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Fermionic representation of a symmetrically frustrated SU(3) model: Application to the Haldane-gap antiferromagnets

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ABSTRACT

The one-dimensional spin 1 bilinear–biquadratic model is re-expressed in a symmetrically frustrated SU(3) model, which facilitates us to introduce a fermionic representation and related bond-operator mean-field theory. By analyzing the gap and the static spin susceptibility, we shows that this treatment can easily capture the commensurate and incommensurate Haldane gap phases.

One-dimensional quantum antiferromagnets exhibit fascinating properties in many situations [1]. The spin 1 bilinear–biquadratic chain is extensively studied in the context of Haldane gap phase [2–8]. Intensive studies based on both theoretical analysis and numerical simulations have been able to reveal their delicate properties and the well-known properties have become the testing ground for various methods. In a previous study, we had proposed a class of symmetrically frustrated SU(N) models for quantum magnets, and developed a corresponding bond-operator mean-field theory to solve it [9]. Although the theory is not restricted to the dimensionality and we had applied it to the two-dimensional antiferromagnets [10], but how good is such a mean-field type theory for one-dimensional systems? Here we apply it to the famous Haldane chain problem to show the main properties of the system is well described by this simple mean-field theory.

The generalized frustrated SU(N) model reads

$$H = J_1 \sum_{\langle ij\rangle,\mu\nu} \mathcal{J}_\nu^\mu(r_i)\mathcal{J}_\mu^\nu(r_j) - J_2 \sum_{\langle ij\rangle,\mu\nu} \mathcal{J}_\nu^\mu(r_i)\mathcal{J}_\nu^\mu(r_j), \tag{1}$$

where J_1 and J_2 are two coupling constants for nearest neighbors, $\mathcal{J}_\nu^\mu(r_i)$'s are the N^2-1 generators of SU(N) group and satisfy the algebra $[\mathcal{J}_\beta^\alpha(r_i), \mathcal{J}_\nu^\mu(r_j)] = \delta_{ij}(\delta_\nu^\alpha \mathcal{J}_\beta^\mu(r_i) - \delta_\beta^\mu \mathcal{J}_\nu^\alpha(r_i))$. The first term exhibits the SU(N) symmetry [11]. While the second term exhibits SU(N) symmetry only on bipartite lattices. The existence of both terms makes the model deviate from the SU(N) symmetries [9]. One can choose $\mathcal{J}_\nu^\mu(r_i)$ as the fundamental representation with a single box in Young tableau. We introduce a set of creation and annihilation operators to rewrite the Hamiltonian in the second quantization representation. In the SU(N) representation each site has N quantum states $|\mu\rangle$ so that we may introduce N pairs of operators $f_{i\mu}^\dagger$ and $f_{i\mu}$: $|i,\mu\rangle = f_{i\mu}^\dagger|\rangle$ with the vacuum state $|\rangle$ at site i. In this way we can construct the operator, $\mathcal{J}_\nu^\mu(r_i) \equiv f_{i\nu}^\dagger f_{i\mu}$, with a constraint for single occupancy, $\sum_{\mu=1}^N f_{i\mu}^\dagger f_{i\mu} = 1$, on each site. This is the so-called *hard-core condition* even if the particles are bosons. Interestingly it is found that the generators satisfy the SU(N) algebra for either bosonic or fermionic representation. So the Hamiltonian is rewritten as

$$H = J_1 \sum_{\langle ij\rangle} P_{ij} - J_2 \sum_{\langle ij\rangle} B_{ij}^\dagger B_{ij} + \sum_i \lambda_i \left(\sum_\mu f_{i\mu}^\dagger f_{j\mu} - 1\right), \tag{2}$$

where $P_{ij} \equiv \sum_{\mu\nu} \mathcal{J}_\nu^\mu(r_i)\mathcal{J}_\mu^\nu(r_j)$ serves as the permutation operator, the bond pairing operator $B_{ij} = \sum_\mu f_{j\mu} f_{i\mu}$ and the Lagrangian multipliers λ_j are introduced to realize the constraint of single occupancy. The permutation operator can be expressed as $P_{ij} = \sum_{\mu\nu} f_{i\mu}^\dagger f_{i\nu} f_{j\nu}^\dagger f_{j\mu} = \varsigma{:}F_{ij}^\dagger F_{ij}{:}$ with $F_{ij} = \sum_\mu f_{j\mu}^\dagger f_{i\mu}$, where $::$ de-

