PROBING THE ANTIFERROMAGNETIC LONG-RANGE ORDER WITH GLAUBER SPIN STATES

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Abstract

It is well known that the ground state of low-dimensional antiferromagnets deviates from Néel states due to strong quantum fluctuations. Even in the presence of long-range order, those fluctuations produce a substantial reduction of the magnetic moment from its saturation value. Numerical simulations in anisotropic antiferromagnetic chains suggest that quantum fluctuations over Néel order appear in the form of localized reversal of pairs of neighboring spins. In this paper, we propose a *coherent state* representation for the ground state to describe the above situation. In the one-dimensional case, our wave function corresponds to a two-mode Glauber state, when the Néel state is used as a reference, while the boson fields are associated to coherent flip of spin pairs. The coherence manifests itself through the antiferromagnetic long-range order that survives the action of quantum fluctuations. The present representation is different from the standard zero-point spin wave state, and is asymptotically exact in the limit of strong anisotropy. The fermionic version of the theory, obtained through the Jordan-Wigner transformation, is also investigated.

1 Introduction

The Heisenberg model has been extensively studied for many years as a non trivial many-body problem in quantum magnetism. For low dimensional systems, the ground state deviates from Néel ordering due to strong quantum fluctuations [1]. The determination of this ground state represents a fascinating problem, that in one dimension originated a whole branch of Mathematical Physics based in the so called "Bethe-Ansatz" technique [2]. However, exact solutions are extremely intricate, very often not susceptible of a direct physical intuition, and in the case of the Heisenberg model, they are restricted to one dimension.

In this contribution, we would like to present a novel approach based in a localized description of quantum fluctuations. If one takes as a reference the Ising limit, with a ground state of Néel type, switching the transverse part of the Heisenberg Hamiltonian may be visualized as a disordering process, where pairs of neighboring spins are simultaneously flipped, the ground state being a quantum superposition of admixtures contained in the manifold of total $S_z = 0$. This effect has been systematically observed in numerical simulations for anisotropic Heisenberg chains [3], and was used by Lagos and the author as the heuristic base for the construction of a trial solution [1]. To fix ideas, we will concentrate in the case of spin 1/2, and most of the examples will refer to a one-dimensional system. The theory can be extended to arbitrary dimension [4],

and to arbitrary value of the spin [5]. The antiferromagnetic Heisenberg Hamiltonian with axial anisotropic exchange can be written as:

$$\mathcal{H} = J \sum_{<ij>} \left[S_z(i)S_z(j) + \frac{\alpha}{2} \left\{ S_+(i)S_-(j) + S_-(i)S_+(j) \right\} \right], \tag{1}$$

where i, j are site indexes for nearest neighbors, $J > 0$ is the antiferromagnetic exchange, the S's are spin 1/2 operators, and α is the axial anisotropy parameter. Special cases of Hamiltonian (1) are: i) $\alpha = 0$, the Ising case; ii) $\alpha = 1$, the isotropic Heisenberg model; iii) $\alpha \to \infty$, the so called 'XY-model'.

It is important to stress that the approach that will be proposed here is not perturbative, in spite that the Ising limit is considered as a departure point for its formulation. The method works successfully in the axial anisotropic regime, and is asymptotically exact for high anisotropy. Near the isotropic point, however, a delocalization transition occurs, and the linear spin wave theory becomes a better approximation when compared with exact results or numerical simulations [6]. However, the treatment can be extended in a variational way to account for the isotropic case, or the Heisenberg-XY regime [7]. In particular, for two dimensions, isotropic exchange, and spin $S = 1/2$, the ground energy deviates less than 0.5% [7] from results obtained by elaborate Monte Carlo calculations [8].

2 The Wave Function

The Hamiltonian (1) is said to represent the so called XXZ model, with the axial-anisotropy region confined to the interval $0 \leq \alpha < 1$. In the Ising limit ($\alpha = 0$), the ground state is of Néel type. For the infinite chain, there is a broken symmetry, and one of the two possible Néel states has to be chosen as a reference state. They both are connected by time inversion, the ground state of the infinite system being a doublet in the anisotropic region. The phase transition, with the presence of long-range order and a symmetry broken ground state, requires degeneracy. In contrast, in finite chains, the spectrum is not degenerate and the ground state is an eigenstate of the time-inversion operator (symmetric or antisymmetric, depending on the number of spins), with equal admixtures of both Néel kets.

For our developments here, we will choose the Néel state $|\mathcal{N}\rangle$, where the eigenvalues of the $S_z(m)$ operators for the linear chain are $\frac{1}{2}(-1)^m$. With the usual definition of spin ladder operators $S_\pm(m)$, we define boson-like operators by:

$$\phi_e^\dagger = \sqrt{\frac{2}{N}} \left\{ \frac{1}{4}\alpha N + \sum_{m\ even} S_+(m+1)S_-(m) \right\}, \tag{2}$$

$$\phi_o^\dagger = \sqrt{\frac{2}{N}} \left\{ \frac{1}{4}\alpha N + \sum_{m\ odd} S_+(m)S_-(m+1) \right\}, \tag{3}$$

where N is the total number of sites in the chain. Operators defined by (2) and (3) flip pairs of neighboring spins when applied to the reference Néel state $|\mathcal{N}\rangle$. Two sequences with translational symmetry are possible, which we label by *even* and *odd*. It is apparent that a similar construction

can be realized with the other Néel state $|\mathcal{N}\rangle'$ with $S_z \to \frac{1}{2}(-1)^{m+1}$, interchanging the roles of operators (2) and (3).

