Diagrammatic approach in the variational coupled-cluster method

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Abstract

Recently, as demonstrated by an antiferromagnetic spin-lattice application, we have successfully extended the coupled-cluster method (CCM) to a variational formalism in which two sets of distribution functions are introduced to evaluate Hamiltonian expectation. We calculated these distribution functions by employing an algebraic scheme. Here we present an alternative calculation based on a diagrammatic technique. Similar to the method of correlated-basis functionals (CBF), a generating functional is introduced and calculated by a linked-cluster expansion in terms of diagrams which are categorized and constructed according to a few simple rules and using correlation coefficients and Pauli exclusion principle (or Pauli line) as basic elements. Infinite resummations of diagrams can then be done in a straightforward manner. One such resummation, which includes all so-called ring diagrams and ignores Pauli exclusion principle, reproduces spin-wave theory (SWT). Approximations beyond SWT are also given. Interestingly, one such approximation including all so-called super-ring diagrams by a resummation of infinite Pauli lines in additional to resummations of ring diagrams produces a convergent, precise number for the order-parameter of the one-dimensional isotropic model, contrast to the well-known divergence of SWT. We also discuss the direct relation between our variational CCM and CBF and discuss a possible unification of
the two theories.

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I. INTRODUCTION

A microscopic quantum many-body theory is mainly to study correlations between the constituent particles of a quantum system. One of the most successful quantum many-body theories is the method of correlated basis functionals (CBF) [1] which includes real-space many-body correlation functions in the ground state and employs similar techniques as in classical statistical mechanics to calculate the corresponding distribution functions. The CBF has proved to be one of very few many-body theories capable of dealing with strongly correlated boson systems in liquid phase. Another successful quantum many-body theory is the coupled-cluster method (CCM) [2–4] in which excitation operators with respect to an uncorrelated model state are employed to construct the many-body correlations in an exponentiated operator factor in the ket ground-state. The distribution functions are not needed in the CCM as the Hamiltonian expectation value is straightforwardly calculated as a finite order polynomial in terms of the correlation coefficients. This is because the bra ground-state in the CCM is not the hermitian conjugate of the ket ground-state but is in a simple, linear form [5]. The CCM has proved to be one of most powerful techniques in calculating ground-state energy for many non-liquid fermion systems such as atoms, molecules and electron gas [6]. However, a general many-body theory capable of dealing with strongly correlated fermion systems in liquid phase is still needed.

In our earlier papers [7], by an application to bipartite quantum antiferromagnetic lattice systems, we have extended the CCM to a variational formalism where, in contrast to the traditional CCM, the bra and ket ground-states are hermitian conjugate to one-another. Two sets of the distribution functions were introduced to evaluate Hamiltonian expectation. We developed an algebraic scheme to calculate these distribution functions through self-consistent sets of equations. In this paper, we present an alternative scheme based on diagrams to calculate these distribution functions. As in the CBF, a generating functional is introduced and calculated by a linked-cluster expansion in terms of diagrams. These diagrams are constructed according to a few simple rules and using only three basic elements:
(a) dots representing the ket-state correlation coefficients, (b) exchange lines representing
the bra-state correlation coefficients, and (c) Pauli line representing Pauli exclusion prin-
ciple manifested by the spin-1/2 operator property \((s^\pm)^2 = 0\) in our spin model example. In
this fashion, infinite diagrams can be resummed in a straightforward manner. As a simple
application in our spin model, the spin-wave theory (SWT) \([8,9]\) is reproduced by including
all so-called ring diagrams without any Pauli line. Approximations beyond SWT by resum-
mations including Pauli lines are also given. One such approximation, which includes all
so-called super-ring diagrams by a resummation of infinite Pauli lines in addition to resum-
mations of ring diagrams, produces a convergent, precise result for the order-parameter of
the one-dimensional isotropic model, contrast to the well-known divergence of SWT. Fur-
thermore, the diagrammatic analysis discussed here forms a basis for a possible combination
of the variational CCM and CBF. Such a unified theory may prove to be capable of dealing
with strongly-correlated fermion system in liquid phase.