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notes normal ordering of operators, and $\varsigma = 1$ for bosons and -1 for fermions. For $N = 2, 3, 4$, the model above is equivalent to the spin 1/2 XXZ model, the spin 1 bilinear–biquadratic model, and the $\mathrm{SU}(2) \times \mathrm{SU}(2)$ spin–orbital model [12], respectively. Here we focus on the case of $N = 3$, i.e. we study the Haldane-gap phase of the one-dimensional spin 1 bilinear–biquadratic model. We choose fermionic representation, i.e. $\{f_{i\mu}, f_{j\nu}^\dagger\} = \delta_{ij}\delta_{\mu\nu}$, and the reason will be discussed appropriately later.

For spin 1, each site has three states $|m_i\rangle$ with $m_i = -1, 0, +1$ according to the eigenvalues of S_i^z. We reorganize the three states and define three operators,

$$f_{i1}^\dagger|0\rangle = \frac{i}{\sqrt{2}}\big(|m_i = -1\rangle + |m_i = 1\rangle\big), \tag{3}$$

$$f_{i2}^\dagger|0\rangle = |m_i = 0\rangle, \tag{4}$$

$$f_{i3}^\dagger|0\rangle = \frac{1}{\sqrt{2}}\big(|m_i = -1\rangle - |m_i = 1\rangle\big). \tag{5}$$

In terms of f operators, the three spin operators can be written as

$$S_i^x = \psi_i^\dagger \Omega^x \psi_i, \tag{6}$$

$$S_i^y = \psi_i^\dagger \Omega^y \psi_i, \tag{7}$$

$$S_i^z = \psi_i^\dagger \Omega^z \psi_i, \tag{8}$$

where

$$\psi_i^\dagger = \begin{pmatrix} f_{i1}^\dagger & f_{i2}^\dagger & f_{i3}^\dagger \end{pmatrix}, \tag{9}$$

$$\Omega^x = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \Omega^y = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$
$$\Omega^z = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}. \tag{10}$$

Then, up to a constant, the above model is transformed to the spin 1 bilinear–biquadratic model,

$$H = J_\phi \sum_{\langle ij\rangle} \big[\cos\phi\, \mathbf{S}_i \cdot \mathbf{S}_j + \sin\phi (\mathbf{S}_i \cdot \mathbf{S}_j)^2\big], \tag{11}$$

with the couplings transformed as $J_1 = J_\phi \cos\phi$ and $J_2 = J_\phi \times (\cos\phi - \sin\phi)$. Its ground state phase diagram has been established in great detail [7]. The gapped phase of Eq. (11) can be divided into two intervals: the "commensurate" Haldane phase for $-\pi/4 < \phi < \phi_{\mathrm{VBS}}$ and the "incommensurate" Haldane phase for $\phi_{\mathrm{VBS}} < \phi < \pi/4$, where $\phi_{\mathrm{VBS}} = \tan^{-1} 1/3$ is the valence-bond-solid (VBS) point [13]. It can be analyzed by the shifting peak of the static spin susceptibility $\chi(q, \omega = 0)$.

