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LETTER TO THE EDITOR

Self-consistent mean-field approximation for the square-lattice frustrated Heisenberg model

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Abstract. A self-consistent mean-field method is used to obtain the phase diagram of the frustrated antiferromagnetic Heisenberg model with next-nearest-neighbour exchange couplings on a square lattice at zero temperature starting with a Holstein–Primakoff transformation. It is suggested that the Néel-type order is not destroyed for any value of the ratio of the nearest- to next-nearest-neighbour exchange couplings for $S \geqslant 1$, while for $S = \frac{1}{2}$ there may exist a disordered phase for strong frustration.

Recently the two-dimensional frustrated antiferromagnetic (AF) Heisenberg models have attracted much interest. Chandra and Doucot [1] first studied the square lattice AF Heisenberg model with frustration introduced by next-nearest-neighbour exchange coupling (called the NNN model heaeafter) with linear spin-wave (LSW) theory [2] and suggested that its ground state is spin liquid around a point where the classical ground state is heavily degenerate. Since then, the nature of the ground state of this model has been studed by various authors [3–18]. Several states have been proposed for the ground states of this NNN model: the spin liquid state [3], the dimer state [4–9], the chiral spin state [10], the twisted spin state [11], and so on. However, there is controversy as to which exists truly as the ground state of the NNN model.

In a previous work [19], the present author used the spin-wave expansion to evaluate the staggered magnetization of the square-lattice NNN model to order $O(1/S^2)$ at zero temperature. It is shown that the corrections to the LSW theory due to the higher-order terms in the Hamiltonian based on the spin-wave expansion of the Holstein–Primakoff (HP) transformation [20] are very important. If we deal with these terms properly, we can get reasonable approximate results. For this reason we have decided to carry out a further study of the NNN model using a self-consistent mean-field method developed by Chu and Shen [21] to deal with the non-linear terms of the quantum AF Heisenberg Hamiltonian based on AF spin-wave theory.

Consider the NNN model defined on a square lattice of N sites [1]:

$$H = \sum_{\langle ij \rangle} S_i \cdot S_j + \alpha \sum_{\langle ii' \rangle} S_i \cdot S_{i'} + \alpha \sum_{\langle jj' \rangle} S_j \cdot S_{j'} \tag{1}$$

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where the sites $\{ii'\} \in$ A and the sites $\{jj'\} \in$ B. The notation $\langle ij \rangle$ denotes the nearest-neighbour (NN) pairs on the square lattice, and $\langle ii' \rangle$ and $\langle jj' \rangle$ denote the nearest-neighbour pairs on the sublattices A and B, respectively. The lattice constant is taken to be equal to unity. The parameter α is assumed to be positive and thus the NN and NNN exchange couplings compete with each other.

Classically, for $\alpha < 0.5$ the ground state of this system has the conventional two-sublattice Néel-type long-range order. If α exceeds 0.5, the system splits into interpenetrating square lattices, in each of which two-sublattice order exists. Following [4] we call the latter order the four-sublattice Néel order. In the quantum case these conclusions are modified even at zero temperature due to zero-point fluctuations. The order parameter vanishes in certain cases, where the conventional long-range order may be unstable, leading to a new spin state. The phase diagram giving the critical value of the spin below which the order parameter ceases to be a function of α has been determined [1, 13–16] with LSW theory, modified spin wave (MSW) theory [22] and Schwinger-boson mean-field (SMBF) theory [23]. The purpose of this letter is to obtain a phase diagram within a self-consistent mean-field approximation starting with the HP transformation. The self-consistent mean-field approximation starting with Dyson–Maleev transformation [24] is also applicable to the NNN model. Using the latter transformation we can obtain a completely identical set of self-consistent equations. Since the Hamiltonian of the Dyson–Maleev transformation is not Hermitian, we choose the HP transformation as our starting point. As we shall show, the $1/S - \alpha$ phase diagram obtained differs significantly from that obtained by LSW, MSW and SMBF theories [1, 13–16].