II. THE VARIATIONAL COUPLED-CLUSTER METHOD

We take the spin-1/2 antiferromagnetic XXZ model on a bipartite lattice as our example.
The Hamiltonian is given by

\[
H = \frac{1}{2} \sum_{l,\rho} H_{l,l+n} = \frac{1}{2} \sum_{l,n} \left( A s^z_l s^z_{l+n} + \frac{1}{2} s^+_l s^-_{l+n} + \frac{1}{2} s^-_l s^+_{l+n} \right),
\]

where \(A > 0\) is the anisotropy constant, the index \(l\) runs over all lattice sites, \(n\) runs
over all \(z\) nearest-neighbour sites, and \(s^\pm\) are the usual spin raising (+) and lowering (−)
operators. As in our earlier work using the traditional CCM \([10]\), we take the model state
as the classical Néel state with alternating spin-up and spin-down sublattices. As before,
we shall exclusively use index \(i\) for the spin-up sublattice and the index \(j\) for the spin-down
sublattice. The many-spin correlations in its ground state of Eq. (1) can then be included by
considering the excited states with respect to the uncorrelated model state. These excited
states are constructed by applying the so-called configuration creation operators \(C^i_j\) 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 $s^-_i$ and $s^+_j$; 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 $C_{ij}^\dagger = s^-_i s^+_j / 2s$, and their destruction counterpart, $C_{ij} = s^+_i s^-_j / 2s$, where $s$ is the spin quantum number. Although we are mainly interested in $s = 1/2$ in this article, we keep the factor of $1/2s$ for the purpose of comparison with the large-$s$ expansion.

As discussed in details in our earlier paper [7], we use Coester representation for both the ket and bra ground-states and write

$$ |\Psi\rangle = e^S|\Phi\rangle, \quad S = \sum_I F_I C_I^\dagger; \quad \langle \tilde\Psi | = \langle \Phi | e^{\tilde S}, \quad \tilde S = \sum_I \tilde F_I C_I, \quad (2) $$

with

$$ \sum_I F_I C_I^\dagger = \sum_{n=1}^{N/2} \sum_{i_1,...,j_1,...} f_{i_1,...,j_1,...} \frac{s_{i_1}^- s_{j_1}^+ s_{i_2}^- s_{j_2}^+ \cdots s_{i_n}^- s_{j_n}^+}{(2s)^n}, \quad (3) $$

for the ket state and the corresponding hermitian conjugate of Eq. (3) for the bra state, using notation $\tilde F_I = \tilde f_{i_1,...,j_1,...}$ for the bra-state coefficients. The coefficients $\{F_I, \tilde F_I\}$ are then determined by the usual variational equations as

$$ \frac{\delta \langle H \rangle}{\delta \tilde F_I} = \frac{\delta \langle H \rangle}{\delta F_I} = 0, \quad \langle H \rangle \equiv \frac{\langle \tilde\Psi | H | \Psi \rangle}{\langle \tilde\Psi | \Psi \rangle}. \quad (4) $$

We define the so-called bare distribution functions as

$$ g_I = \langle C_I \rangle, \quad \tilde g_I = \langle C_I^\dagger \rangle, \quad (5) $$

where we have exchanged the definition of $g_I$ with that of $\tilde g_I$ as compared with those in Ref. 7 for purely notational reason. The Hamiltonian expectation $\langle H \rangle$ is shown, in general, to be a function containing up to linear terms in $g_I$ and $\tilde g_I$ and finite order polynomial in $F_I$ (or in $\tilde F_I$) in Eq. (21) of Ref. 7:

$$ \langle H \rangle = \mathcal{H}(g_I, \tilde g_I, F_I) = \mathcal{H}(\tilde g_I, g_I, \tilde F_I). \quad (6) $$
Two systematic schemes have been developed for calculating the distribution functions of Eqs. (5): one is algebraic and the other is diagrammatic. In the algebraic approach, by taking the advantage of the properties of the operators, it is straightforward to derive the following self-consistent sets of equations for the distribution functions

\[ g_I = G(\tilde{g}_J, F_J), \quad \tilde{g}_I = G(g_J, \tilde{F}_J), \quad (7) \]

where \( G \) is a function containing up to linear terms in \( \tilde{g}_J \) (or \( g_J \)) and finite order polynomial in \( F_J \) (or \( \tilde{F}_J \)). Eqs. (7) are solved for \( g_I \) and \( \tilde{g}_I \) as a function of \( F_I \) and \( \tilde{F}_I \). The variational Eqs. (4) are then carried to determined the optimum \( F_I \) and \( \tilde{F}_I \). In this algebraic calculation, direct comparison with the traditional CCM can be made. It is shown that the CCM is a linear approximation to one set of distributions as simply \( \tilde{g}_I \approx \tilde{F}_I \), which is a poor approximation for the spin-spin correlation function and low-lying excitations. More detailed comparison was given in Ref. 7. Here we present the diagrammatic scheme similar to that in CBF to calculate these distribution functions. We like to point out that Eqs. (2) and (4)-(7) are the main general equations of the variational CCM.