As we mentioned above, we choose fermionic representation. This choice is related to the mean fields and the decomposition scheme we are going to introduce. We define the two mean fields as the thermodynamic average of the bond operators, $F = \langle F_{ij}\rangle$ and $B = i\langle B_{ij}\rangle$, $i = \sqrt{-1}$. Now that we have non-negative decompositions,

$$:F_{ij}^\dagger F_{ij}: \geqslant 0, \tag{12}$$

$$B_{ij}^\dagger B_{ij} \geqslant 0, \tag{13}$$

and we are dealing with the Haldane gap phase with $J_1, J_2 > 0$, we had to take $\varsigma = -1$ (i.e. the fermionic representation) to make sure that

$$P_{ij} = \varsigma J_1 :F_{ij}^\dagger F_{ij}: \leqslant 0, \tag{14}$$

$$-J_2 B_{ij}^\dagger B_{ij} \leqslant 0, \tag{15}$$

so that nonzero mean fields are reasonable to mimic the low energy sectors of the Hamiltonian (2). In this case, we say the decomposition scheme is semi-negative and the mean fields are nontrivial if nonzero mean fields solutions are presented in the end.

The Hubbard–Stratonovich transformation [14] is performed to decouple the Hamiltonian into a bilinear form. The chemical potential λ_i is taken to be site-independent, $\lambda_i = \lambda$, which can be also regarded as a mean field. In the momentum space the mean-field Hamiltonian is

$$H = \sum_{k,\mu} \epsilon(k) f_{k\mu}^\dagger f_{k\mu} - \frac{1}{2}\sum_k \Delta_B(k)\big(f_{k\mu} f_{-k\mu} + f_{-k\mu}^\dagger f_{k\mu}^\dagger\big)$$
$$- \lambda N_\Lambda + N_\Lambda J_1 F^2 + N_\Lambda J_2 B^2, \tag{16}$$

where $\epsilon(k) = \lambda - \Delta_F(k)$, N_Λ is the total number of lattice sites, and we have defined

$$\Delta_F(k) = 2J_1 F \cos k; \tag{17}$$

$$\Delta_B(k) = 2J_2 B \sin k. \tag{18}$$

The Hamiltonian (16) is of a Bardeen–Cooper–Schrieffer (BCS) type and needs to be diagonalized. By performing the Bogoliubov transformation,

$$\gamma_{k\mu} = u_k f_{k\mu} - v_k f_{-k\mu}^\dagger; \qquad \gamma_{-k\mu}^\dagger = u_k f_{-k\mu}^\dagger + v_k f_{k\mu} \tag{19}$$

with the coherence factors satisfying

$$u_k^2 = \frac{1}{2}\left[1 + \frac{\epsilon(k)}{\omega(k)}\right], \tag{20}$$

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon(k)}{\omega(k)}\right], \tag{21}$$

$$2u_k v_k = \frac{\Delta_B(k)}{\omega(k)}, \tag{22}$$

one can diagonalize the Hamiltonian as

$$H = \sum_{k,\mu} \omega(k) \gamma_{k\mu}^\dagger \gamma_{k\mu} + E_0, \tag{23}$$

where the spectrum and the ground state energy are

$$\omega(k) = \sqrt{\epsilon(k)^2 + \Delta_B^2(k)}, \tag{24}$$

$$E_0 = -\frac{3}{2}\sum_k \omega(k) + \frac{1}{2}\lambda N_\Lambda + N_\Lambda J_1 F^2 + N_\Lambda J_2 B^2. \tag{25}$$

We have $N = 3$ degenerate spectra for quasi-fermions. By optimizing the free energy

$$F = -\frac{3}{\beta}\sum_k \ln\big(1 + e^{-\beta\omega(k)}\big) + E_0 \tag{26}$$

with respect to the mean fields F, B, and λ, we obtain a set of the mean-field equations,

$$\int \frac{dk}{2\pi}\frac{\epsilon(k)}{\omega(k)} \tanh\frac{\beta\omega(k)}{2} = \frac{1}{3}, \tag{27}$$

$$\frac{3}{2}\int \frac{dk}{2\pi}\frac{-\epsilon(k)\cos k}{\omega(k)} \tanh\frac{\beta\omega(k)}{2} = F, \tag{28}$$

$$\frac{3}{2}\int \frac{dk}{2\pi}\frac{\Delta_B(k)\sin k}{\omega(k)} \tanh\frac{\beta\omega(k)}{2} = B. \tag{29}$$

Thus the mean-field Hamiltonian is solved together with the self-consistent equations for the three types of mean fields.