Quantum phase transition in the frustrated Heisenberg antiferromagnet

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Using the J_1-J_2 model, we present a description of quantum phase transition from Néel ordered to the spin-liquid state based on the modified spin-wave theory. The general expression for the gap in the spectrum in the spin-liquid phase is given.

There has been recently considerable interest in magnetically disordered states in quantum spin models. Much of this interest stems from the connection of this problem to high-T_c superconductivity. The ground state of undoped compound has long range antiferromagnetic order. It is well described by the Heisenberg model and has been studied by numerous methods.[1] However, introducing a small number of holes leads to destruction of long range order. The resulting state is still not fully understood.

Destruction of long range order can be studied by introducing some frustration into the Heisenberg model. We will focus on the simplest possible model of such kind which is the J_1-J_2 model defined by

$$H = J_1 \sum_{\rm NN} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} + J_2 \sum_{\rm NNN} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'}. \tag{1}$$

In this Hamiltonian, the J_1 term describes the usual Heisenberg interaction of nearest neighbor spins ($S = \frac{1}{2}$) on a square lattice, while the J_2 term introduces a frustrating interaction between next nearest neighbor sites. The J_1-J_2 model itself is hardly applicable to any real materials[2] (although it was originally proposed[3] to describe high-T_c superconductors). However, it is valuable for demonstrating how long range order can be destroyed. For convenience, we set $J_1 = 1$ and denote $\alpha \equiv J_2/J_1$ (the notation of Ref. 1 is used whenever possible).

For small α, the ground state is Néel ordered. For large α the system is decomposed into two Néel ordered sublattices which, however, have the same quantization axis. This is the so-called collinear state. Whether or not the Néel and collinear states are separated in parameter space by a state without long range order has been the subject of many discussions. Besides the many spin-wave calculations,[4-8] the model has been studied by the Schwinger boson mean field theory,[9] analysis of small lattices,[10] a series expansion,[11] a mean field theory of bond operators,[12] and other methods.[13] Despite the numerous efforts, a strict answer has not been obtained. Nevertheless, since only the mean field spin-wave theory and the essentially equivalent Schwinger boson mean field theory predict a first order transition from the Néel to the collinear state, while all other methods provide support for the existence of a different intermediate state, the latter scenario appears far more probable (this is also supported by a recent calculation of corrections to the mean field solution[8]). In this work we assume that the system undergoes a second order quantum phase transition at a certain $\alpha = \alpha_c$ from the Néel to a spin-liquid state.

For the Néel phase we will use the spin wave theory which gives the following description. The staggered magnetization $m^\dagger = |\langle 0|S^z_{\mathbf{r}}|0\rangle|$ is equal to

$$m^\dagger = \frac{1}{2} - \frac{2}{N} \sum_{\mathbf{k}} \sinh^2 \theta_{\mathbf{k}}, \tag{2}$$

where N is the number of sites on the lattice, the summation is performed over the Brillouin zone of one sublattice ($|k_x| + |k_y| \le \pi$), and $\theta_{\mathbf{k}}$ is the parameter of the Bogolubov transformation determined in the linear spin-wave theory[4] (LSWT) by

$$\tanh 2\theta_{\mathbf{k}} = \frac{\gamma_{\mathbf{k}}}{1 + \alpha(\eta_{\mathbf{k}} - 1)}, \tag{3}$$

or in the mean field spin-wave theory[5] (MFSWT) by the self-consistent solution of Eq. (2) together with

$$\tanh 2\theta_{\mathbf{k}} = \frac{(m^\dagger + g_1)\gamma_{\mathbf{k}}}{(m^\dagger + g_1) + \alpha(m^\dagger + g_2)(\eta_{\mathbf{k}} - 1)}, \tag{3$'$}$$

$$g_1 = \frac{2}{N} \sum_{\mathbf{k}} \frac{1}{2} \gamma_{\mathbf{k}} \sinh 2\theta_{\mathbf{k}}, \quad g_2 = \frac{2}{N} \sum_{\mathbf{k}} \eta_{\mathbf{k}} \sinh^2 \theta_{\mathbf{k}}.$$

We have defined

$$\gamma_{\mathbf{k}} = \frac{1}{2}(\cos k_x + \cos k_y) \quad \text{and} \quad \eta_{\mathbf{k}} = \cos k_x \cos k_y.$$

Numerical values of $m^\dagger$ in LSWT, MFSWT, and other approximations are shown in Fig. 1.