### III. DIAGRAMMATIC REPRESENTATION OF GENERATING FUNCTIONAL

In this section, we calculate the bare distribution functions \( g_I \) and \( \tilde{g}_I \) of Eq. (5) by employing a diagrammatic scheme. As a demonstration, we consider a simple truncation approximation in which the correlation operators \( S \) and \( \tilde{S} \) of Eqs. (2) retain only the two-spin flip operators as (the so-called SUB2 approximation as defined in Ref. 10),

\[ S \approx \sum_{ij} f_{ij} C_{ij}^\dagger = \sum_{ij} f_{ij} s_i^- s_j^+ / 2s, \quad \tilde{S} \approx \sum_{ij} \tilde{f}_{ij} C_{ij} = \sum_{ij} \tilde{f}_{ij} s_i^+ s_j^- / 2s. \quad (8) \]

Using the usual angular momentum commutations \([s_i^z, s_j^{\pm}] = \pm s_i^{\pm} \delta_{ij}, [s_i^+, s_j^-] = 2s_i^z \delta_{ij}\), 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 any physical operators in terms distribution functions of Eqs. (5). In this approximation, for example, the expectation value of Eq. (1) is given by
\begin{align}
\langle H_{ij} \rangle &= A \langle s_i^z s_j^z \rangle + \frac{1}{2} (g_{ij} + \tilde{g}_{ij}) ,
\end{align}

where $\langle s_i^z s_j^z \rangle$ is calculated as

\begin{align}
\langle s_i^z s_j^z \rangle &= -s^2 + s \left( \sum \rho_{ij} + \sum \rho_{ij}^j \right) - \left( \sum \rho_{ij',ij}^j + \rho_{ij} \right) ,
\end{align}

$\rho_{ij}$ is the usual full one-body distribution function defined as

\begin{align}
\rho_{ij} &\equiv f_{ij} \tilde{g}_{ij} = f_{ij} \frac{\langle s_i^- s_j^+ \rangle}{2s} ,
\end{align}

and where $\rho_{ij,i',j'}$ is the full two-body distribution function defined as

\begin{align}
\rho_{ij,i',j'} &\equiv f_{ij} f_{i'j'} \tilde{g}_{ij,i'j'} = f_{ij} f_{i'j'} \frac{\langle s_i^- s_j^+ s_i'^- s_j'^+ \rangle}{(2s)^2} .
\end{align}

The order parameter is given by

\begin{align}
\langle s_i^z \rangle &= s - \rho ,
\end{align}

where $\rho = \sum_j \rho_{ij}$, taking the advantage of translational invariance.

We define a generating functional $W$ in the usual fashion as,

\begin{align}
W &\equiv \ln \langle \tilde{\Psi}|\Psi \rangle ,
\end{align}

so that the bare and full distribution functions can be simply expressed as functional derivatives of $W$. For example, the one-body and two-body bare functions are given by

\begin{align}
\tilde{g}_1 &= \langle C_1^i \rangle = \frac{\delta W}{\delta f_1} , \quad \tilde{g}_{12} = \langle C_1^i C_2^j \rangle = \frac{\delta^2 W}{\delta f_1 \delta f_2} + \tilde{g}_1 \tilde{g}_2 ,
\end{align}

where, for simplicity, we have employed notation $1 \equiv (i_1, j_1)$ so that $f_1 = f_{i_1j_1}$ etc.; and the structure function $S_{12}$ has the usual relation as in the CBF as

\begin{align}
S_{12} &\equiv f_1 \frac{\delta \rho_2}{\delta f_1} = \rho_1 \delta_{12} + \rho_{12} - \rho_1 \rho_2 ,
\end{align}

where $\rho_1 = \rho_{ii,jj}$, etc.

We now write $W$ in terms of a linked-cluster expansion.
\[ W = \text{sum of all linked cluster contributions}. \] (17)

The main task of this section is to find a diagrammatic scheme to categorize this expansion. We first expand the ket-state operator in the simplified notation, 
\[ e^S = 1 + S + \frac{1}{2!} S^2 + \cdots = 1 + f_1 C_1^\dagger + \frac{1}{2!} f_1 f_2 C_1^\dagger C_2^\dagger + \cdots, \]
where in the last equation, the summation over all indices is understood. The normalization integral,
\[ \langle \tilde{\Psi} | \Psi \rangle = 1 + \delta f_1 \delta f_1 \] (18)
can be evaluated straightforwardly for the first few terms. In the above series, the primed indices are used for bra state expansion. We notice that each term of Eq. (18) contains equal number of creation and destruction operators (otherwise, the expectation is zero).

