THEORY OF VALENCE-BOND LATTICE ON SPIN LATTICES*

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Abstract. Quantum spin-lattice systems in low dimensions exhibit a variety of interesting zero-temperature phases, some of which show non-classical (i.e., non-magnetic) long-range orders, such as dimer or trimer valence-bond order. These symmetry-breaking systems with localized valence bonds are referred to as valence-bond lattices (VBL) in this article. A review of our systematic microscopic formalism based on a proper set of composite operators for the ground and excited states of the VBL systems is given. The one-dimensional (1D) spin-$\frac{1}{2}$ frustrated model is investigated in detail. Several possible VBL systems on the 1D spin-1 chains, the 2D square and \textit{kagomé} lattices are also discussed. That our microscopic theory guarantees the rotational symmetry of the VBL systems is emphasized.

1. INTRODUCTION

Spontaneous symmetry breaking (SSB) (the symmetries of a many-body Hamiltonian not being preserved by its ground state) has always been a fascinating phenomenon in physics. Spin-lattice systems provide ample evidence for such SSB. Perhaps the most well-known example is the ferromagnetic (FM) Heisenberg models which have the classical ground state with all spins pointing in the same direction, say, along the $z$-axis, thereby breaking the rotational symmetry of its Hamiltonian.

The antiferromagnetic (AFM) counterparts, however, prove much more complicated in quantum mechanics. This is well demonstrated by the fact that even on
a bipartite lattice the classical Néel state consisting of two alternating spin-up and spin-down sublattices is no longer the eigenstate of the Hamiltonian. Despite that, a number of AFM systems show a nonzero, albeit reduced, Néel-like order. For example, the 2D spin-$\frac{1}{2}$ AFM Heisenberg model on the square lattice, which has been under intensive study since the discovery of high-temperature superconductors, is now widely believed to possess in its ground state a Néel-like order which is reduced to about two-thirds of the classical value due to quantum correlations [1,2].

In addition to the FM phase and Néel-like AFM phase, quantum spin models also exhibit SSB of non-classical (i.e., non-magnetic) types in their ground states, such as the dimerization in a spin chain with two adjacent atoms forming a spin-singlet valence-bond (VB), thereby breaking the chain lattice symmetry. Since the total spin vector of an isotropic spin system is also a good quantum number, those ground states with zero total spin vector certainly have no classical counterparts. Any long-range order in such a many-body ground state must be quantum mechanical in origin and the corresponding broken symmetry is likely to be the lattice symmetry because the rotational symmetry is preserved by such a ground state.

Working in the sector of zero total spin vector has a long history. In fact, the seminal Bethe ansatz, which provides exact solutions for the spin-$\frac{1}{2}$ Heisenberg chain, was first proved by Hulthén [3] through finite-size calculations within the framework of resonant valence-bonds (RVB), although the term “RVB” was not used then. Anderson extended this concept of RVB (originally due to Pauline) to frustrated spin-lattice systems [4], and later to the high-temperature superconductor materials [5]. More relevant to the present purposes, Majumdar and Ghosh [6] found that the perfect dimer VB configuration which breaks the lattice translational symmetry is the exact ground state of the important 1D spin-$\frac{1}{2}$ Heisenberg chain at a particular ratio of nearest-neighbour and next-nearest-neighbour coupling constants. In the last six years or so, the VB basis of low-dimensional quantum spin-lattice systems has attracted a lot of theoretical interest [7,8]. In particular, Affleck et al. [7] discovered that a homogeneous VB configuration is the exact ground state of a particular spin-1 Heisenberg-biquadratic chain. This finding sheds considerable light on the well-known Haldane conjecture [9] on the nonzero gap in the spin-1 Heisenberg chain. (The term “valence-bond solid” was then used for such a VB state, although it has no conventional symmetry breaking [10].)

An important rigorous result of quantum long-range orders is provided by a series of spin-$s$ $SU(n)$ ($n = 2s + 1$) chains (or the $SU(2)$ spin-$s$ chains with Hamiltonians which project out singlet states). This series of Hamiltonians has been solved by a mapping to the spin-$\frac{1}{2}$ $XXZ$ chain which is integrable by Bethe ansatz [11]. By the same mapping, it has been shown that the ground state of the $SU(n)$ model for any $n > 2$ breaks the lattice symmetry with a double degeneracy [12]. The exact values of the corresponding dimerization order parameter have been obtained. In particular, the dimerization order parameters for the $SU(3)$ and $SU(4)$ models are reduced to about 42% and 68% respectively [12].

Although there are no exactly-known examples, it seems possible that spontaneous trimerization, which is characterised by a sequence of spin-singlet states formed from three adjacent spins, may occur for some systems with integer spin quantum numbers since the trimer state is also a rather stable configuration. Recently this possibility has been discussed for the spin-1 Heisenberg-biquadratic chains over an
extended region of the coupling constants [13]. Furthermore, the spontaneous dimerization or trimerization may also occur in higher-order dimensionalities. For example, it has been proposed that the 2D spin-$\frac{1}{2}$ frustrated Heisenberg model on the square lattice may show a column dimer VB order over a small but nonzero region of the coupling constants [14]. A more complicated dimerization picture was suggested for the spin-$\frac{1}{2}$ Heisenberg model on the $kagomé$ lattice [15]. The trimerization of spin-1 models on the $kagomé$ lattice is also a subject to be discussed in this article.

For convenience, the term “valence-bond lattice” (VBL) is used in this article to represent collectively all those quantum spin-lattice systems in which the simple VB configurations (i.e., dimer or trimer, etc.) are localized with the broken lattice symmetry. One defines a perfect VBL as a regular array of isolated simple VB configurations on a lattice. In general, one expects that the perfect VBL is not the ground state of a given quantum spin-lattice Hamiltonian under consideration. But if the system possesses a VBL long-range order in its ground state, the perfect VBL should be a good starting point. The quantum correlations can then be analyzed on the basis of the perfect VBL. This same strategy was employed in 1952 by Anderson [1] in his AFM spin-wave theory, in which the quantum fluctuations from the classical Néel state are described by collective motions of two sets of bosons. The VBL systems are not unlike the quantum Néel-like systems, despite the complication of their ground states being in the sector of zero total spin vector rather than of zero total spin along the $z$-axis. Similar to the Néel-like systems, where the quantum fluctuations are described by the spin-flip operators (i.e., spin raising and lowering operators) with respect to the Néel model state, a proper set of composite operators first developed by Parkinson in 1979 [16] is used to describe the quantum correlations with respect to the perfect VBL model state. A similar spin-wave theory can then be made by a bosonization scheme for those composite operators. But a more systematic approach is provided by a powerful microscopic quantum many-body theory, namely the coupled-cluster method [17], based on those composite operators themselves. The restriction in the sector of zero total spin vector is guaranteed by a very useful and important theorem of the CCM.

