Variational Wavefunction for Quantum Antiferromagnets

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We present here a new approach to determine an accurate variational wavefunction for general quantum antiferromagnets, completely defined by the requirement to reproduce the simple and well known spin-wave expansion. By this wavefunction, it is possible to obtain the correct behavior of the long distance correlation functions for the one dimensional $S = 1/2$ antiferromagnet, i.e. a system without long range order. The qualitative difference between the integer and half integer case is also easily understood with this variational approach. Finally we present numerical results for the 2D XY model, showing that the present wavefunction has an overlap $> 0.99$ to the exact ground state of the $S = 1/2$ model for finite system up to $6 \times 6$ clusters.

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Since the discovery of High-Tc superconductivity an increasing attention has been devoted to the study of strongly correlated systems. In particular, the role of antiferromagnetic (AF) correlations in such electronic systems was soon clear as it may lead to superconductivity.

In the present paper we define a simple strategy to build a variational wavefunction for general quantum spin Hamiltonians, without restriction on dimensionality, spin, and existence or non existence of long range (AF) order.

In order to simplify the discussion, we restrict the forthcoming analysis to the general anisotropic $xxxx$ model on a finite lattice with $L$ sites and with periodic boundary conditions:

\[ H = \sum_{i,j} -J_{i,j}(S_i^z S_j^z + S_i^x S_j^x) + J_{i,j}^z S_i^z S_j^z, \]  

where $\vec{S}$ is usual notation for spin $S$ operators and the couplings $J_{i,j}, J_{i,j}^z$ depend only on the distance between the sites $i$ and $j$, in order to define a translation invariant Hamiltonian. It is also assumed that the couplings $J$s allow a stable ferromagnetic (FM) solution on the xy-plane, at the classical level. Within these notations, the spin isotropic Heisenberg model corresponds to nearest neighbor couplings with $J_{i,j} = J$ for the AF case (after the usual transformation $S_i^+ = (-1)^i S_i^+$ to change the sign of $J$ in a bipartite lattice) and $J_{i,j}^z = -J_{i,j}$ for the FM case. The isotropic condition is obtained by continuity for $|J^z| \to J$.

For this general Hamiltonian, standard spin-wave (SW) theory can be applied, where for convenience we set the order parameter along the $y -$axis and apply Holstein-Primakoff transformation rules at leading order in $\frac{1}{S}$:

\[ S_i^y = -S + a_i^+ a_i, \]
\[ S_i^x = \sqrt{\frac{S}{2}} (a_i^+ + a_i), \]
\[ S_i^z = i \sqrt{\frac{S}{2}} (a_i^+ - a_i). \]

Here the boson $a_i^+$ creates a spin fluctuation at the site $i$ over the FM state $|F >$.

By introducing standard Fourier transformed variables $\tilde{a}_q, J(q)$ and $J^z(q)$, and after a little algebra, the linear SW Hamiltonian can be written in the compact form

\[ H = S \sum_q \left[ D_q \tilde{a}_q \tilde{a}_q^+ + \frac{\eta_q}{2} (\tilde{a}_q \tilde{a}_q^+ + h.c.) \right], \]

where $D_q = 2J(0) - j(q) + j^z(q)$ and $\eta_q = -(j(q) + j^z(q))$. Each $q$ component of the above Hamiltonian can be dealt independently and easily diagonalized by introducing the Bogoliubov transformation $\tilde{a}_q = u_q \beta_q^+ + v_q \beta_q$, with simple expressions for $u_q$ and $v_q$ in terms of $D_q$ and $\eta_q$. In a finite lattice system, a special care should be paid to the uniform $q = 0$ mode corresponding to the conservation of the total spin component along the $z -$axis. As shown in Fig. 9, the Bogoliubov transformation is singular for $q = 0$. Nevertheless, this mode can be dealt systematically, because it is exactly equivalent to a standard projection of the SW ground state to the subspace of vanishing total spin projection $S_{tot}^z = 0$. Note that, in fact, the classical state $|F >$ has not a definite $S_{tot}^z$ and after the above projection, indicated in the following by $P_{S_{tot}=0}$, the order parameter is uniformly distributed in the $x - y$ plane, as is, of course, expected in a finite lattice.

In view of the above discussion, the ground state wavefunction has the following Gaussian form:

\[ |\psi_G > = P_{S_{tot}=0} \prod_{q \neq 0} \left( \frac{1}{\sqrt{2\pi i u_q^2}} \frac{1}{u_q} e^{\frac{i}{2} u_q S_q a_q^+ a_q} \right) |F >. \]

The SW result is very simple because it represents the solution of a quantum oscillator for $S \to \infty$; however, in this limit the constraint, that the boson excitations on a
single site obey $a_i^\dagger a_i \leq 2S$, is obviously violated in the wavefunction \( \psi_0 \).