The first-order expectation is easily calculated as
\[ \langle C_1^\dagger C_1 \rangle = \frac{1}{(2s)!} \langle \Phi | s_{j_1}^+ s_{i_1}^- s_{j_2}^+ s_{i_2}^- | \Phi \rangle = \delta_{i_1, j_2} \delta_{i_2, j_1}. \]
Hence we have, writing out the summation explicitly,
\[ \text{1st order} = \sum_i f_i \tilde{f}_i. \] (19)

The calculation of the second-order expectation \[ \langle C_2 C_1^\dagger C_2^\dagger C_1 \rangle \] is slightly more complicated. We first consider the case of \( i_1 \neq i_2 \) (i.e., \( i_1 \neq i_2 \) and \( j_1 \neq j_2 \)). There are four nonzero terms
\[ \left( \delta_{i_1, i_2} \delta_{i_2, i_1} + \delta_{i_1, i_2} \delta_{i_2, i_1} \right) \left( \delta_{j_1, j_2} \delta_{j_2, j_1} + \delta_{j_1, j_2} \delta_{j_2, j_1} \right) = \left( \delta_{i_1, i_2} \delta_{i_2, i_1} + \delta_{i_1, i_2} \delta_{i_2, i_1} \right) \left( \delta_{j_1, j_2} \delta_{j_2, j_1} + \delta_{j_1, j_2} \delta_{j_2, j_1} \right). \]
The cases when \( i_1 = i_2 \) and/or \( j_1 = j_2 \) can be easily accounted for by introducing a factor involving the usual delta functions as,
\[ \left( 1 - \frac{1}{2s} \delta_{i_1 i_2} \right) \left( 1 - \frac{1}{2s} \delta_{j_1 j_2} \right) = 1 + \Delta_{12}, \]
with a definition,
\[ \Delta_{12} \equiv -\frac{1}{(2s)} \delta_{i_1 i_2} + \delta_{j_1 j_2} + \frac{1}{(2s)^2} \delta_{i_1 i_2} \delta_{j_1 j_2}. \] (20)
This is because \( s_{i_1}^- \) \( s_{i_2}^- = (s_{i_2}^+)^2 = 0 \) for \( s = 1/2 \), a manifestation of Pauli exclusion principle. The second-order contribution is hence derived as
\[
\frac{1}{(2l)!^2} \tilde{f}_2 \tilde{f}_1 f_1 f_2 \left( \delta_{i_1' i_1} \delta_{j_1' j_1} + \delta_{i_2' i_2} \delta_{j_2' j_2} \right) \left( \delta_{j_1' j_1} \delta_{j_2' j_2} + \delta_{i_1' i_2} \delta_{j_1' j_2} \right) \left( 1 + \Delta_{12} \right)
\]

\[
\frac{1}{2!} \left[ \left( f_1 \tilde{f}_1 \right) \left( f_2 \tilde{f}_2 \right) + f_1 f_2 \tilde{f}_{i_1 j_2} \tilde{f}_{i_2 j_1} \right] \left( 1 + \Delta_{12} \right)
\]

where the second term inside the square brackets clearly represents the so-called exchange contributions. We notice that we did not consider explicitly the Pauli exclusion principle for the bra-state operators in the above derivations as the delta functions for the ket state operators also take this principle into account due to the fact that each of the bra-state operators always need to match one of the ket-state operators in order to give nonzero contribution. This is also true for higher-order terms. We also notice the expression of Eq. (20) is in fact also correct for spin quantum number \( s > 1/2 \) because, for a general \( s \),

\[
\frac{1}{2(2s)^2} \langle \Phi | (s_i^+)^2 (s_i^-)^2 | \Phi \rangle = \left( 1 - \frac{1}{2s} \right)
\]

etc. For higher-order terms in the expansion of Eq. (18), the extension of Pauli exclusion principle can be simply written as a product of two-body factors as

\[
\prod_{n>m} \left( 1 + \Delta_{nm} \right)
\]

We notice that the above product in general is not exact any more but an approximation for \( s > 1/2 \) as the three-body effects (e.g., from \( (s_i^-)^3 \) when \( i_1 = i_2 = i_3 \)) have been ignored.