We assume, as is usual, that the staggered magnetization is parallel to the z direction. To obtain, within the self-consistent spin-wave theory, the ground-state properties for the NNN model given by (1), we follow the standard procedure for the two-sublattice and four-sublattice cases. Using the HP transformation, the Hamiltonian can be rewritten in terms of the Bose operators of the spin deviation on the sublattices. For the two-sublattice case, by the HP transformation [20]:

$$S_i^z = S - a_i^\dagger a_i \qquad S_i^+ = (S_i^-)^+ = \sqrt{2S}(1 - a_i^\dagger a_i/2S)^{1/2} a_i$$
$$S_j^z = -S + b_j^\dagger b_j \qquad S_j^+ = (S_j^-)^+ = \sqrt{2S} b_j^\dagger (1 - b_j^\dagger b_j/2S)^{1/2} \tag{2}$$

the Hamiltonian (1) can be written as H^{HP}

$$H^{\mathrm{HP}} = H_0 + H_1 + \dots \tag{3}$$

where S is the magnitude of the spin, and a_i and b_j are Bose annihilation operators. In (3) the quadratic part H_0 is

$$H_0 = -2NS^2(1-\alpha) + S\sum_{\langle ij \rangle}(a_i^\dagger a_i + b_j^\dagger b_j + a_i^\dagger b_j + a_i b_j^\dagger) - \alpha S \sum_{\langle ii' \rangle}(a_i^\dagger a_i - a_{i'}^\dagger a_{i'})$$
$$- \alpha S \sum_{\langle jj' \rangle}(b_j^\dagger b_j - b_{j'}^\dagger b_{j'}) \tag{4}$$

and the quartic part H_1 is

$$H_1 = -\frac{1}{4}\sum_{\langle ij \rangle}(a_i^\dagger a_i a_i b_j + b_j^\dagger b_j b_j a_i + 2a_i^\dagger a_i b_j^\dagger b_j) \frac{\alpha}{4}\sum_{\langle ii' \rangle}(a_i^\dagger a_{i'}^\dagger a_{i'} a_{i'} - a_i^\dagger a_{i'}^\dagger a_i a_{i'})$$
$$- \frac{\alpha}{4}\sum_{\langle jj' \rangle}(b_j^\dagger b_{j'}^\dagger b_{j'} b_{j'} - b_j^\dagger b_{j'}^\dagger b_j b_{j'}) + \mathrm{HC}. \tag{5}$$

The key step is the method of processing the quartic part given by (5). Here we apply the self-consistent mean-field approximation [21] for these non-linear terms to obtain the mean-field Hamiltonian. Let

$$\langle a_i a_i \rangle = \langle a_i^\dagger a_i^\dagger \rangle = \langle a_i a_{i'} \rangle = \langle a_i^\dagger a_{i'}^\dagger \rangle = \langle b_j b_{j'} \rangle = \langle b_j^\dagger b_{j'}^\dagger \rangle = \langle b_j b_j \rangle = \langle b_j^\dagger b_j^\dagger \rangle = 0$$
$$\langle a_i^\dagger b_j \rangle = \langle a_i b_j^\dagger \rangle = 0. \tag{6}$$

We can directly linearize the non-linear terms in H_1 as

$$a_i^\dagger a_i a_i b_j = \langle a_i^\dagger a_i \rangle a_i b_j + \langle a_i b_j \rangle a_i^\dagger a_i - \langle a_i^\dagger a_i \rangle \langle a_i b_j \rangle$$
$$b_j^\dagger b_j b_j a_i = \langle b_j^\dagger b_j \rangle b_j a_i + \langle b_j a_i \rangle b_j^\dagger b_j - \langle b_j^\dagger b_j \rangle \langle b_j a_i \rangle$$
$$a_i^\dagger a_{i'}^\dagger a_{i'} a_{i'} = \langle a_{i'}^\dagger a_{i'} \rangle a_i^\dagger a_{i'} + \langle a_i^\dagger a_{i'} \rangle a_{i'}^\dagger a_{i'} - \langle a_i^\dagger a_{i'} \rangle \langle a_{i'}^\dagger a_{i'} \rangle$$
$$b_j^\dagger b_{j'}^\dagger b_{j'} b_{j'} = \langle b_{j'}^\dagger b_{j'} \rangle b_j^\dagger b_{j'} + \langle b_j^\dagger b_{j'} \rangle b_{j'}^\dagger b_{j'} - \langle b_j^\dagger b_{j'} \rangle \langle b_{j'}^\dagger b_{j'} \rangle \tag{7}$$

