$

where function $\mathcal{H}_{\mathrm{CCM}}$ is linear in $\tilde{F}_I$ and finite order in F_I. In our spin model calculation of Sec. IV, within the similar truncation involving only up to two-spin flip correlations (the so-called SUB2 approximation), the corresponding CCM calculation is to ignore all two-body and higher-order many-body distribution functions in Eq. (31). The two-spin correlation function thus calculated has unphysical behaviors as

discussed in Ref. 8. Furthermore, F_I and $\tilde{F}_I$ are not longer hermitian conjugate to one another and the energy thus calculated can not be guaranteed to be real, as is well known.

In Arponen's extension of the CCM[5], while keeping the ket state in the traditional CCM form, the bra state, also not manifestly hermitian to ket state, is parametrized by a nonlinear factor as

$$\langle\tilde{\Psi}| = \langle\Psi| e^{\tilde{S}} e^{-S}, \tag{45}$$

where correlation operators S and $\tilde{S}$ are give as in Eqs. (8)-(9). Within our variational formalism, as can be demonstrated, this representation of the bra state is equivalent to applying the random-phase approximation to the g_I equation to obtain g_I as finite-order polynormial of $\{\tilde{f}_J\}$,

$$g_I \approx g_I(\{\tilde{f}_J\}). \tag{46}$$

A detailed calculation in our spin model revealed that in the similar SUB2 truncation in Arponen's approach, the random-phase results of Eq. (40) for the two-body distribution function is reproduced. While it is clearly an improvement over the traditional CCM, Arponen's extension is also known to be poor for the strongly correlated systems (e.g., quantum Helium-4 fluid) even when high-order many-body contributions are considered. This may be related to the random-phase approximation of Eq. (46).

In conclusion, our variational extension of the CCM provides a general many-body theory in which the traditional CCM represents a simple linear approximation and Arponen's extension represents a random-phase approximation. The traditional CCM is well known to be efficient in obtaining accurate ground state energy for a finite system with a large energy gap separating the ground and excited states[12]; but, as pointed out earlier, it is poor when long-range correlations in the system are important; and Arponen's extension provides a remedy in producing the physical long range behaviors. But both these two methods are known to be poor in dealing with strongly correlated systems which demand correct description at short-range, in most cases, strongly repulsive. We believe the variational formalism represented here may provide an effective approach to the strongly correlated systems. Furthermore, its strong overlap with other well known many-body theories such as the method of correlated basis functionals can provide useful clues in making suitable approximations in practical calculations. As the necessary further truncation in our technique is flexible, different truncation approximations may be required for different physical systems and we hope to gain experience by applying the technique to a variety of systems. In this regard, we are encouraged to read a recent preprint[13] in which a fully variational approach has been employed to study several weakly interacting boson systems using the so-called independent pair correlation functions, which, in fact, is the corresponding SUB2 truncation of the Eq. (23) but writing in the real space. We like to point out that a clear advantage of the algebraic approach presented here is that it is straightforwardly extendible to include higher-order many-body correlations beyond the SUB2 level and as well as to other systems as electrons.

ACKNOWLEDGMENTS

Many useful discussions with J. Arponen, R.F. Bishop, F. Coester, and H. Kümmel are acknowledged.

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