In order to extend to higher-order calculations including the exchange contributions, we need a systematic graph representation. For this purpose, as shown in Fig. 1, we use a solid dot to represent the ket state coefficient \( f_1 \) with \( 1 = (i_1 j_1) \) as defined earlier; a (directed) exchange line drawing from \( i_1 \) to \( j_2 \) to represent the bra state coefficient \( \tilde{f}_{i_1 j_2} \); and a Pauli (dashed) line drawing between any two dots to represent delta function \( \Delta_{12} \) of Eq. (20).

With these graphic notations, a linked contribution is represented by a connected diagram. After the detailed calculations up to 5th order, we have established the following simple and complete rules for construction of these diagrams in the normalization integral of Eq. (18):

- The \( k \)th-order contribution consists of all possible diagrams involving \( k \) dots;
• In each diagram the number of dots equal to number of exchange lines;
• A dot is always connected by exchange lines (leaving and coming) hence exchange lines always form loops;
• Between any pair of dots one can draw at most one Pauli line;
• The contribution of each diagram is divided by its symmetry factor;
• Summations over all indices involved.

We first consider the case without any Pauli line, $\Delta_{nm} = 0$. (This is equivalent to turning spin operators to boson operators as will be shown later.) For example, the first-order contribution of Eq. (19) is simply a dot with an exchange line leaving and coming as shown as diagram $a$ in Fig. 2, where the direction of exchange line is clockwise as in most other diagrams (we therefore do not show arrows of exchange lines explicitly). The second-order contribution with $\Delta_{12} = 0$ is given by two diagrams $b$ and $c$ in Fig. 2, namely $\frac{1}{2!}(b + c)$. The 3rd-order contribution is calculated as $\frac{1}{3!}(a + 3b + 2c)$ and is shown in Fig. 3, where factor 3 for diagram $b$ is due to the three equivalent diagrams by rotation and the factor 2 for diagram $c$ comes from the two equivalent diagram with opposite directions, one clockwise the other counter-clockwise (this is referred to as parity symmetry). In similar fashion one can write down the 4th-order contribution as shown in Fig. 4 for the corresponding diagrams as

$$4\text{th order} = \frac{1}{4!}(a + 6b + 8c + 3d + 6e) ,$$

(22)

where the coefficient numbers are the symmetry factors of the corresponding diagrams. For example, the factor 6 for diagram $e$ is due to the fact that there are three equivalent diagrams each with parity symmetry factor of 2. The 5th-order contributions include 7 independent diagrams, as shown in Fig. 5, namely

$$5\text{th order} = \frac{1}{5!}(a + 10b + 20c + 15d + 30e + 20f + 24g) .$$

(23)
We notice that, in all these results, the last term represents a ring diagram with $k$ dots in the $k$th order contribution. We use $R_k$ to represent this ring diagram with the symmetry factor $(k-1)!/k! = 1/k$. For example, the 4th-order ring contribution is, writing out the summations explicitly

$$R_4 = \frac{1}{4} \sum_{1,2,3,4} f_1 \tilde{f}_{ij} f_2 \tilde{f}_{ij} f_3 \tilde{f}_{ij} f_4 \tilde{f}_{ij} .$$

(24)

Furthermore, the other terms in these $k$-order contributions are simply a product of smaller ring contributions. This property can be extended to higher order. (For this purpose one needs to apply symmetric group $S_n$ to count the number of diagrams. See, for example, Ref. 11). We are now in position to write all contributions without any Pauli line in terms of these ring diagrams. The normalization integral of Eq. (18) is then written as

$$\langle \tilde{\Psi} | \Psi \rangle_{\Delta_{nm}=0} = \sum_{k=0}^{\infty} \frac{1}{k!} \nu_1! (R_1)^{\nu_1} \frac{1}{\nu_2!} (R_2)^{\nu_2} \cdots \frac{1}{\nu_k!} (R_k)^{\nu_k} = \exp(R_1 + R_2 + R_3 + \cdots) .$$

The corresponding generating functional $W'$ without any Pauli line is simply

$$W' \equiv W \bigg|_{\Delta_{nm}=0} = \sum_{k=1}^{\infty} R_k .$$

(25)

To include Pauli lines (i.e. $\Delta_{nm} \neq 0$), we use notation $L_k$ to represents the contribution of all linked $k$-clusters and write

$$W = \ln \langle \tilde{\Psi} | \Psi \rangle = L_1 + L_2 + L_3 + \cdots .$$

(26)

Using the simple rules discussed earlier, without much difficulty, we can list all $k$-cluster contributions of $L_k$ in terms of a ring diagram $R_k$ plus all possible ways of drawing Pauli lines between any pair of $k$ dots of rings, including those pairs of dots between rings and those pairs of dots inside rings. In Fig. 6 we list all 3rd-order contributions in $L_3$ except $R_1, R_2$ and $R_3$. 