$$\begin{aligned} a_i^\dagger a_i b_j^\dagger b_j &= (1-\lambda)[\langle a_i^\dagger a_i \rangle b_j^\dagger b_j + \langle b_j^\dagger b_j \rangle a_i^\dagger a_i - \langle a_i^\dagger a_i \rangle \langle b_j^\dagger b_j \rangle] \\ &\quad + \lambda[\langle a_i^\dagger b_j^\dagger \rangle a_i b_j + \langle a_i b_j \rangle a_i^\dagger b_j^\dagger - \langle a_i^\dagger b_j^\dagger \rangle \langle a_i b_j \rangle] \\ a_i^\dagger a_{i'}^\dagger a_i a_{i'} &= (1-\lambda')[\langle a_i^\dagger a_i \rangle a_{i'}^\dagger a_{i'} + \langle a_{i'}^\dagger a_{i'} \rangle a_i^\dagger a_i - \langle a_i^\dagger a_i \rangle \langle a_{i'}^\dagger a_{i'} \rangle] \\ &\quad + \lambda'[\langle a_i^\dagger a_{i'} \rangle a_{i'}^\dagger a_i + \langle a_{i'}^\dagger a_i \rangle a_i^\dagger a_{i'} - \langle a_i^\dagger a_{i'} \rangle \langle a_{i'}^\dagger a_i \rangle] \\ b_j^\dagger b_{j'}^\dagger b_j b_{j'} &= (1-\lambda')[\langle b_j^\dagger b_j \rangle b_{j'}^\dagger b_{j'} + \langle b_{j'}^\dagger b_{j'} \rangle b_j^\dagger b_j - \langle b_j^\dagger b_j \rangle \langle b_{j'}^\dagger b_{j'} \rangle] \\ &\quad + \lambda'[\langle b_j^\dagger b_{j'} \rangle b_{j'}^\dagger b_j + \langle b_{j'}^\dagger b_j \rangle b_j^\dagger b_{j'} - \langle b_j^\dagger b_{j'} \rangle \langle b_{j'}^\dagger b_j \rangle] \end{aligned} \tag{8}$$

where $0 \leqslant \lambda, \lambda' \leqslant 1$ are Lagrange multipliers introduced by us, which will be determined later by minimizing the energy of the ground state.

Now, using the Bogoliubov transformation, the Fourier transform of the mean-field Hamiltonian can be easily diagonalized. After a straightforward calculation we have the following results. The ground-state energy is given by

$$E_0 = -2N(1-\alpha)S^2 + 2Ne_0. \tag{9}$$

The staggered magnetization is

$$\langle S_0^z \rangle = S - A \tag{10}$$

and the spin-wave excitation energy is

$$\hbar\omega(k) = 4A_k/\Delta_k \tag{11}$$

where

$$A_k = (1-\alpha+\alpha\eta_k)S - (1-\alpha-\lambda+\alpha\lambda'+(\alpha/2)\eta_k)A - \alpha(1/2-\lambda'\eta_k)B - C/2 \tag{12}$$

$$B_k = (S - A/2 - \lambda C)\gamma_k \tag{13}$$

$$\Delta_k = [1 - B_k^2/A_k^2]^{-1/2} \tag{14}$$

$$e_0 = (A + C)(2S - A + \lambda A - \lambda C) - \alpha(A - B)(2S - A + \lambda' A + \lambda' B) \tag{15}$$

with

$$A = \frac{1}{N}\sum_k (\Delta_k - 1) \tag{16}$$

$$B = \frac{1}{N}\sum_k \Delta_k \eta_k \tag{17}$$

$$C = -\frac{1}{N}\sum_k \Delta_k B_k \gamma_k / A_k \tag{18}$$

and

$$\gamma_k = \frac{1}{4}\sum_\delta \exp(\mathrm{i}k\delta) = \frac{1}{2}(\cos k_x + \cos k_y) \tag{19}$$

$$\eta_k = \frac{1}{4}\sum_\Delta \exp(\mathrm{i}k\Delta) = \cos k_x \cos k_y . \tag{20}$$

Here δ and Δ are vectors to nearest and next-nearest neighbours of a given site respectively. The above equations are solved with the constraint of choosing the Lagrange multipliers λ and λ' to minimize the ground-state energy.

A similar procedure to that described above for the two-sublattice case can be taken for the four-sublattice case (collinear case). In the latter case, as long as one takes note of the fact that four types of Bose operators should be introduced, then following the same procedure as above we can obtain the corresponding equations within the self-consistent mean-field approximation, which will not be given here for brevity. We will see below that for the four-sublattice case there is no qualitative difference from the LSW theory.