Recently, Bishop, Parkinson and Xian [18] have successfully applied the CCM to a number of quantum spin systems, including the spin-$\frac{1}{2}$ AFM Heisenberg model on the square lattice. In their analysis, the Néel state was taken as a model state for the anisotropic-Heisenberg AFM systems. Upon the Néel model state the many-spin correlations are incorporated via a so-called correlation operator consisting of the spin raising and lowering operators with respect to the model state. Within a well-defined systematic approximation scheme amenable to computer-algebraic techniques, they have obtained excellent results for the ground-state energy, excitation spectra, and staggered magnetization as functions of the anisotropy parameter. Their CCM analysis not only produces the numerical results which are among the best estimates available today, but also enables them to study the quantum phase transition of the anisotropic-Heisenberg systems in an extremely systematic fashion [19]. From these experiences, one expects that the CCM analysis should yield similar good quantitative results for the VBL systems.

Because of its simplicity, our microscopic analysis for the spin-$\frac{1}{2}$ frustrated chains is first given. Then the same analysis is extended to other systems, including some spin models on the 2D square and $kagomé$ lattices. The outline of this article is as follows.
Sec. 2 considers the few-body systems and introduces the corresponding composite operators and their boson transformations. Sec. 3 is devoted to the study of the 1D spin-$\frac{1}{2}$ frustrated model, firstly by the spin-wave approximation via a bosonization of those composite operators, secondly by the more systematic CCM analysis based on the composite operators themselves. Extensions of the same analysis to the other systems, including the spin-1 Heisenberg-biquadratic chains and the some 2D models on the square lattice and the kagomé lattice, are discussed in Sec. 4. A general discussion is given in Sec. V to conclude this article. A brief proof of the important symmetry theorem of the CCM is given in the Appendix.

2. FEW-ATOM SYSTEMS AND VALENCE-BONDS

As outlined in Sec. 1, our microscopic theory for a VBL system is based on a set of composite operators which are defined according to the Hilbert space of the corresponding few-atom system. Our discussion here is restricted to the two-atom and three-atom systems. The boson transformation of those composite operators and the spin VB notations are also given.

2.1 Two-Atom Systems

A two-atom system, each with spin $\frac{1}{2}$, has four states, a singlet and triplet states. The singlet state can be written, in the obvious notation, as

$$|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle); \quad (2.1)$$

and the triplet states are, respectively

$$|1\rangle = |\uparrow\uparrow\rangle, \quad |2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad |3\rangle = |\downarrow\downarrow\rangle. \quad (2.2)$$

In a matrix representation, one denotes each of these four states by a column matrix with a single nonzero element. Any operator in this Hilbert space can then be written as a $4 \times 4$ matrix. Following Parkinson [16], operator $A_{mn}$ is introduced as having only a single non-zero element in a $(4 \times 4)$ matrix, namely $\langle m'|A_{mn}|n'\rangle = \delta_{mm'}\delta_{nn'}$. All single spin operators can now be written in terms of these sixteen, namely

$$s_1^z = \frac{1}{2}(A_{02} + A_{20} + A_{11} - A_{33}), \quad s_2^z = \frac{1}{2}(-A_{02} - A_{20} + A_{11} - A_{33}), \quad (2.3a)$$

$$s_1^- = \frac{1}{\sqrt{2}}(A_{30} - A_{01} + A_{21} + A_{32}), \quad s_2^+ = \frac{1}{\sqrt{2}}(A_{01} - A_{30} + A_{21} + A_{32}), \quad (2.3b)$$

$$s_1^+ = \frac{1}{\sqrt{2}}(A_{03} - A_{10} + A_{12} + A_{23}), \quad s_2^- = \frac{1}{\sqrt{2}}(A_{10} - A_{03} + A_{12} + A_{23}). \quad (2.3c)$$

The inverse transformations are clearly nonlinear. Therefore $A_{mn}$ has been referred to as a composite operator [13]. In particular, $A_{00}$ corresponds to the spin-singlet projection operator, namely $A_{00} = 1/4 - s_1 \cdot s_2$. 

4
We notice that $A_{10}$ ($A_{30}$) is an operator which increases (decreases) $s^z_{\text{total}}$ ($\equiv s^z_1 + s^z_2$) by one unit, while $A_{20}$ leaves $s^z_{\text{total}}$ unchanged; their Hermitian conjugates (i.e., transpose matrices) have the opposite effects. Since any of the triplet states can be generated by letting $A_{n0}$ ($n = 1, 2, 3$) operate on the singlet state $|0\rangle$, $A_{n0}$ play the role of creation operators with respect to $|0\rangle$; their transpose matrices correspond to the destruction operators. Using the following algebra

$$A_{mn}A_{kl} = A_{ml}\delta_{nk}, \quad (2.4)$$

which follows by definition, it is easy to see that any $A_{mn}$ can be expressed by a product of $A_{m0}$ and $A_{0n}$.

For a two-atom system each with spin 1, the dimension of the Hilbert space is nine. The total number of composite operators $A_{mn}$ ($m, n = 0, 1, 2, \ldots, 8$) is eighty-one. Among them are eight pairs of creation and destruction operators with respect to the singlet state. As in the spin-$\frac{1}{2}$ case, if one chooses the the singlet state

$$|0\rangle = \frac{1}{\sqrt{3}}(|1, -1\rangle + |-1, 1\rangle - |0, 0\rangle), \quad (2.5)$$

the eight pairs of the creation and destruction operators with respect to $|0\rangle$ are then denoted as $A_{n0}$ and $A_{0n}$ ($n = 1, 2, \ldots, 8$) respectively.

### 2.2 A Three-Atom System

Similar to the two-atom systems discussed above, in order to construct the composite operators of a three-atom system, one should list all of its states. Consider the spin-1 case. There are $3^3 = 27$ states. Ref. [13] lists all of them in detail. Again, the singlet state

$$|0\rangle = \frac{1}{\sqrt{6}}(|0, 1, -1\rangle + |1, -1, 0\rangle + |-1, 0, 1\rangle - |0, -1, 1\rangle - |-1, 1, 0\rangle - |1, 0, -1\rangle), \quad (2.6)$$

is the first state, and the nine states of $s^z_{\text{total}} = 1$ ($s^z_{\text{total}} \equiv s_1 + s_2 + s_3$) follow, and so on, until the last state with all three down spins.

As before, $A_{00}$ for the present case is also the spin singlet projection operator by definition, and can be written as

$$A_{00} = \frac{1}{18}S_{123}(6 + S_{123} - S^2_{123}), \quad S_{123} \equiv s_1 \cdot s_2 + s_2 \cdot s_3 + s_3 \cdot s_1; \quad (2.7)$$

the creation and destruction operators with respect to the singlet state $|0\rangle$ of Eq. (2.6) are similarly given by $A_{n0}$ and $A_{0n}$ ($n = 1, 2, \ldots, 26$). In Ref. 13, an approximation is made by truncating the Hilbert space from twenty-seven states to the first ten (i.e., restricting to the subspace of $s_{\text{total}} = 0$ and 1). In this subspace, there are only nine pairs of creation and destruction operators which can be easily managed.