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IV. DIAGRAM RESUMMATIONS, SPIN-WAVE THEORY AND BEYOND

We first consider all diagrams without any Pauli line, namely all the ring diagram contributions $R_k$ with $k = 1, 2, \cdots$, and show that the spin-wave theory is thus reproduced. As can be seen from Eq. (20), these ring diagrams represent the first order approximation in the large-$s$ limit. In fact, in this limit, operators $s_i^{-}$ and $s_j^{+}$ behave like bosons as $s_i^{-} \rightarrow \sqrt{2s} \ a_i^\dagger$, $s_j^{+} \rightarrow \sqrt{2s} \ b_j^\dagger$ [8,9]. The corresponding wavefunction by Eq. (8) becomes the spin-wave function as

$$|\Psi\rangle \rightarrow |\Psi_{sw}\rangle = \exp \left(\sum_{ij} f_{ij} a_i^\dagger b_j^\dagger\right) |\Phi\rangle = \prod_q \exp \left(f_q a_q^\dagger b_{-q}^\dagger\right) |\Phi\rangle ,$$

where the Néel state $|\Phi\rangle$ should be considered as the vacuum state for the two sets of bosons $a_i^\dagger$ and $b_j^\dagger$ and where, in the last equation, we have made Fourier transformations using the translational symmetry as,

$$a_i^\dagger = \sqrt{\frac{2}{N}} \sum_q e^{-iq \cdot r_i} a_q^\dagger, \quad b_j^\dagger = \sqrt{\frac{2}{N}} \sum_q e^{-iq \cdot r_j} b_q^\dagger$$

$$f_{ij} = \frac{2}{N} \sum_q e^{-i(q \cdot (r_j - r_i))} f_q ,$$

with summation over $q$ restricted to the magnetic zone. The normalization integral of Eq. (27) can be easily calculated as the wavefunction is uncoupled in $q$-space. Using expansion $\exp(f_q a_q^\dagger b_{-q}^\dagger) = \sum_n (f_q a_q^\dagger b_{-q}^\dagger)^n / n!$ and a simple algebra $\langle \Phi | a_q^n (a_q^\dagger)^n | \Phi \rangle = n!$, we have the following well-known result (see, for example, Chapter 2 of Ref. 12),

$$\langle \Psi_{sw} | \Psi_{sw} \rangle = \prod_q \frac{1}{1 - f_q \bar{f}_q} .$$

The corresponding generating functional is hence given by,

$$W_{sw} = \ln \langle \Psi_{sw} | \Psi_{sw} \rangle = - \sum_q \ln \left(1 - \bar{f}_q f_q\right) = \sum_q \left[\bar{f}_q f_q + \frac{1}{2} (\bar{f}_q f_q)^2 + \cdots\right] ,$$

which is precisely the result of Eq. (25) after Fourier transformation, namely

$$W' = W_{sw} .$$
Distribution functions without any Pauli line can be easily calculated using functional derivatives of Eq. (15)-(16) with diagrammatic representation. For example, the one-body bare distribution function, \( \tilde{g}'_1 = \delta W' / \delta f_1 \), is simply represented by Fig. 7, where the action of partial derivative is equivalent to unfolding the ring. Writing out the summations explicitly, we have the expansion of Fig. 7 as,

\[
\tilde{g}'_1 = \tilde{f}_1 + \sum_2 \tilde{f}_{i_1 j_2} \tilde{f}_{i_2 j_1} + \sum_{2,3} \tilde{f}_{i_1 j_2} \tilde{f}_{i_2 j_3} \tilde{f}_{i_3 j_1} + \cdots ,
\]

(31)

and similar expansion for \( g'_1 \). A close inspection of \( \tilde{g}'_1 \) and \( g'_1 \) expansions yields self-consistency equations as

\[
\begin{align*}
\tilde{g}'_1 &= \tilde{f}_1 + \sum_2 \tilde{f}_{i_1 j_2} g'_2 \tilde{f}_{i_2 j_1} , \\
g'_1 &= f_1 + \sum_2 f_{i_1 j_2} \tilde{g}'_2 f_{i_2 j_1} ,
\end{align*}
\]