We introduce here a simple wavefunction $|\psi_T\rangle$ which is for any $S$ defined in the correct Hilbert space and only asymptotically for $S \to \infty$ reduces to the known form \( \psi_0 \):

$$|\psi_T\rangle = P_{S_{tot}=0} e^{\frac{1}{2} \sum q < a_q S_q^z a_q^\dagger} |F\rangle.$$  \hspace{1cm} (4)

This is a generalization of the Manousakis wavefunction \( \psi_0 \) obtained only for the isotropic AF model in 2D. The unknown function $g_q$ is then determined by requiring that the eigenvalue equation

$$H|\psi_T\rangle = E|\psi_T\rangle$$  \hspace{1cm} (5)

is satisfied for $S \to \infty$. Note that, due to the presence of the projector, the direction of the FM order parameter in the $x-y$ plane is irrelevant. It is thus convenient to direct it in the $x$–axis direction before projection. In the state $|F\rangle = \prod_q |S_q^z = S\rangle$ each site has maximum spin along the $x$–axis, and in a basis diagonal with $S_z|\sigma\rangle = \sigma |\sigma\rangle$, this state can be expanded as $|S_q^z = S\rangle = 2^{-S} \sum_{m=-S}^{S} \sqrt{\binom{2S}{S-m}} |\sigma\rangle$. It is therefore evident that the many-spin state $P_{S_{tot}=0}|F\rangle$ can be generally written as a sum of classical configurations $|C_i\rangle = |\sigma_1, \sigma_2, \ldots, \sigma_L\rangle$, with $\sum_i \sigma_i = 0$ with all positive, non vanishing coefficients. For instance, for $S = 1/2$, $P_{S_{tot}=0}|F\rangle = \sum S_z = 0$ spin configurations $|C\rangle$.

The exponential form in \( \psi_0 \) (commuting with $P_{S_{tot}}$) represents a classical Jastrow factor $\exp \left( \frac{1}{2} \sum_{i,j} v(i-j)|\sigma_i\sigma_j\rangle \right)$ over the possible configurations $|C_i\rangle$ with a proper two-body potential $v(r) = 2\pi S S_q^z a_q^\dagger a_q$ acting on the classical spins. The positiveness of the wavefunction over all such configurations guarantees that \( \psi_0 \) is not orthogonal to the true ground state, for any finite $S$, and therefore it will necessarily collapse to it, provided \( \psi_0 \) is verified.

We expect that the linear spin-wave approximation is quite accurate to determine the self-consistency in the eigenvalue equation \( \psi_0 \), because this is determined only by the short range correlations, for which there is always some kind of order, needed to apply the basic approximation \( \psi_0 \). Provided the physics of the ground state wavefunction is correctly described by \( \psi_0 \), also long distance spin-spin correlations are expected to be correctly determined. For instance, the spin-wave estimate is meaningless for the order parameter $m = S - \langle a^\dagger a \rangle \to -\infty$ for the 1D $S = 1/2$ Heisenberg model, whereas with the present approach the long range order (LRO) of the wavefunction $P_{S_{tot}=0}|F\rangle$ is readily destroyed by the long range potential $v(r) \sim \ln r$, consistently determined (see later) in the large $S$ limit. This approach allows therefore to define a spin-wave expansion even for models without a true LRO, which represents a remarkable extension of this powerful technique for quantum spin systems. \( \psi_0 \)

In order to determine the function $g_q$, or equivalently to solve \( \psi_0 \) for $S \to \infty$, we just notice that each $q$ and $-q$ couple of wavevectors in \( \psi_0 \) can be linearized by introducing complex auxiliary fields $z_q$:

$$2 e^{\frac{1}{S} g_q S_q^z S_{-q}^z} = \int \frac{dz_q}{\pi} e^{-|z_q|^2} + \sqrt{\frac{2g_q}{S}} (z_q S_q^z + z_{-q} S_{-q}^z).$$  \hspace{1cm} (6)

The above expression has to be applied to the vacuum of the spin waves $a_q |F\rangle = 0$. Since is, in this representation, $S_q^z = i \sqrt{\frac{S}{2}} (a_q^\dagger - a_{-q})$, one easily obtains that, for large spin,

$$|\psi_T\rangle \propto P_{S_{tot}=0} e^{\frac{1}{2} \sum q \neq 0 - \frac{g_q}{1 - g_q} a_q^\dagger a_{-q}} |F\rangle.$$  \hspace{1cm} (7)

By matching the two wavefunctions \( \psi_0 \) and \( \psi_0 \), we determine $g_q = v_q / (v_q - u_q)$ for $S \to \infty$.