Further, the dispersion of the Goldstone spin-wave excitations is

$$\epsilon_{\mathbf{k}} = \begin{cases} 2\,[1 + \alpha(\eta_{\mathbf{k}} - 1)](1 - \tanh^2 2\theta_{\mathbf{k}})^{1/2}, & \text{LSWT}, \\ 4\left[(m^\dagger + g_1) + \alpha(m^\dagger + g_2)(\eta_{\mathbf{k}} - 1)\right](1 - \tanh^2 2\theta_{\mathbf{k}})^{1/2}, & \text{MFSWT}. \end{cases} \tag{4}$$

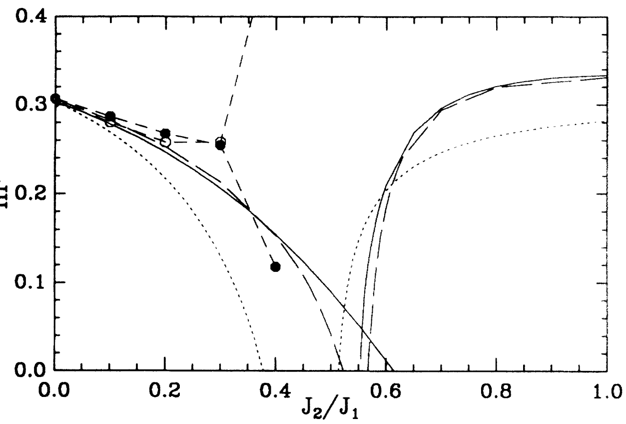

FIG. 1. Staggered magnetization $m^\dagger$ as a function of α in the Néel and collinear states. Dotted line is the LSWT result (Ref. 4), solid line the MFSWT result (Ref. 5), long dashed line the improved MFSWT result (Ref. 8), and dashed line obtained by the $1/S$ expansion (Ref. 7) in the first (○) and second (•) order.

For $k \ll 1$, it is $\epsilon_{\mathbf{k}} = ck$. We calculate $Z_c = c/c_0$ ($c_0 = \sqrt{2}$ is the spin-wave velocity at $\alpha = 0$ calculated by LSWT),

$$Z_c = \begin{cases} (1-2\alpha)^{1/2}, & \text{LSWT}, \\ 2(m^\dagger + g_1)\left(1 - 2\alpha\frac{m^\dagger+g_2}{m^\dagger+g_1}\right)^{1/2}, & \text{MFSWT}. \end{cases} \tag{5}$$

The numerical value of Z_c is given in Fig. 2. Note the remarkable agreement of the mean field solution and the $1/S$ expansion when the latter is converging.

Let us now examine the accuracy of the spin-wave theory as the staggered magnetization $m^\dagger$ decreases. The spin-wave theory starts with transforming the spin operators $\mathbf{S}_{\mathbf{r}}$ to bosonic operators $a_{\mathbf{r}}^\dagger$ and $a_{\mathbf{r}}$ using the Dyson-Maleev or Holstein-Primakoff transformation. In either case, $S_{\mathbf{r}}^z = \frac{1}{2} - \hat{n}_{\mathbf{r}}$ with $\hat{n}_{\mathbf{r}} = a_{\mathbf{r}}^\dagger a_{\mathbf{r}}$ (a spin up sublattice is considered). The physical states are those with $n_{\mathbf{r}} = 0$

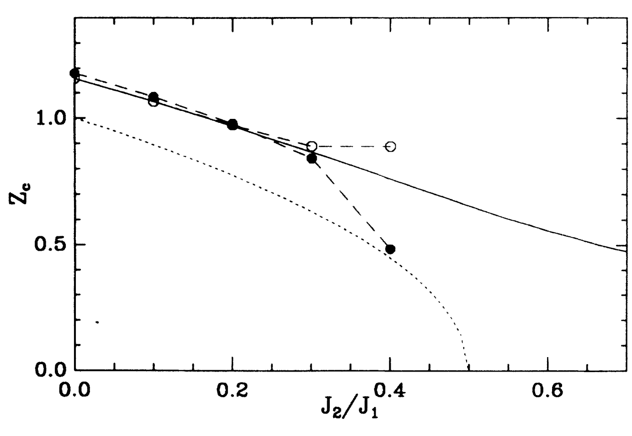

FIG. 2. Spin-wave velocity renormalization Z_c as a function of α. Dotted line is the LSWT result (Ref. 4), solid line the MFSWT result (Ref. 5), and dashed line obtained by the $1/S$ expansion (Ref. 7) in the first (○) and second (•) order.