(32)

agreed exactly with Eq. (31) of Ref. 7 in this SWT approximation. The two-body functions in this approximation can also be easily obtained in this fashion as given in Ref. 7. The spontaneous magnetization of Eq. (13) is given by \( \langle s^z_i \rangle = s - \rho' \), with \( \rho' \) given by

\[
\rho' = \sum_j \rho'_{ij} = \sum_q \frac{\tilde{f}_q f_q}{1 - f_q f_q} = \frac{1}{2} \sum_q \left( \frac{1}{\sqrt{1 - \gamma_q^2}} - 1 \right) ,
\]

(33)

where we have used the reproduced SWT results of Ref. 7,

\[
\tilde{f}_q = f_q = \frac{A}{\gamma_q} (\sqrt{1 - \gamma_q^2}) , \\
\gamma_q = \frac{1}{z} \sum_n e^{i q \cdot r_n} ,
\]

(34)

where \( z \) is the coordination number and \( n \) is the nearest-neighbour index of the bipartite lattice. For one-dimensional (1D) model at isotropic point \( A = 1 \), the integral of Eq. (33) diverges, contrast to the well-known exact result of \( \rho = 1/2 \) for \( s = 1/2 \) by Bethe ansatz (see Ref. 10 for references).

To go beyond SWT, we need to include Pauli lines. Using the similar resummation technique as discussed above, we express the expansion of bare one-body distribution function \( \tilde{g}_1 \) in terms of diagrams as shown in Fig. 8, similar to the expansion in Chap. 9 of Ref. 12 and in Ref. 13, after multiplying \( f_1 \) on both sides of the equation,

\[
\rho_1 = f_1 \tilde{g}_1 = f_1 \frac{\delta W}{\delta f_1} = \text{Fig. 8} ,
\]

(35)
where we have done all resummations of ring diagrams as in Eq. (31) and hence all exchange lines in the diagrams of Fig. 8 are now function $g'_{ij}$, not the original exchange line function $f_{ij}$. For a simple approximation, we consider the first two diagrams of Fig. 8 as

$$\rho_1 \approx \rho'_1 + \rho'_1 \sum_2 \Delta_{12} \rho'_2.$$  \hspace{1cm} (36)

We notice that, after ignoring the higher-order term, Eq. (36) (without the common $f_1$ factor) agrees with the expression $\langle s_i^+ s_j^- \rangle = \langle s_i^- s_j^+ \rangle$ of SWT in Ref. 9 and with Eq. (31) of our earlier paper Ref. 7 (after changing the sign of both 5th and 6th terms in the equation as they were typos). After summing over index $j_1$ with $\rho = \sum_{j_1} \rho_{1,j_1}$, we have, using Eq. (20) for $\Delta_{12}$,

$$\rho = \rho'_1 - \frac{2}{(2s)^2} (\rho')^2 + \frac{1}{(2s)^2} \sum_j \left( \rho'_{ij} \right)^2.$$  \hspace{1cm} (37)

For $s = 1/2$ and isotropic point $A = 1$, we obtain $\rho \approx 0.127$ for the square lattice and 0.067 for the cubic lattice. They are smaller than $\rho' = 0.197$ and 0.078 of SWT respectively. This is not surprising because SWT is known to have over estimated the quantum fluctuations. The best numerical values for the square lattice vary from $\rho = 0.16$ to 0.19, including results from extrapolation of high-order localized CCM calculations [14]. For the 1D isotropic model, however, $\rho$ of Eq. (37) diverges as $\rho'$ diverges as mentioned earlier.

We next consider an approximation involving higher-order Pauli lines by including all higher-order diagrams similar to that of Eq. (36), as shown in Fig. 9. This infinite series can again be resummed in a closed form as a self-consistency equation, equivalent to replacing $\rho'_2$ in Eq. (36) by $\rho_2$ itself as

$$\rho_1 = \rho'_1 + \rho'_1 \sum_2 \Delta_{12} \rho_2.$$  \hspace{1cm} (38)

The resummation in Eq. (38) is similar to the resummation of rings in Eqs. (31)-(32), we therefore refer it as super-ring resummation. The numerical results for $\rho$ thus obtained at the isotropic point for high dimensions improve slightly, as $\rho = 0.145$ for the square lattice and 0.068 for the cubic lattice. However, for the 1D isotropic model, Eq. (38) produces a
convergent, precise number $\rho = 1/2$. This is interesting indeed, as the divergence of SWT has troubled theorists for many years. It is worth mentioning that the traditional CCM SUB2 approximation [15] also produced a convergent result for the 1D model but at $A = 0.373$, not at the isotropic point $A = 1$. We leave more discussion to the following section, and leave detailed calculations including other higher-order terms and resummations in two-body function $\rho_{12}$ and structure function $S_{12}$ of Eq. (16) somewhere else.