### 2.3 Bosonization of Composite Operators

A bosonization scheme for a set of operators usually starts from a reference. The reference of the bosonization scheme (e.g., Holstein-Primakoff transformation) in the
conventional spin-wave theory [1] is either the spin-up state or spin-down state. The reference for our present purpose is clearly the singlet state $|0\rangle$ of the corresponding few-spin system. Therefore, the similarities between operators $s^z$ and $A_{00}$ and between $s^+ (s^-)$ and $A_{n0} (A_{0n})$ can be clearly seen.

While $s^z$ and $s^\pm$ obey the usual $SU(2)$ angular momentum algebras, from Eq. (2.4), it is easy to see that $A_{mn}$ obey the following pseudo-spin algebra,

$$[A_{mn}, A_{kl}] = A_{ml} \delta_{nk} - A_{kn} \delta_{lm}. \quad (2.8)$$

Therefore, $A_{mn}$ has also been referred to as a pseudo-spin operator. From Eq. (2.8) one can make the following Dyson-Maléciv-like transformation,

$$A_{00} = 1 - \sum_{n=1}^{d-1} a_n^+ a_n; \quad A_{n0} = a_n^+ A_{00}, \quad A_{0n} = a_n; \quad A_{mn} = a_m^+ a_n, \quad (2.9)$$

where $m, n = 1, 2, \ldots, d-1$ with $d$ the Hilbert space dimensionality of the few-atom system, and where $a_n, a_n^+$ are $(d-1)$ sets of boson operators, obeying the usual boson commutation, $[a_m, a_n^+] = \delta_{mn}$.

By definition, the singlet state $|0\rangle$ is the vacuum state of the bosons, namely, $a_n|0\rangle = 0, n = 1, 2, \ldots, d-1$. The physical states correspond to the vacuum state $|0\rangle$ and the $(d-1)$ states with only one boson excited. Furthermore, as the matrix elements between the physical and unphysical subspaces are equal to zero, the transformation given by Eqs. (2.9) is exact at zero temperature just as in the case of the conventional spin-wave theory [1].

### 2.4 Valence Bonds

In the above analysis, the singlet state is always taken as the reference with respect to which creation and destruction operators are defined. This is the essence of our microscopic theory for the VBL systems.

As is well known, spin singlet states can be conveniently represented in terms of VB which in turn can be expressed by Schwiniger bosons [7,8]. Schwiniger boson representation is given by the following transformation,

$$s^+ = a^+ b, \quad s^- = a b^+, \quad s^z = \frac{1}{2}(a^+ a - b^+ b), \quad (2.10)$$

where $a, a^+$ and $b, b^+$ obey the usual boson commutations. It should be emphasized that Schwiniger bosons are used here purely for the notational purpose. They should not be confused with the bosonization scheme of Eq. (2.9). A spin-$s$ state with $s^z = m (-s \leq m \leq s)$ is written in the Schwiniger representation as

$$|s, m\rangle = \frac{(a^+)^{s+m} (b^+)^{s-m}}{\sqrt{(s+m)!} \sqrt{(s-m)!}} |V\rangle, \quad (2.11)$$

where $|V\rangle$ is the vacuum state of the bosons. A spin VB between atoms $i$ and $j$ is defined by a number of the so-called VB operators [8]

$$C_{ij}^+ = a_i^+ b_j^+ - a_j^+ b_i^+, \quad (2.12)$$
Figure 1. Three VB configurations: (a) spin-$\frac{1}{2}$ dimer, (b) spin-$1$ dimer and (c) spin-$1$ trimer. A single bond is defined by $C^+_{ij}$ of Eq. (2.12).

acting on the vacuum state $|V\rangle$. Using Eq. (2.11), it is easy to see that the spin-singlet states of Eqs. (2.1), (2.5) and (2.6) can be conveniently written respectively, apart from the trivial normalization factors, as one-bond $C^+_{12}|V\rangle$, two-bond $(C^+_{12})^2|V\rangle$, and three-bond $C^+_{12}C^+_{23}C^+_{31}|V\rangle$ configurations.

A general VB configuration can be easily drawn for a spin-$s$ many-spin system. In Fig. 1, two dimer and one trimer configurations are shown. A many-spin ground state with zero total spin vector $s_{\text{total}} \equiv \sum_i s_i = 0$ is in general given by a linear summation of all independent VB configurations in which each atom is linked by $2s$ VBs [7,8]. In general, different many-spin VB states are not orthogonal to one another. This makes working in the VB basis very difficult. But the ground state of some interesting quantum systems is dominated by a particular VB state consisting of an array of independent simple VBs such as those shown in Fig. 1. These are the VBL systems defined in Sec. 1. In the following sections, a systematic microscopic theory is developed by taking these perfect VBLs as the reference state and by employing the creation and destruction operators $A^+_{n0}$ and $A_{0n}$ with respect to this reference.

3. THE SPIN-$\frac{1}{2}$ FRUSTRATED CHAINS

3.1 Spin-Wave Theory

The 1D spin-$\frac{1}{2}$ frustrated model is perhaps the simplest model with spontaneous dimerization. The model consists of $N$ atoms each with spin $\frac{1}{2}$ on a chain with nearest-neighbour and next-nearest-neighbour interactions. The Hamiltonian is simply

$$H = \sum_{i=1}^{N} (s_i \cdot s_{i+1} + J s_i \cdot s_{i+2}),$$

where $J$ is the coupling constant, the usual periodic boundary condition is assumed, and even $N$ and a unit lattice spacing are also chosen for convenience. At $J = 0$, $H$ is the well-known Heisenberg model which was solved exactly by Bethe ansatz [3]; its ground state is gapless and has no long-range order. At $J = 1/2$, the ground state is given by the dimer VB configuration as shown in Fig. 1 (a) with a double degeneracy.
\[ |D\rangle = \prod_{r=1}^{N/2} |0\rangle_{2r-1,2r}, \]

where the notation \( |0\rangle_{i,j} \) represents the singlet state of the pair given by Eq. (2.1).

Let \( r \) denote each dimer in Fig. 1 (a), and \( s_1(r) \) and \( s_2(r) \) the two spins of the dimer, Eq. (3.1) becomes

\[ H = \frac{N}{2} \sum_{r=1}^{N/2} [s_1(r) \cdot s_2(r) + s_2(r) \cdot s_1(r+1) + Js_1(r) \cdot s_1(r+1) + Js_2(r) \cdot s_2(r+1)]. \]

One can then express \( H \) in terms of the composite operators \( A_{mn} \) by Eqs. (2.3).

As discussed in Sec. 2, since the fluctuations with respect to \( |D\rangle \) can be described by operators \( A_{00} \) and \( A_{0n}^n \) (\( n = 1, 2, 3 \)), one can derive the equations of motion for all of these three sets of pairs. By employing the usual decoupling approximations and taking \( A_{00} \approx 1 \), it is easy to derive the spin-wave spectra (i.e., eigen modes). Parkinson [16] employed this method to obtain the triplet spectrum for the Heisenberg model \((J = 0)\).