We have numerically solved the self-consistent equations for both the two-sublattice and four-sublattice cases for various values of α and S. The Lagrange multipliers λ and λ' are chosen so as to minimize the energy E_0 of the lowest-energy state, i.e., the ground state. We obtain a phase diagram on the $1/S - \alpha$ plane as shown in figure 1. For the two-sublattice case the phase boundary goes noticeably beyond $\alpha = 0.5$ and for $S \to \infty$ the boundary turns back on itself to reach the classical limit $\alpha = 0.5$ and does not drop vertically to $\alpha \sim 0.56$, which is quite different from the results obtained by Chandra and Doucot [1] with LSW theory, but which agrees qualitatively with the calculations of [13–16] using MSW and SMBF theories. For the four-sublattice case our calculation shows that there is no qualitative difference between the LSW, MSW and SMBF theories. In figure 1 the lines A(A′) and B(B′) are solutions for $\langle S_0^z \rangle = 0$ corresponding to the two-sublattice case and the

four-sublattice case, respectively. Thus two-sublattice Néel order exists below A and above B′ and the four-sublattice counterpart exists below B and above A′. As for the region below A′ and B′ there exists either two-sublattice or four-sublattice Néel order. To determine which state is more stable in this coexistent region we have numerically computed the ground-state energies of both cases and compared them. The energy of the two-sublattice case is equal to that of the four-sublattice case on the boundary line C. This means that there is a first-order phase transition between both cases on line C. In the region between lines B′ and C the energy of the two-sublattice case is less than that of the four-sublattice case, while in the region between lines C and A′ the energy of the two-sublattice case exceeds that of the four-sublattice case. Therefore, the system has two-sublattice Néel order in the region below A and above C, and in the region below B and above C four-sublattice Néel order exists. A first-order phase transition occurs on line C between the two-sublattice and the four-sublattice Néel states. Above lines A and B no Néel-type long-range order exists.

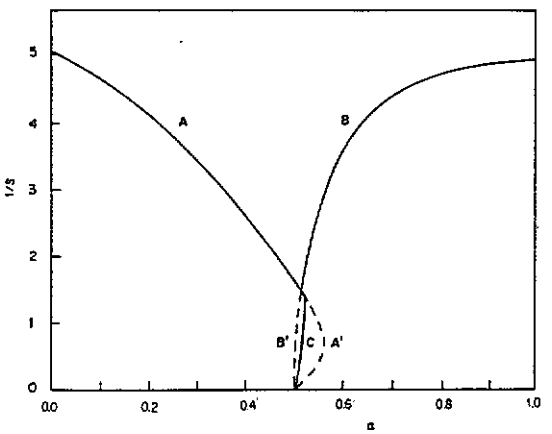

Figure 1. Phase diagram of the NNN model at zero temperature obtained within the self-consistent mean-field approximation based on the Holstein–Primakoff transformation. The lines A(A′) and B(B′) show the critical values below which the order parameter vanishes, corresponding to the two-sublattice and four-sublattice cases, respectively. The line C is the first-order transition boundary.

As seen in figure 1, we have found that for $S \geqslant 1$ there is no qualitative difference between our theory and the MSW theory [13–15] or the SMBF theory [16]: the Néel order is not destroyed at any value of α. On the contrary, for $S = 1/2$ at a certain α ($\simeq 0.47$) the staggered magnetization vanishes, which is considerably different from results obtained [13–16] using MSW and SMBF theories. This also occurs within LSW theory, but in this case $\langle S_0^z \rangle$ vanishes at a larger value of α (~ 0.47 within present approximation but ~ 0.38 within LSW theory [1]). It is reasonable to speculate that long-range order is destroyed around $\alpha = 0.5$ for two-dimensional spin-$\frac{1}{2}$ NNN frustrated Heisenberg systems. Thus a number of interesting ideas about quantum disordered antiferromagnets could be tested experimentally for spin-$\frac{1}{2}$ systems.

In summary, we have obtained a phase diagram of the two-dimensional NNN frustrated antiferromagnetic Heisenberg model within the self-consistent mean-field approximation starting with the Holstein–Primakoff transformation. It is suggested

that for $S \geqslant 1$ the system has either two-sublattice or four-sublattice order at any value of the ratio of nearest- and next-nearest-neighbour exchange couplings. At $\alpha \sim 0.5$ a first-order phase transition exists between the states. On the contrary, for $S = \frac{1}{2}$ it seems very likely that a disordered state exists around $\alpha = 0.5$ for the NNN frustrated AF Heisenberg model. The nature of this state is still controversial. These conclusions are based on the calculation of the self-consistent mean-field approximation of the Holstein–Primakoff transformation. Of course, the present approximate calculations need to be improved; for example, first, our approximation is a mean-field theory and it is difficult to control; second, the terms in H^{HP} higher than quartic and the kinematic interactions are also very important, and these must be considered if a quantitatively more reliable result is to be obtained.

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