and 1. However, the Hamiltonian is in fact simplified so that it connects the physical states to unphysical (see discussion in Ref. 1). To estimate the amount of unphysical states introduced to the wave function we calculated averages of higher powers of the $\hat{n}_{\mathbf{r}}$ operator,

$$\begin{aligned} \langle 0|\hat{n}_{\mathbf{r}}|0\rangle &= m \equiv \frac{1}{2} - m^\dagger, \\ \langle 0|\hat{n}_{\mathbf{r}}^2|0\rangle &= m + 2m^2, \\ \langle 0|\hat{n}_{\mathbf{r}}^3|0\rangle &= m + 6m^2 + 6m^3, \end{aligned} \tag{6}$$

where m is defined by Eq. (2). If only $n_{\mathbf{r}} = 0$ and 1 were present, we would have $\hat{n}_{\mathbf{r}}^l = \hat{n}_{\mathbf{r}}$ ($l \geq 1$). The problem of unphysical states becomes serious as m increases. To estimate the weight of the states with $n_{\mathbf{r}} > 1$, we proceed as follows. Expand the state obtained in the spin-wave theory in states with a definite number of bosonic excitations at site $\mathbf{r}$,

$$|0\rangle = \sum_{n=0}^{\infty} c_n |n_{\mathbf{r}}\rangle, \tag{7}$$

where $\hat{n}_{\mathbf{r}}|n_{\mathbf{r}}\rangle = n_{\mathbf{r}}|n_{\mathbf{r}}\rangle$. Obviously, the correlators of Eqs. (6) can now be expressed as

$$\langle 0|\hat{n}_{\mathbf{r}}^l|0\rangle = \sum_{n=0}^{\infty} n^l c_n^2, \quad l = 0,1,2,3,\ldots\ . \tag{8}$$

Now we truncate the series (7) at c_4 and with the truncated series we solve the first four of Eqs. (8) taking the left-hand-side from Eq. (6). The results are presented in Table I. Because a truncated series is used, negative weights sometimes appear. However, for the purpose of estimating, the method is adequate. We see that at $m = 0.5$ unphysical states constitute about 20% of the wave function and we conclude that the spin-wave approximation should be quite reasonable even at this point. (However, we must restrict ourselves to considering only low powers of the operators $a_{\mathbf{r}}^\dagger$ and $a_{\mathbf{r}}$ since high powers have large contributions from unphysical states and may lead to absolutely unphysical results.)

We assume that the system undergoes a second order transition into a liquid state at $\alpha = \alpha_c$ (the point when the sublattice magnetization becomes zero). In terms of the initial ($\alpha = 0$) ground state, zero sublattice magnetization means that the ground state is a condensate of many spin waves $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$. To describe the emerging phase we must take into account their nonlinear interaction. We cannot do this exactly. However, there is

TABLE I. The weight of unphysical states when the series (7) is truncated at c_4.

m	c_0^2	c_1^2	c_2^2	c_3^2
0.100	0.852	0.209	−0.074	0.013
0.196[a]	0.738	0.350	−0.112	0.023
0.300	0.659	0.412	−0.100	0.029
0.400	0.635	0.357	−0.020	0.028
0.500	0.675	0.167	0.142	0.017

[a]The m for $\alpha = 0$.

an approximate method using the suggestion made by Takahashi[14] for the Heisenberg model at nonzero temperature.