Application of bosonization scheme not only provides a more systematic means to obtain the excitation spectra, but also allows one to study the ground-state properties as well. By Eqs. (2.9), one can further express \( H \) in terms of the three sets of bosons (a polynomial up to sixth order). Diagonalization of the quadratic parts of \( H \) by the usual Bogoliubov transformations, one can easily obtain the ground-state energy \( E_0 \) and excitation spectra \( \omega_q \) within the spin-wave approximation. They are given by respectively

\[ \frac{E_0}{N} = \frac{3}{4} \int_0^\pi dq \frac{2}{\pi} [\sqrt{1 - (1 - 2J) \cos 2q} - 1] - \frac{3}{8}, \]

and

\[ \omega_q = \sqrt{1 - (1 - 2J) \cos 2q}. \]

Eq. (3.5) agrees with that of Parkinson at \( J = 0 \) [16]. A discussion of these results is left to the end of this section.

3.2 The Coupled-Cluster Method

The CCM has been successfully applied to a wide range of quantum many-body problems in both physics and quantum chemistry [17]. The interested reader is referred to Ref. [17] for the general formalism of the CCM and to Ref. [18] for its particular application to the spin systems with the Néel-like order. Here its extension to the VBL systems is considered.

(a). The Ground State

The CCM ansatz for the ground ket state is \( |\Psi_g\rangle = e^S|\Phi\rangle \), where \( |\Phi\rangle \) is the so-called model state which is usually chosen as an uncorrelated many-body wavefunction, and where \( S \) is the many-body correlation operator consisting purely of the creation operators with respect to \( |\Phi\rangle \). For the VBL problem under consideration,
it is quite natural to choose the perfect VBL state as the model state. The creation operators with respect to this model state are clearly given by any combination of those operators $A_{n0}^r$ with $n = 1, 2, \ldots, d - 1$, where $d$ is the dimensionality of the corresponding few-spin system and $r$ denotes its vector position in the VBL. Their Hermitian conjugates $A_{n0}^r$ are the corresponding destruction operators.

The Schrödinger equation of the ground state, after a simple manipulation, can then be written as

$$e^{-S}He^{S}|\Phi\rangle = E_g|\Phi\rangle,$$

where $E_g$ is the ground-state energy, and where the similarity-transformed Hamiltonian can be expressed as a series of nested commutators, namely

$$e^{-S}He^{S} = H + [H, S] + \frac{1}{2!}[H, S, S] + \cdots,$$

which usually terminates at the fourth-order for most Hamiltonians with pair-interaction potentials [17,18]. For the present case, the series of Eq. (3.7) terminates because Hamiltonians always contain a finite-order polynomial of the destruction operators.

Now let us focus on the spin-$\frac{1}{2}$ dimerization. The model state is the given by the dimer state, $|\Phi\rangle = |D\rangle$. There are three sets of creation operators, namely $A_{10}^r$, $A_{20}^r$, and $A_{30}^r$. If one restricts to the sector of zero $s^z_{\text{total}} (\equiv \sum_i s^z_i)$, the correlation operator $S = \sum_{n=1}^{N/2} S_n$, with

$$S_1 = \sum_{r=1}^{N/2} S_r A_{20}^r,$$

$$S_2 = \sum_{r,r'} \left[ S_{r,r'}^{(1)} A_{10}^r A_{30}^r - \frac{1}{2!} S_{r,r'}^{(2)} A_{20}^r A_{20}^r \right],$$

etc. In Eq. (3.8) the primes on the summations imply exclusion of the terms with any pair of indices being equal.

The ground-state energy is obtained by taking the inner product of the Schrödinger equation (3.6) with the model state $|D\rangle$ itself, namely

$$E_g = \langle D|e^{-S}He^{S}|D\rangle;$$

and the correlation coefficients $\{S_{r,r',...}\}$ in Eqs. (3.8) are determined by the coupled set of equations obtained by taking inner products of Eq. (3.6) with states constructed from the corresponding destruction operators, namely

$$\langle D|A_{n0}^r e^{-S}He^{S}|D\rangle = 0, \quad \forall r,$$

for the one-body equation; and

$$\langle D|A_{n1}^r A_{n2}^r e^{-S}He^{S}|D\rangle = 0, \quad \langle D|A_{n2}^r A_{n0}^r e^{-S}He^{S}|D\rangle = 0, \quad \forall r, r' (\neq r)$$

for the two-body equations. The three-body equations and higher-order many-body equations are obtained in a similar fashion.

9
The exact energy equation (3.9) can be straightforwardly derived as
\[
\frac{E_g}{N} = \frac{1}{8}[(1 - 2J)(2b_1^{(1)} + b_1^{(2)}) - a] - 3, \tag{3.12}
\]
where the lattice symmetry is used to set accordingly \( S_r = a \), \( S_{r_1,r_2}^{(l)} = S_{r_2,r_1}^{(l)} = b_r^{(l)} \), with \( l = 1, 2 \) and \( r = r_2 - r_1 \).

The exact one-body equation (3.10) can also be easily derived. It couples only to the two-body and three-body coefficients. Similarly, the two-body equations (3.11) couple only to the one-body, three-body and four-body coefficients, and so on. One clearly needs to employ an approximation scheme for a practical calculation. The most common approximation of the CCM is the \( \text{SUB}_n \) scheme which retains up to \( n \)-body correlation operators. Here the \( \text{SUB}_2 \) scheme is considered, namely \( S_{\text{SUB}_2} = S_1 + S_2 \) and \( S_n = 0 \) for \( n \geq 3 \). The one-body equation (3.10) yields an interesting solution, \( a = 0 \), implying no one-body correlations for the dimerization problem. Furthermore, the two-body equations (3.11) provide a solution in which the two sets of two-body coefficients are identical, namely
\[
b_r^{(1)} = b_r^{(2)} \equiv b_r. \tag{3.13}
\]
We notice that the model state \( |D\rangle \) is in the sector of \( s_{\text{total}} = 0 \), and the one-body correlation operator \( S_1 \) will take the state out of this sector. We also notice that the two-body correlation operator \( S_2 \) commutes with \( s_{\text{total}} \) if and only if Eq. (3.13) is satisfied. All these imply that the ground state in our \( \text{SUB}_2 \) approximation remains in the sector of \( s_{\text{total}} = 0 \) despite the fact that we started with operators in the sector of \( s_z^{\text{total}} = 0 \). In fact, this nice property also holds at higher-order approximations in the above CCM analysis. Appendix provides a brief proof for a general theorem which states that the CCM coupled equations [e.g., Eqs. (3.10) and (3.11)] at any level of approximations always provide at least a solution which guarantees the symmetry of the model state if this symmetry is one of those belonging to the model Hamiltonian. This is certainly a big advantage because it is much more difficult to work in the sector of \( s_{\text{total}} = 0 \) than of \( s_z^{\text{total}} = 0 \).