The function $g_q$, given by the above expression, turns singular only for $q \to 0$ and behaving as $\frac{m}{\gamma_0}$ with $\gamma_0 = -\sqrt{2}$ for the nearest neighbor model. By expanding the exponential \( \psi_0 \) in real space, we recover the wavefunction from Ref. \( \psi_0 \) with logarithmic interaction between the spins. As shown in this paper and related comments, this is precisely the condition to have Luttinger liquid behavior, or anomalous large distance exponents in 1D. The spin-spin correlation functions, according to the Luttinger liquid analysis, decay as a power low: $<S_0^z S_r^z> \sim r^{-\mu_z}$ and $<S_0^z S_r^x> \sim r^{-\mu_x}$. Analogously to what was found in Ref. \( \psi_0 \), we have obtained that $\mu_z$ and $\mu_x$ depend only on the Jastrow coefficient $\gamma$: $\mu_z = \frac{1}{\gamma}$, $\mu_x = \frac{1}{\gamma^2}$, in good agreement with the data shown in Fig. \( \psi_0 \). For the isotropic model the prefactor is not the exact one which is consistent with $<\hat{S}_0^z \cdot \hat{S}_r^> \sim \frac{1}{r}$ correlations. However, if we determine $g_q$ by applying the SW expansion to the well known Haldane-Shastry model \( \psi_0 \)

$$J(q) = \frac{1}{2} q^2 \text{ and } J_z(q) = -\frac{1}{2} \left( \sigma - q \right)^2 \text{ mod}(0, \pi),$$

we find $\gamma_0 = -\frac{1}{2}$, i.e. the exact value. The wavefunction $|\psi_T\rangle$ is the exact ground state of the model for particular $v(r) = 2 \ln (\sqrt{L})$ to which our spin estimate is asymptotically converging for $L \to \infty$ ( $g_0 = -\frac{1}{2\pi} + \text{const.}$).

Let us now consider the spin one model, again in 1D. In our approach, the function $g_q$ is insensitive to the spin $S$, apart for a prefactor. However, the wavefunction changes dramatically, compared to the $S = 1/2$ case, due to the change of the Hilbert space, determined not only by two spins with opposite magnitude ($S_z = \pm 1$), but also by vacancy sites with $S_z = 0$, that are completely decoupled.
from the non-vanishing spins. It is not difficult to realize that in the $S = 1$ case the model corresponds to an one dimensional Coulomb gas model with charge $S_z = \pm 1$ since the vacancy sites can be considered as an empty space between the charges.

FIG. 1. Log-log plot of the $S = 1/2$ spin-spin correlation functions $c(L)$ for the spin operators in a plane ($< S^+_0 S^-_{L/2} >$) and in the direction orthogonal to it ($< S^+_0 S^z_{L/2} >$) and for two values of $\gamma$. The triangles refer to exact diagonalization data and squares to Monte Carlo estimates (error bars are much smaller than size of the points). The curves are obtained by fitting the data to the power law behavior 
\[ \log c(L) = \mu \log L + a + b/L; \]

| $\gamma$ | $< S^+_0 S^-_{L/2} >$ | $< S^+_0 S^z_{L/2} >$ |
|----------|----------------------|---------------------|
| 1.0      | $1.59 \pm 0.03$      | $0.64 \pm 0.09$     |
| 1.1      | $1.43 \pm 0.01$      | $0.6 \pm 0.1$       |

The Coulomb gas model with logarithmic interaction has been encountered several times in the literature and its phase diagram, probably complete, has been established. But the mapping to this model is not orthodox, since with a little algebra the cos term in the Kane and Fisher Hamiltonian is replaced by a log(cos$^2 S$ (g$\Phi$)) which differs from the usual model because there are infinite potential barriers between the valleys. However, we have found that the qualitative features of the cos model and the present log cos$^2$ one are the same. Note also that the mapping to a model with a local defect is possible for integer $S$ and not for half integer spin, where our wavefunction displays only one phase.