In the quasi-Ising limit, the ground state is close to $|\mathcal{N}\rangle$, and under this assumption we obtain the following algebra for the ϕ's:

$$\left[\phi_e, \phi_e^\dagger\right] = \left[\phi_o, \phi_o^\dagger\right] = 1, \quad [\phi_e, \phi_o] = \left[\phi_o, \phi_e^\dagger\right] = 0, \tag{4}$$

which are boson-like commutation relations. Within the same approximation, and restricting ourselves to the manifold $S_z = 0$, the Heisenberg Hamiltonian (1) can be written as a two-mode harmonic oscillator Hamiltonian [1]:

$$\mathcal{H} = J\left(\phi_e^\dagger \phi_e + \phi_o^\dagger \phi_o\right) + E_g(\alpha), \tag{5}$$

where $E_g(\alpha)$ is the ground state energy.

The Néel state satisfies the relations:

$$\phi_e|\mathcal{N}\rangle = \frac{1}{2}\alpha\sqrt{\frac{N}{2}}|\mathcal{N}\rangle, \quad \phi_o|\mathcal{N}\rangle = \frac{1}{2}\alpha\sqrt{\frac{N}{2}}|\mathcal{N}\rangle, \tag{6}$$

showing that the Néel state, or quasi-classical state, can be represented as a *Glauber state* [9], in terms of the ϕ's operators. The eigenvalue in (6), that also enters in the definitions (2,3), has been chosen so as to cancel the linear terms in Hamiltonian (5). Using a standard notation, we define *translation* operators by:

$$D(z) = \exp\left\{z\phi - z^*\phi^\dagger\right\}, \tag{7}$$

where ϕ may be the *even* or *odd* operator. A coherent state is thus obtained as:

$$|z_1, z_2\rangle = \exp\left\{z_1\phi_e - z_1^*\phi_e^\dagger\right\}\exp\left\{z_2\phi_o - z_2^*\phi_o^\dagger\right\}|0\rangle, \tag{8}$$

with z_1, z_2 two arbitrary complex numbers. If we write

$$z_1 = z_2 = \frac{1}{2}\alpha\sqrt{\frac{N}{2}},$$

we get a closed expression for the Néel state as a *minimum uncertainty wave packet* of the ϕ's operators. Of course, an equivalent representation can be constructed with the Néel ket as the vacuum, just by shifting the definitions of the ϕ's in a constant, and thus introducing linear terms in Hamiltonian (5).

Since the Néel state is a well defined state, we would like to represent the ground $|0>$, in terms of fluctuations over the Néel state $|\mathcal{N}\rangle$. This can be accomplished in closed analytic form, by inverting expression (8):

$$|0\rangle = \exp\left\{-\alpha\sqrt{\frac{N}{8}}\left(\phi_e^\dagger - \phi_e\right)\right\}\exp\left\{-\alpha\sqrt{\frac{N}{8}}\left(\phi_o^\dagger - \phi_o\right)\right\}|\mathcal{N}\rangle. \tag{9}$$

The structure displayed by (9) is quite interesting. Quantum fluctuations over the quasi-classical state $|\mathcal{N}\rangle$ are induced by the ϕ's operators. The distribution of fluctuations is Poissonian, the

anisotropy parameter α being related to the width of the wave packet. For α sufficiently small, the state (9) displays long-range order in spite of quantum fluctuations, but the effective magnetic moment is reduced from its saturation value. A vanishing magnetic moment signals at a phase transition as a function of the parameter α.

In spite that the algebra given by (4) is obtained in the Ising limit, the trial state (9) results to be extremely accurate in describing the energy and correlation functions in the whole interval $0 \leq \alpha < 1$. The one dimensional case represents the most stringent test for the wave function, since, as we will sketch below, the accuracy of the method improves with the dimension [4]. The energy *per spin* and the staggered magnetic moment corresponding to our trial state (9) can be put in closed analytical form in terms of Bessel functions of integer order [5]:

$$E_g = \langle 0|\mathcal{H}|0\rangle = -\frac{J}{4}\left[J_0^2(2\alpha) + J_1^2(2\alpha) + 2\alpha J_1(2\alpha)\right], \tag{10}$$

$$M_z = \langle 0|S_z(m)|0\rangle = \frac{(-1)^m}{2} J_0(2\alpha). \tag{11}$$

The generalization to higher dimensions is rather straightforward [4]. If one assumes that the lattice is *bipartite*, *i.e.* not *frustrated* for Néel ordering, the corresponding boson-like operators are defined as:

$$\phi_\delta^\dagger = \sqrt{\frac{2}{N}} \sum_{\mathbf{R}} S_+(\mathbf{R} + \delta)S_-(\mathbf{R}) + \frac{\alpha}{2(z-1)}\sqrt{\frac{N}{2}} \tag{12}$$

where $\mathbf{R}$ labels sites in a sublattice, $\{\delta\}$ the set of nearest neighbors, and z is the coordination number. The reference Néel state $|\mathcal{N}>$, in this case, assigns *up* spins to the $\mathbf{R}$ sublattice, and *down* spins to $\mathbf{R} + \delta$. The interesting formula is the analogue of (9) for the ground state:

$$|0\rangle = \exp\left\{-\frac{\alpha}{2(z-1)}\sqrt{\frac{N}{2}}\sum_\delta \left(\phi_\delta^\dagger - \phi_\delta\right)\right\} |\mathcal{N}\rangle. \tag{13}$$

Due to the $\frac{\alpha}{2(z-1)}$ factor in the exponential of (13), one realizes that the importance of quantum fluctuations diminishes with the coordination number z, and correspondingly with the dimensionality. However, closed form expression for arbitrary dimension and spin have not been obtained yet, even for the simplest lattice structure (like the square lattice) [10]. In spite of the above fact, using the Hellmann-Feynman theorem [5], one can show that the error in the energy, as calculated with the state (13), is proportional to α^4. To go towards the isotropic point and to the Heisenberg-XY region, one has to generalize the theory in a variational way [7].

3   The Jordan-Wigner transformation

The one-dimensional Heisenberg model for spin 1/2 can be mapped onto a spinless fermion model through the so called Jordan-Wigner transformation [11]. The two spin states are mapped onto fermion states with occupation numbers 0 and 1. Two fermions can not occupy a single site (one may think in a very large on-site Coulomb repulsion), and they hop in a lattice with nearest neighbors interactions. The transformation is accomplished by:

$$S_-(n) = \exp\left\{-i\pi \sum_{m<n} C_m^\dagger C_m\right\} C_m, \tag{14}$$

where the $C, C^\dagger$ are fermion operators. We readily obtain the relations:

$$S_+(m) \quad S_-(m+1) = C_m^\dagger C_{m+1},$$

$$S_+(m) \quad S_-(m) = S_z(m) + \frac{1}{2} = C_m^\dagger C_m = N_m,$$

that substituted in (1) yield the following fermion Hamiltonian:

$$\mathcal{H} = t \sum_m \left(C_m^\dagger C_{m+1} + h.c. \right) + V \sum_m \left(N_m - \frac{1}{2} \right) \left(N_{m+1} - \frac{1}{2} \right), \tag{15}$$

where $t = J\alpha/2$, $V = J$. If $J > 0$, the fermion interaction V is repulsive. For positive α, Hamiltonian (15) describes hole-like fermions. An electron-like system is obtained by changing $\alpha \to -\alpha$. We already know that the properties of the Heisenberg Hamiltonian (1) are invariant under such a change [12]. Antiferromagnetic ordering implies that the total number of fermions is $\frac{N}{2}$, and the fermion ket that corresponds to the Néel state is the one with

$$\langle N_m \rangle = \frac{1}{2} \left[1 + (-1)^m \right].$$

We will call this state $|\mathcal{N}>$ to keep continuity with the previous sections. If one translates our ground state (9) into fermion language, one gets:

$$|0\rangle = \exp\left(-\frac{\alpha}{2} \mathcal{U} \right) |\mathcal{N}\rangle, \tag{16}$$

with

$$\mathcal{U} = \sum_m (-1)^m \left(C_{m+1}^\dagger C_m - C_m^\dagger C_{m+1} \right),$$

and mean occupation number given by

$$\langle 0 | N_m | 0 \rangle = \frac{1}{2} \left[1 + (-1)^m J_0(2\alpha) \right],$$

where $\alpha = 2t/V$. As in the spin case, most physical interesting quantities can be calculated in closed analytical form using the trial ket (16). For the fermion-fermion correlation functions, this has been done in Ref.[13]. A quantity which is important to investigate possible Fermi liquid behavior, is the one-particle momentum distribution [14]. In our case, this can be obtained analytically with (16), yielding:

$$\langle N_k \rangle_{holes} = \frac{1}{2} \left[1 - \sin \left(2\alpha \cos k \right) \right], \tag{17}$$

for hole-like fermions, and

$$\langle N_k \rangle_{part} = \frac{1}{2} \left[1 + \sin \left(2\alpha \cos k \right) \right], \tag{18}$$

for a particle-like system. The above distributions display a soft variation with the wave number k, and therefore no Fermi liquid behavior. The highly correlated limit $\alpha \to 0$, yields the constant value $1/2$, with the complete destruction of the Fermi surface of non-interacting particles.

4 Acknowledgments

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