V. DISCUSSION

In this article, we present a diagrammatic scheme for the calculations of distribution functions of the variational CCM, as an alternative to the algebraic scheme published in our earlier papers [7]. The results of SWT are reproduced by an approximation which resums all ring diagrams without any Pauli line. Approximations beyond SWT can also easily be made by including diagrams with Pauli lines. One such approximation, which includes all super-ring diagrams by a resummation of infinite Pauli lines in addition to resummations of all ring diagrams, produces a convergent, precise number for the order parameter of the 1D isotropic model, contrast to the divergence of SWT. This cure of SWT divergence is also interesting to 2D models (including square and triangle lattices) as naive higher-order calculations within the framework of SWT are also likely to produce divergent results, despite the fact that the first order results are reasonable. We believe that similar resummations of super-ring diagrams as Fig. 9 and Eq. (38) may provide a solution for such divergent problems. We leave more detailed calculations to somewhere else.

It is also possible to include in the ground state higher-order many-body correlations such as 4-spin-flip operators, in additional to the 2-spin-flip operators of Eqs. (8). Furthermore, as demonstrated here by the diagrammatic approach, a direct link between our variational CCM and the powerful CBF has now been established, as both rely on determination of distribution functions through functional derivatives of a generating functional. In particular, as given by Eq. (13), particle density $\rho$ in CBF is equivalent to the order
parameter of our spin models as \( \langle s^z_i \rangle = s - \rho \). Its diagrammatic expansions in two theories are similar (see Chap. 9 of Ref. 12 and Ref. 13 for more CBF details). For 2D and 3D lattice models, the values of density \( \rho \) are small compared with \( s \). Such spin systems can therefore be described as dilute gases (dilute gases of quasiparticle magnons of spin waves). For the isotropic 1D model, density \( \rho \) is saturated, corresponding to the order parameter equal to zero, a critical value. Our approximation including a resummation of super-ring diagrams is capable of reproducing precisely such number. It is also interesting to know that our diagrammatic analysis of the variational CCM is for the translational invariance lattice system while similar analysis in CBF is for inhomogeneous systems \([12,13]\).

Clearly, for more accurate results in general, we need to include correlations between those quasiparticles in our ground state, and the CBF is well known to be one of most effective theories for dealing with such particle correlations (even when they are very strong as in a Helium-4 quantum liquid \([1]\)) by systematic calculations of the important two-body distribution functions. We therefore propose a unified trial wavefunction \( |\Psi_U\rangle \) as, including a generalized Jastrow correlation operator \( S^0 \) involving quasiparticle density operator \( s^z \),

\[
|\Psi_U\rangle = e^{S^0/2} |\Psi\rangle , \quad S^0 = \sum_{ij} f^0_{ij} s^z_i s^z_j ,
\]

where \( \{ f^0_{ij} \} \) are the new additional variational parameters and \( |\Psi\rangle \) is our variational CCM state of Eq. (2). The diagrammatic scheme as discussed in this article is useful for calculating the expansion of the new generating functional of Eq. (39). We have made progress in such calculations and wish to report results soon. We also believe such a unified many-body theory may prove to be capable of dealing with strongly correlated fermion systems in general.

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FIGURES

Fig. 1. Three basic elements for construction of diagrams, where simplified index notations \( i_1, j_1 \) etc. are used.

Fig. 2. First- and Second-order contributions in the expansion of Eq. (18).

Fig. 3. Diagrams of third-order contributions in the expansion of Eq. (18).

Fig. 4. Similar to Fig. 3 but for the 4th-order contributions.

Fig. 5. Similar to Fig. 3 but for the 5th-order contributions.

Fig. 6. Diagrams of up to third-order contributions to the generating functional \( W \) of Eq. (26) except ring diagrams \( R_1, R_2, R_3 \). The corresponding symmetry factors are, in the same order as the list of diagrams, \( 1/2, 1/2, 1, 1/2, 1, 1/2, 1, 1/3!, 1/2, 1/3 \).

Fig. 7. The ring expansion of the one-body bare distribution function \( \tilde{g}_1 \) of Eq. (31).

Fig. 8. First few contributions to the full one-body distribution function \( \rho_1 \) of Eq. (35), where open dots indicating no summations over its indices while solid dots indicating such summations as before.

Fig. 9. Super-ring diagram expansion, similar to the ring diagram expansion of Fig. 7 but now involving Pauli lines and with resummations of ring diagrams already carried out in all exchange lines. See texts for more details.