The energy equation is now reduced to
\[
\frac{E_g}{N} = \frac{3}{8}[(1 - 2J)b_1 - 1], \tag{3.14}
\]
and, after simplification, the two equivalent two-body equations in the \( \text{SUB}_2 \) scheme are given by
\[
\frac{1}{2} \sum_{\rho = \pm 1} (K_3 \delta_{r \rho} + K_2 b_r - 2K_1 b_{r+\rho} + K_1 \sum_{r' \neq 0} b_r b_{r+\rho-r'}) = 0, \quad r \neq 0 \tag{3.15}
\]
with \( K_1 \equiv 1 - 2J \), \( K_2 \equiv 4(1 - 2K_1 b_1) \), and \( K_3 \equiv K_1 (1 + 4b_1^2) - 2(1 + 2J)b_1 \). A simpler approximation can be made from Eq. (3.15), namely the \( \text{SUB}_2 \)-2 scheme which retains only the single coefficient, \( b_1 \). Eq. (3.15) then reduces to
\[
1 - 2J + 2(3 - 2J)b_1 - 9(1 - 2J)b_1^2 = 0, \tag{3.16}
\]
which is easily solved. The full SUB2 equation (3.15) can also be solved analytically by a Fourier transformation method in a similar fashion as described in Ref. 18. Here only the final result is given by the following self-consistency equation for \( b_1 \),

\[
b_1 = \frac{1}{3K_1} \left( 2 - \frac{K_2}{2} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq \sqrt{1 - k_1 \cos 2q + k_2 \cos^2 2q} \right),
\]

(3.17)

where the constants \( k_1 \) and \( k_2 \) are defined by

\[
k_1 \equiv \frac{1}{K_2^2} (4K_1 K_2 + 8K_1^2 b_1 - 4K_1^2 X), \quad k_2 \equiv \frac{4K_1 (K_1 - K_3)}{K_2^2},
\]

(3.18)

and where \( X \equiv \sum_{r=1}^{N/2} b_r b_{r+1} \), which can be calculated self-consistently as \( b_1 \) of Eq. (3.17). After \( b_1 \) is determined as a function of \( J \), the ground-state energy is obtained by Eq. (3.14). Again the discussion of these results is left to the end.

(b). The Excited States

The CCM ansatz for the excited state is \( |\Psi_e⟩ = X |\Psi_g⟩ = X e^S |Φ⟩ \), where \( |\Psi_g⟩ \) is the ground state as determined above and \( X \) is the excitation correlation operator consisting only of the creation operators as \( S \) does. Using the Schrödinger equations for the ground and excited states, one obtains

\[
e^{-S} [H, X] e^S |Φ⟩ = e X |Φ⟩, \quad e \equiv E_e - E_g.
\]

(3.19)

In the so-called SUB(2,1) scheme, one retains up to two-body correlations in \( S \) and one-body correlations in \( X \), namely, \( S \to S_{\text{SUB2}} = S_1 + S_2 \) and \( X \to X_1 \). Therefore one writes, \( X_1 = \sum_r X_r A'^{r}_{10} \). The other two one-body excitation operators are given by replacing \( A'^{r}_{10} \) by \( A^{r}_{20} \) and \( A^{r}_{30} \) respectively. The coefficient \( X_r \) is determined by the inner product of Eq. (3.19) with the state \( A'^{r}_{10} |Φ⟩ \). A Fourier transformation readily yields the following excitation spectrum with a lattice momentum \( q \),

\[
e_q = \frac{K_2}{4} \sqrt{1 - k_2 \cos 2q + k_2 \cos^2 2q},
\]

(3.20)

where the constants \( K_2, k_1 \) and \( k_2 \) are as defined before. The other two excited states with operator \( A^{r}_{50} \) and \( A^{r}_{50} \) produce the same spectrum. Therefore \( e_q \) is a triplet spectrum as expected.

3.3 Discussion

Fig. 2 shows the results of the ground-state energy per atom as a function of \( J \) from the spin-wave approximation, and from the SUB2-2 and full SUB2 schemes of the CCM. The numerical results [20] of Tonegawa and Harada, obtained by extrapolating the finite-size calculations for \( J < 1/2 \), and the exact results by Parkinson of the \( N = 20 \) system for \( J > 1/2 \), are also included for comparison. At \( J = 1/2 \) (i.e., the Majumdar-Ghosh point) both spin-wave theory and the CCM approximations give the exact result of \(-3/8\). This is not surprising because both take the dimer state \( |D⟩ \) as
their model state. At $J = 0$ (the Heisenberg point), spin-wave theory yields $-0.4498$, while the SUB2-2 and full SUB2 schemes yield $-0.4268$, $-0.4298$ respectively. They all agree with the exact result of $-0.4432$ by the Bethe ansatz [3]. But we notice that at $J = 0$ spin-wave theory produces divergent results for other physical quantities such as the dimerization parameter discussed later. Furthermore, as can be seen from Fig. 2, the energy curve of spin-wave theory is symmetric about $J = 1/2$, while the extremely simple SUB2 scheme gives much better results for a wide range of the coupling constant $J$ when compared with the numerical results of Ref. [20].

We notice that both spin-wave theory and the SUB2 scheme have two terminating points $J_c^{(1),(2)}$, beyond which, namely for $J < J_c^{(1)}$ and $J > J_c^{(2)}$, there is not real solution. For spin-wave theory, the two points are given by $J_c^{(1)} = 0$ and $J_c^{(2)} = 1$, while $J_c^{(1)} = -0.4443$ and $J_c^{(2)} = 1.591$ from the SUB2 scheme. The corresponding energy values of the SUB2 scheme are $-0.5172$ and $-0.6977$ respectively. In the past we had identified the SUB2 terminating points as the phase transition critical points for the anisotropic-Heisenberg models [18]. This is strongly supported by the calculations of the spin correlation functions and order parameters within the same CCM analysis. The following discussion of the triplet spectra of the spin-wave excitations also supports that the two terminating points $J = J_c^{(1),(2)}$ of the present dimerization case may again correspond to the quantum phase transitions of the frustrated systems.