FIG. 2. Plot of the $S = 1$ spin-spin correlation function $< S^+_0 S^-_{L/2} >$, for Monte Carlo data, as a function of $\gamma$. When $\gamma$ increases, the system is going from a disordered (plasma) phase, with a typical configuration $0 + + - - - - 0000 + - +000 -00 +0 - 0$, to an ordered (dielectric) phase, with short range bound states with opposite spins $- - - - - - - - - - - - - - - -$. The symbols $+, 0, -$ represent the values $(S_z^i =1, 0, -1)$. For the larger system size, the change of the phase is more pronounced, implying a true phase transition as expected (see text).

FIG. 3. Log-log plots and L-log plots of the $S = 1$ in-plane spin-spin correlation function $< S^+_0 S^-_{L/2} >$ for $\gamma = 1.0$ and $\gamma = 1.8$ (for the Monte Carlo data, with $\gamma = 1.0$ error bars are smaller than the size of points). In the disordered phase ($\gamma = 1.0$), the spin-spin correlation function clearly decays as a power low, whereas the exponential decay assumption is much worse.
In the $S = 1$ case, for large $\gamma$, there is a dielectric phase (see Fig. 2) that reminds the Haldane phase with an hidden order parameter. Here the order is not hidden and of course the wavefunction is quantitatively meaningless. The remaining phase, where the charges are confined, is again characterized by a power law decay in the spin-spin correlations. This suggests that, for small $\gamma$, when our approximation is more reliable, a spin one magnet has power law correlations (Fig. 3) and remains gapless. Indeed, the phase diagram of the $S = 1$ model displays the power law behavior close to the $J_z \simeq 0$ point, which is consistent with our findings as the estimated $\gamma$ decreases for smaller $J_z$. In the Kane and Fisher model, correlation functions fall off with a power law in both regions. In the present model we cannot exclude the existence of a correct finite correlation length (gap) for integer spins, but we have not been able to find a clear numerical evidence, as shown in Fig. 3) for $\gamma = 1.8$. Nevertheless, we believe that the emerging picture in the integer spin case is qualitatively sound and correctly describes the possible gapless phases, present also in the $S = 1$ models.

| Bosons | $4 \times 4$ | $6 \times 6$ |
|--------|-------------|-------------|
| $E_V - E_{ex}$ | $\langle \psi_T | \psi_G \rangle > |^2$ | $E_V - E_{ex}$ | $\langle \psi_T | \psi_G \rangle > |^2$ |
| 2 | 0.99997 | 0.00008 | 0.99994 |
| 3 | 0.99988 | 0.00014 | 0.99993 |
| 4 | 0.99960 | 0.00034 | 0.99987 |
| 5 | 0.99937 | 0.00071 | 0.99973 |
| 6 | 0.99889 | 0.00126 | 0.99954 |
| 7 | 0.99820 | 0.00198 | 0.99832 |
| 8 | 0.99762 | 0.00288 | 0.99906 |
| 9 | 0.99876 | 0.00396 | 0.99876 |
| 10 | 0.99840 | 0.00524 | 0.99840 |
| 11 | 0.99798 | 0.00674 | 0.99798 |
| 12 | 0.99750 | 0.00842 | 0.99750 |

**TABLE I.** Difference between variational energy $E_V$ and exact one $E_{ex}$, and overlap square of the corresponding wavefunctions for various clusters and number $N$ of bosons. In this case the density of bosons was fixed by adding to the spin Hamiltonian a magnetic field term $-HS_\text{tot}$ and determining the value of $H$ by requiring: $2S(\frac{1}{2} - \rho) = \langle S_{\text{tot}}^z \rangle$ with $\rho = \frac{1}{2}$ fixed and consistently $S \to \infty$. The direction of the order parameter has to be canted from the $xy$ plane in order to determine a stable classical solution.

Finally, we want to show a simple application of this variational wavefunction to a system of hard core bosons in the two dimensional case. Provided the system has LRO for $\rho = N/L = 1/2$ [12], the spin-wave approximation is expected to be accurate. Still, it was amazing for us to see so much accuracy (see table) in the ground state wavefunction, yielding practically an exact numerical solution of this correlated model. Notice that, at fixed number of bosons, the accuracy improves with size, showing that the low density limit [3] is fulfilled exactly, by this wavefunction. This is a non trivial fact because in this limit the Jastrow factor diverges logarithmically. Our numerical results shows that the spin-wave function is very accurate for any density, especially in the low density limit. We find therefore a clear evidence that the superfluid condensate exists, for any density, extending the rigorous proof in Ref. [12] for $\rho = 1/2$.

To conclude we have presented here a very promising method to build unbiased variational wavefunctions for spin systems, which are quite reliable for gapless phases because we reproduce in this case all the known results for 1D systems where the spin wave theory is worst. We believe that this wavefunction open new possibilities to understand strongly correlated systems.

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