Following Takahashi, we impose an additional condition that sublattice magnetization is zero,

$$\langle 0|S_A^z - S_B^z|0\rangle = \langle 0|\tfrac{1}{2} - a_{\mathbf{r}}^\dagger a_{\mathbf{r}} + \tfrac{1}{2} - b_{\mathbf{r}}^\dagger b_{\mathbf{r}}|0\rangle = 0, \qquad (9)$$

where A and B are the spin up and down sublattices. In essence it means an effective cutoff of unphysical states. In fact, Eq. (9) together with conservation of the z component of the total spin is equivalent to

$$\left\langle 0\left|\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right|0\right\rangle = \left\langle 0\left|\sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}\right|0\right\rangle = \frac{N}{4}\,. \qquad (10)$$

The total number of single spin-wave states in the magnetic Brillouin zone is $N/2$. Therefore, after introducing Eq. (9) the effective number of allowed states in the Hilbert space of the system is

$$\left(\frac{(N/2)!}{(N/4)!(N/4)!}\right)^2 \sim \frac{4}{\pi N}2^N,$$

so that with logarithmic accuracy the correct dimensionality (2^N) is restored.

The constraint (9) is introduced into the Hamiltonian via a Lagrange multiplier λ. Now we must diagonalize

$$H_\lambda = H - \lambda\left(\sum_A a_{\mathbf{r}}^\dagger a_{\mathbf{r}} + \sum_B b_{\mathbf{r}}^\dagger b_{\mathbf{r}}\right). \qquad (11)$$

The simple (linear) second term here [taken together with Eq. (9)] takes account of nonlinear interaction of spin waves. Diagonalizing Eq. (11) we get the spectrum of excitations which has a gap $\Delta \propto \sqrt{\lambda}$. When $\Delta \ll 1$, the spectrum is

$$E_{\mathbf{k}} = (\Delta^2 + \epsilon_{\mathbf{k}}^2)^{1/2}, \qquad (12)$$

where $\epsilon_{\mathbf{k}}$ is the dispersion from Eq. (4) and Δ is determined from (for clarity, we present now equations only in the form they have in LSWT)

$$m^\dagger + 2\iint \frac{d^2\mathbf{k}}{(2\pi)^2}\left(\frac{1}{\epsilon_{\mathbf{k}}} - \frac{1}{E_{\mathbf{k}}}\right) = 0 \qquad (13)$$

[here $m^\dagger < 0$ is calculated from Eq. (2)]. The integral in Eq. (13) converges at small k where $\epsilon_{\mathbf{k}} \approx ck$. After integration we have for $\alpha > \alpha_c$

$$\Delta = \pi|m^\dagger|c^2. \qquad (14)$$

The correlation length in this state is $\xi \propto 1/\Delta$.

In the vicinity of the transition, $\Delta = \pi c_c^2 A(\alpha - \alpha_c)$, where c_c is the spin-wave velocity at the critical point ($c_c \approx 0.71$ whether LSWT or MFSWT is used; see Fig. 2) and $A = -\partial m^\dagger/\partial\alpha$ is the slope of dependence of $m^\dagger$ versus α (Fig. 1). We can estimate A from LSWT or the improved MFSWT (Ref. 8) and we obtain $\Delta \approx 3.3(\alpha - \alpha_c)$.

It is easy to generalize the consideration to nonzero temperatures. In this case the gap Δ will be determined from

$$m^\dagger + 2\iint \frac{d^2\mathbf{k}}{(2\pi)^2}\left[\frac{1}{\epsilon_{\mathbf{k}}} - \frac{1}{E_{\mathbf{k}}}\coth\left(\frac{E_{\mathbf{k}}}{2T}\right)\right] = 0. \qquad (15)$$

Similarly to the $T = 0$ case, the integration can be performed exactly for $T, \Delta \ll 1$ yielding

$$\frac{T}{2\pi}\ln\left(2\sinh\frac{\Delta}{2T}\right) = -\rho_s, \qquad (16)$$

where

$$\rho_s = \frac{1}{4}m^\dagger c^2.$$

Equation (16) has been obtained in the $\mathcal{N} = \infty$ limit of the nonlinear σ model[15] ($\mathcal{N} = 3$ is the number of components of the order parameter) which describes the long range behavior of near-critical spin systems using several phenomenological parameters. Solutions of Eq. (16) in different regimes have been discussed[15] (see also Ref. 16) and we will not dwell on this issue.

To summarize, we have presented a description of quantum melting of long range antiferromagnetic order in the frustrated Heisenberg model. The suggested approach can be used for many systems, in particular the doped t-J model.[17]

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