Figure 2. Ground-state energy per atom as a function of $J$. Shown are the results from the spin-wave theory (dotted), the SUB2-2 scheme (short-dashed), and the full SUB2 scheme (long-dashed). The terminating points are indicated. The numerical results from Ref. [20] are also included (solid).
The triplet spectra of Eq. (3.5) and Eq. (3.20) have the same qualitative behaviour. Fig. 3 shows the schematic plot of the spectrum from the SUB(2,1) scheme of the CCM at several values of \( J \). The spectrum clearly shows a nonzero gap between the two terminating points and the gap collapses at both the terminating points. In particular, the triplet spectrum is flat with a gap value of 1 at \( J = 1/2 \). This flatness implies no coupling between pairs of spins (dimers) at \( J = 1/2 \) within the approximations. Since the simple dimer state \( |D⟩ \) is the exact ground state at this point, the two-body correlation can be easily included in the excitation operator \( X \) and the corresponding two-body coefficients can be determined by a simple variational procedure similar to the well-known Feynman theory for the excitation spectrum of the \(^4\)He superfluid [21]. Hence the excitation operator with a lattice momentum \( q \) is written as,

\[
X_q = \sum_r e^{2iqr} A^r_{10} + \sum_{r,r'} f_q(r, r') A^r_{10} A^{r'}_{20}. \tag{3.21}
\]

Taking \( f_q(r, r') \) as the variational parameter to optimise the expectation value of the Hamiltonian, it is found that the gap in the spectrum is reduced by half at \( q = 0 \) and \( \pi \), but remains at 1 at \( q = \pi/2 \) [22]. (The preliminary calculations of the similar SUB(2,2) scheme not only yield similar results at \( J = 1/2 \) but the whole spectrum as a function of \( J \) [22].) These results of the triplet spectrum from such a low-order approximation seem to agree with a more substantial calculation at \( J = 1/2 \) by Shastry and Sutherland [23]. They obtained the spectrum of a soliton-like excitation with a minimum gap of 0.25 at \( q = 0 \) and \( \pi \) and a maximum gap of about 1 at \( q = \pi/2 \). Tonegawa and Harada’s numerical calculations [20] confirmed the nonzero gap at \( J = 1/2 \) and in the nearby region. They predicted that the gap collapses at \( J_0 \approx 0.3 \), while Haldane [24], who used a fermion representation, predicted this value to be about 1/6. Recently, \( J_0 \) has been estimated by the conformal field theory to be about 0.2411 [25]. In any case, this gapless point may correspond to a phase transition from the dimerized phase to a critical phase similar to the Heisenberg model at \( J = 0 \).

A more intriguing situation occurs for \( J > 1/2 \), where the triplet spectrum of both spin-wave theory and the SUB(2,1) scheme has a minimum at \( q = \pi/2 \). This certainly reminds us of the magneto-roton excitations in the fractional quantum Hall effects [26]. As \( J \) increases, the minimum (spin-roton gap) decreases and finally at \( J = J_c^{(2)} \), it collapses at \( q = \pi/2 \). Whether or not this suggests a phase change in the spatial periodicity of the system from double to four-fold, for example, is still unclear. The numerical calculations of the spin-spin correlation function [20] certainly show a more complicated feature for \( J > 1/2 \). In particular, the short-range four-fold Néel order (\( \uparrow \downarrow \uparrow \downarrow \cdots \)) is observed for \( J > 1/2 \), contrast to the case of \( J < 1/2 \) where the ordinary short-range two-fold Néel order (\( \uparrow \downarrow \cdots \)) is observed [27]. As we know, at \( J = \infty \), the model Hamiltonian of Eq. (3.1) becomes two uncoupled Heisenberg chain with a double lattice spacing showing a four-fold spatial periodicity. Clearly, higher-order calculations are needed to obtain a clearer picture.

To conclude this section, it should be pointed out that the dimerization order parameter, defined by \( D \equiv \langle s_{i-1} \cdot s_i \rangle - \langle s_i \cdot s_{i+1} \rangle \), can be easily obtained within spin-wave theory and the SUB2 scheme of the CCM. In spin-wave theory, for example, \( D \) is found to be nonzero in the region of \( 0 < J < 1 \) and gradually diminish when \( J \) moves toward the two terminating points; but at the two terminating points (\( J = 0, 1 \)), \( D \) diverges to \(-\infty\), implying a breakdown of spin-wave theory. The SUB2 scheme of
the CCM, however, yields converging results even at the two terminating points, as it is the case in our previous CCM analysis for the 1D anisotropic-Heisenberg model [18]. Since it also involves the ground bra state which is not manifestly the Hermitian conjugate of the ground ket state in the CCM, our CCM analysis for the dimerization order parameter and correlation functions will appear elsewhere.

4. OTHER SYSTEMS

4.1 The Spin-1 Chains

Recently, the 1D Heisenberg-biquadratic spin-1 chain has attracted much attention because it provides very rich and interesting quantum phases. The model Hamiltonian is given by

\[ H = \cos \theta \sum_i s_i \cdot s_{i+1} + \sin \theta \sum_i (s_i \cdot s_{i+1})^2, \quad s = 1 \]  \hspace{1cm} (4.1)

where the coupling between spins is parametrized by \( \theta \). The FM phase is restricted to the region of \( \pi/2 \leq \theta \leq 5\pi/4 \), and the rest is non-FM.

There are a number of exact results available at several values of \( \theta \). In particular, at \( \theta = -\pi/2 \), the system is exactly known to be dimerized with a nonzero gap and the corresponding order parameter is about 42% of the perfect dimer state [11,12]. At \( \tan \theta = 1/3 \), the ground state is given by a homogeneous VB configuration with a nonzero energy gap but with no lattice symmetry breaking [7]. At \( \theta = \pi/4 \), the model is again integrable, the ground state clearly shows a triple spatial periodicity and the excitation spectrum becomes gapless at the lattice momentum \( q = 0 \) and 2\( \pi/3 \).
Figure 4. Expectation values of the 1D spin-1 Hamiltonian as a function of θ with respect to the three simple VB states: homogeneous (dotted), dimer (short dashed), and trimer (long dash). Also shown are the results from finite-size exact calculations (solid).

[28]. Based on these exact results, one tends to conclude that the system may show different phases representing by the three VB states respectively, namely the dimer state as shown in Fig. 1 (b), the trimer state in Fig. 1 (c) and the homogeneous VB state discussed in Ref. [7]. The expectation values of the Hamiltonian with respect to these three trial wavefunctions can be straightforwardly obtained as

\[
E_0 = \begin{cases} 
-\frac{4}{3} \cos \theta + 2 \sin \theta, & \text{homogeneous;} \\
-\cos \theta + \frac{8}{3} \sin \theta, & \text{dimer;} \\
-\frac{2}{3} \cos \theta + \frac{10}{9} \sin \theta, & \text{trimer.}
\end{cases}
\] (4.2)

These values are shown in Fig. 4 as a function of θ, together with the numerical results from finite-size exact calculations [18]. One sees that the dimer state has lower energy than that of the homogeneous VB state for θ < tan \(^{-1}(-1/2) \approx -26.6^\circ\); for larger θ, however, the homogeneous VB state has lower energy. In particular, the homogeneous VB state is the exact ground state at tan θ = 1/3 [7]. At even larger θ, it is interesting to see that the trimer state has the lowest energy. This occurs when θ > tan \(^{-1}(3/4) \approx 36.9^\circ\). The lower envelope of the three curves is in general quite close to the ‘exact’ results over the entire non-FM region. This crude approximation certainly seems to give a clear picture for the three-phase diagram of the spin-1 system, so far as the ground-state energy is concerned. Of course, the precise locations of the boundaries between these phases given here are not to be trusted because of the gross simplification.
From the above analysis, it is clear that one can extend our previous calculations to study the dimerization of the chain around the region of $\theta = -\pi/2$ and to study possible trimerization about $\theta \geq \pi/4$. Chubukov [29] applied a dimerized spin-wave theory using the Holstein-Primakoff bosonization to the Hamiltonian of Eq. (4.1) and indeed he found that over an extended region, the dimerized spin-wave excitations are stable. One certainly desires to obtain also other physical quantities, such as the ground-state energy, dimerization order parameter and the corresponding four-spin correlation functions, etc. The CCM analysis described in Sec. 3 for the spin-$1/2$ model can certainly provide a systematic means to obtain these physical quantities.

The possible trimerization of the spin-1 chain was discussed in Ref. [13] where the equations of motion were derived for the creation and destruction operators $A_{r}^{n}$ $(n = 1, 2, \ldots, 26)$ with $r$ denoting each of the trimers in Fig. 1 (c). After a truncation in the Hilbert space, namely restricting to $n = 1, 2, \ldots, 9$, the trimerized spin-wave spectra were obtained. The lowest mode shows a nonzero gap associated with the trimerization, and this gap collapses at precisely $\theta = \pi/4$ and $\theta = \pi/2$. In particular, at $\theta = \pi/4$, the spectrum becomes gapless at lattice momentum $q = 0$ and $2\pi/3$ with a spin-wave velocity of $3/\sqrt{5} \approx 1.342$. This spectrum compares well with the exact result of Sutherland [28], which has a spin-wave velocity of $\sqrt{2}\pi/3 \approx 1.481$. At $\theta = \pi/2$, where the system is known to become FM, a constant zero spectrum was obtained. Again, the CCM analysis using $A_{r}^{n}$ and $A_{0}^{n}$ $(n = 1, 2, \ldots, 26)$ with the trimer model state should provide more systematic and reliable results.

4.2 The Spin-$1/2$ Frustrated Model on the Square Lattice

The 2D spin-$1/2$ frustrated Heisenberg model on the square lattice is described by the following Hamiltonian

$$H = \frac{1}{2} \sum_{i, \rho} s_{i} \cdot s_{i+\rho} + \frac{1}{2} J \sum_{i, \rho'} s_{i} \cdot s_{i+\rho'}, \quad s = \frac{1}{2}$$

where $i$ runs over all lattice sites, and $\rho$ and $\rho'$ over all nearest-neighbour and next-nearest-neighbour (diagonal) sites respectively. Because its possible relevance to the high-temperature superconductors, a variety of techniques has been applied to this model [14]. One now generally believes that the system shows the classical Néel-like order with the ordering wavevector $Q = (\pi, \pi)$ for small $J$ and the collinear magnetic order [$Q = (0, \pi)$] for $J \approx 0.65$ or larger. Between these two phases (i.e., $0.35 < J < 0.6$), however, no magnetic order is observed. Although there is no clear consensus on the zero-temperature structure for this nonmagnetic region, the column dimerized phase shown in Fig. 5 has been proposed [14]. In particular, Chubukov again applied his dimerized spin-wave theory to the Hamiltonian of Eq. (4.3). His results seem to agree with the numerical calculations which suggest that the column dimer VB state may be stable around $J = 1/2$. But it is fair to say that a more systematic approach is needed before one can reach a definite conclusion on the dimerization of the 2D square lattice. It is quite straightforward to extend our CCM analysis for the 1D spin-$1/2$ frustrated chain described in Sec. 3 to the present 2D case. We will report these results soon.
4.3 The Spin-1 Models on the Kagomé Lattice

Spin models on the kagomé lattice are another group of frustrated systems because the ground state of the classical Ising model on the kagomé lattice has infinite degeneracy. In addition to their intrinsic theoretical interest, some spin models on the kagomé lattice may have been realized in experiments. For example, in a layered compound Sr-Cr-Ga-O, the $s = 3/2$ Cr$^{3+}$ ions form a stack of dense kagomé lattices separated by more dilute triangular lattices [30]. And the spin-$\frac{1}{2}$ Heisenberg model on the kagomé lattice has been proposed to explain the interesting phenomena observed in the experiments with $^3$He atoms deposited on the graphite substrate [15].

Here the case of the spin-1 models on the kagomé lattice is considered. It is useful to study the following trimerized Hamiltonian,

$$ H(J) = \left( \sum_{\langle ij \rangle} + J \sum_{\langle ij \rangle} \right) s_i \cdot s_j, \ s = 1, \quad (4.4) $$

where, as shown in Fig. 6, $\langle ij \rangle$ denote the solid bonds and $\langle ij \rangle$ the dashed bond. The symmetric model is given by $J = 1$. At $J = 0$, the perfect trimer VB configuration (i.e., solid bonds in Fig. 6) is the exact ground state. Therefore one expects that the trimerized spin-wave theory discussed in Sec. 4.1 for the spin-1 chain should be a good approximation for at least small values of $J$. The method of equation-of-motion has been applied [31] to the Hamiltonian of Eq. (4.4) for the operators $A_{r0}^n$ and $A_{0n}^r$ with $n = 1, 2, \ldots, 9$, restricting the Hilbert space of each trimer (denoted by the new lattice vector $r$) to the first ten states. The trimerized spin-wave spectra have been obtained as functions of $J$. Unfortunately, the spectra are found to be stable only when $J \leq 1/2$, and the symmetric point $J = 1$ seems to be beyond this simple spin-wave approximation.

However, similar to the 1D spin-1 case discussed earlier, one can in general consider the spin-1 Heisenberg-biquadratic model on the kagomé lattice. This model is given by adding a quadratic term to Eq. (4.4),

$$ H' = J' \sum_{i,\rho} (s_i \cdot s_{i+\rho})^2, \quad (4.5) $$

where, as before, $\rho$ denotes nearest-neighbour sites on the kagomé lattice. From the experience of the 1D spin-1 chain, one expects that the quadratic term of of Eq. (4.5)
may stabilize the trimer VB state over an extended region of $J'$ and even at the symmetric point of $J = 1$. This work is in progress.

5. CONCLUSION

In this article, a microscopic approach to the quantum spin systems with an anticipated VBL long-range order is described. The perfect VBL consisting of independent simple VBs is taken as the model state and the corresponding composite operators first developed by Parkinson are employed. Two approximation schemes are developed, firstly a spin-wave theory via bosonization transformation and secondly the more systematic analysis within the framework of the CCM. The general formalism for the quantum correlations in the ground and excited states of the VBL systems are given. In particular, the simple 1D spin-$\frac{1}{2}$ frustrated model have been investigated in detail as a demonstration. The extensions of our approach to the spin-1 Heisenberg-biquadratic chain and to the 2D frustrated models on the square lattice and kagomé lattice are also discussed. The preliminary results presented in this article are quite promising indeed. There is much more work to do. we wish to report our new results in the near future.

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APPENDIX
SYMMETRY THEOREM OF THE COUPLED-CLUSTER METHOD

In Sec. 3.2, the SUB2 scheme of the CCM provides a solution which preserves
the rotational symmetry (i.e., \( s_{\text{total}} = 0 \)) of the model state \(|D\rangle\), although one started with the operators in the sector of \( s_{\text{total}} = 0 \). We notice that this is true in a general application of the CCM. A brief proof of the following theorem is given in this Appendix: the CCM equations at any level of approximations always provide at least a solution which guarantees the symmetry of the model state if this symmetry is one of those belonging to the Hamiltonian.

Let \( \Lambda \) be a symmetry operator, associated with which the model state \(|\Phi\rangle\) has an eigenvalue \( \lambda_0 \), namely \( \Lambda|\Phi\rangle = \lambda_0|\Phi\rangle \). Let Hamiltonian \( H \) commutes with \( \Lambda \), \([\Lambda, H] = 0\). Therefore, one has

\[
\Lambda H|\Phi\rangle = \lambda_0 H|\Phi\rangle. 
\]

(I). Eigen operator representation. Let \( C_I^+ \) and \( C_J^+ \) be the multi-configurational creation operators with respect to \(|\Phi\rangle\), with the set-indices \( I \) and \( J \) respectively labeling the general multi-particle cluster configurations. The corresponding destruction operators are denoted as \( C_I^- \) and \( C_J^- \) respectively. Assuming that \( C_I^+ \) commutes with \( \Lambda \),

\[
[\Lambda, C_I^+] = 0, \quad \forall I, 
\]

but \( C_J^+ \) does not. Instead, \( C_J^+ \) has the following commutations,

\[
[\Lambda, C_J^+] = \lambda'_1(J) C_J^+, \quad \lambda'_1(J) \neq 0, \quad \forall J. 
\]

Therefore one has for any positive integer \( n \)

\[
\Lambda(C_I^+)^n|\Phi\rangle = \lambda_0(C_I^+)^n|\Phi\rangle, \quad \forall I, 
\]

and

\[
\Lambda C_J^+|\Phi\rangle = \lambda_1(J) C_J^+|\Phi\rangle, \quad \lambda_1(J) \equiv \lambda_0 + \lambda'_1(J). 
\]

The CCM correlation operator \( S \) is defined as

\[
S \equiv \sum'_I S_I C_I^+ + \sum_J S_J C_J^+, 
\]

where the prime implies that the identity term, \( C_0^+ \equiv 1 \), is excluded. The correlation coefficients \( \{S_I, S_J\} \) of Eq. (A.6) are determined by the following sets of the coupled equations,

\[
\langle \Phi| C_I e^{-S} He^S |\Phi\rangle = 0, \quad \forall I \neq 0, 
\]

\[
\langle \Phi| C_J e^{-S} He^S |\Phi\rangle = 0, \quad \forall J, 
\]

where the expansion of the similarity-transformed Hamiltonian

\[
e^{-S} He^S = H + [H, S] + \frac{1}{2!}[H, S][H, S] + \cdots, 
\]

will terminate at a finite order in \( S \) if \( H \) contains a finite number of destruction operators.
We notice that the states \( H|\Phi\rangle, [H, C_I^+]|\Phi\rangle, [[H, C_I^+], C_I^+]|\Phi\rangle, \ldots \), all have the eigenvalue \( \lambda_0 \) for \( \Lambda \) by Eqs. (A.1) and (A.4). However, from Eq. (A.5), the state \( C_I^+|\Phi\rangle \) has a different eigenvalue, \( \lambda_1(J) \neq \lambda_0 \). Therefore they must be orthogonal to one another, namely

\[
\langle \Phi|C_I^+H|\Phi\rangle = 0, \quad \forall J \tag{A.9a}
\]
\[
\langle \Phi|C_I^+[H, C_I^+]|\Phi\rangle = 0, \quad \forall J, I \tag{A.9b}
\]
\[
\langle \Phi|C_I^+[[H, C_I^+], C_I^+]|\Phi\rangle = 0, \quad \forall J, I, I' \tag{A.9c}
\]

etc. Using Eqs. (A.8) and (A.9), one immediately concludes that Eqs. (A.7) have at least a solution given by \( S_I = 0 \) for all \( J \). If this solution is taken, the correlation operator \( S \) of Eq. (A.6) preserves the symmetry of \( |\Phi\rangle \).

(II). Non-eigen operator representation. let \( C_I^+ = (C_I^+(0), C_I^+(1), \ldots, C_I^+(n_I-1)) \) be the multi-configurational creation operators with respect to \( |\Phi\rangle \), with \( n_I \) the dimension of the symmetry \( \Lambda \) within a set \( I \). Assuming \( C_I^+(n) \) do not have the commutations as in Eq. (A.2) or Eq. (A.3). Let the corresponding correlation coefficients be \( S_I = (S_I(0), S_I(1), \ldots, S_I(n_I-1)) \). The CCM correlation operator is then written as

\[
S = \sum_I S_I \cdot C_I^+ = \sum_I [S_I(0)C_I^+(0)+S_I(1)C_I^+(1)+\cdots+S_I(n_I-1)C_I^+(n_I-1)], \tag{A.10}
\]

where the primes again imply exclusion of the identity term, \( I = 0 \).

As before, the correlation coefficients \( \{S_I(i), i = 0, 1, \ldots, n_I - 1\} \) are determined by the following set of coupled equations

\[
\langle \Phi|C_I(i)e^{-S}He^S|\Phi\rangle = 0, \quad i = 0, 1, \ldots, n_I - 1 \text{ and } \forall I \neq 0. \tag{A.11}
\]

Let \( B_I^+ = (B_I^+(0), B_I^+(1), \ldots, B_I^+(n_I-1)) = T_I \cdot C_I^+ \), where \( T_I \) is a \( c \)-number \((n \times n)\) matrix and is chosen such that \( B_I^+(0) \) commutes with the symmetry operator \( \Lambda \), namely

\[
[\Lambda, B_I^+(0)] = 0, \quad \forall I, \tag{A.12}
\]

but

\[
[\Lambda, B_I^+(j)] = \lambda'_j(I)B_I^+(j), \quad \lambda'_j(I) \neq 0, \quad j = 1, \ldots, n_I - 1 \text{ and } \forall I. \tag{A.13}
\]

Multiplying Eq. (A.11) by the corresponding elements of the \( c \)-number Hermitian matrix of \( T_I \), and after a simple summation, one derives the following equivalent equations

\[
\langle \Phi|B_I(j)e^{-S}He^S|\Phi\rangle = 0, \quad j = 0, 1, \ldots, n_I - 1 \text{ and } \forall I \neq 0, \tag{A.14}
\]

where \( S \) can be equivalently written as

\[
S = S'_I \cdot B_I^+, \quad S'_I \equiv S_I \cdot T^{-1}_I. \tag{A.15}
\]

According to (I), there is at least a solution to Eq. (A.14) hence to Eq. (A.11) in which \( S'_I(j) = 0 \) for all \( j \neq 0 \). If this solution is chosen, the symmetry of the model state is preserved. Q.E.D.
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