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Phase diagram of the frustrated square Heisenberg lattice based upon a modified spin-wave theory

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We show that the conventional spin-wave theory cannot give a correct phase diagram for the frustrated square-lattice antiferromagnet. We present a modified spin-wave theory for this model, which is analogous to Takahashi's recent theory of the two-dimensional Heisenberg model without frustrations, and obtain a new phase diagram in which there exists no spin-liquid state for $S=\frac{1}{2}$. Our results agree well with those of recent numerical simulations for small lattices.

The discovery of the layered oxide high-temperature superconductors has led to renewed efforts to get a better understanding of a two-dimensional (2D) antiferromagnetic system. Much of this interest stems from Anderson's claim[1] that the physics of the new materials may be closely related to the existence of the quantum-spin-liquid (QSL) state, which could be generated by spin fluctuations in the 2D spin-$\frac{1}{2}$ Heisenberg model. However, many studies have indicated that there exists a finite zero-temperature staggered magnetization,[2-5] and there is no room to accommodate the nonmagnetic QSL phase in the 2D Heisenberg model. Recently, the frustrated Heisenberg model has been studied by both the conventional-spin-wave (CSW) theory[6] and by numerical techniques.[7,8] From CSW theory[6] a small region in parameter space was found where the long-range Néel order is melted by fluctuations. That may imply the possibility of the existence of a nonmagnetic QSL state in that region. Since the CSW theory[6] is based upon the large-S expansion while numerical simulations[7,8] can only be employed to study a small system with a finite lattice, one thus needs another more reliable approach to analyze the $S=\frac{1}{2}$ model.

In this paper, we present a modified-spin-wave (MSW) theory for the frustrated Heisenberg model. Takahashi[9] has formulated this approach for the 2D Heisenberg model without frustrations that yields excellent agreement with the results of exact diagonalization[10] and the renormalization-group theory.[11] Here we generalize this theory to the 2D frustrated Heisenberg model. It is expected that the MSW approach can be applied not only to the large-S case, but also to the small-S limit because it is a self-consistent spin-wave theory rather than a large-S expansion method.

We consider the 2D frustrated Heisenberg model described by the Hamiltonian

$$H=J_1\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+J_2\sum_{\langle i,k\rangle}\mathbf{S}_i\cdot\mathbf{S}_k\ , \tag{1}$$

where J_1 and J_2 correspond to the nearest- and next-nearest-neighbor coupling constants between spins, respectively. We will refer to Eq. (1) as the J_1-J_2 model.

According to the CSW theory, for $J_2=0$, the ground state is Néel-like. The coupling J_2 introduces frustrations into the problem so that the Néel state cannot be the true ground state for large enough values of J_2. However, in the large-J_2 limit the system decouples into two unfrustrated sublattices, each one with its own Néel order. Classically ($S=\infty$) the change[6] from one regime to another occurs at $J_2/J_1=0.5$. So, $J_2/J_1=0.5$ is the classical transition point (CTP). It is believed that the CSW theory gives the exact results for $S=\infty$, which has been cited often in literature.[6-8,11,12]

In the following we show that with the increase of J_2, the $1/S$ expansion in the CSW theory will diverge near the CTP. According to the CSW theory, the ground state has Néel order for $J_2/J_1<0.5$. A straightforward calculation leads to an expression for the staggered magnetization M_0:[6,11]

$$M_0=S-A-(B/S)(J_2/J_1)+O(S^{-2})\ , \tag{2}$$

with

$$A=-\frac{1}{2}+\frac{1}{N}\sum_k\frac{a_k}{(a_k^2-\gamma_k^2)^{1/2}}\ , \tag{3}$$

$$B=-\frac{1}{N^2}\sum_{k,k'}\frac{\gamma_k^2(1-\gamma_k')}{(a_k^2-\gamma_k^2)^{3/2}}\frac{a_{k'}\gamma_{k'}'-\gamma_{k'}^2}{(a_{k'}^2-\gamma_{k'}^2)^{1/2}}\ , \tag{4}$$

where $\gamma_k=(\cos k_x+\cos k_y)/2$, $\gamma_k'=\cos k_x\cos k_y$, and $a_k=1-(J_2/J_1)(1-\gamma_k')$. The CSW theory predicts that near the CTP, $S\to\infty$, $M_0\to 0$, and $B/S\to 0$. However, from Eqs. (2) and (3), if we neglect the B/S term, $S\approx A\sim\sum_k(a_k^2-\gamma_k^2)^{-1/2}\to\infty$ near the CTP. But, according to Eq. (4), $B/S\sim\sum_k(a_k^2-\gamma_k^2)^{-2}/S\sim S^3$. Thus $(B/S)/A\sim S^2\to\infty$ near the CTP, which indicates that the $1/S$ expansion is invalid. A and B/S have been calculated for several values of J_2/J_1 along the critical line where the staggered magnetization is vanishing within the linear CSW theory. The results are tabulated in Table I.

TABLE I. A and B/S as a function of J_2/J_1.

J_2/J_1	A	B/S
0.00	0.195	0.193
0.05	0.211	0.220
0.10	0.230	0.254
0.15	0.253	0.298
0.20	0.281	0.358
0.25	0.318	0.444
0.30	0.368	0.577
0.35	0.440	0.803
0.40	0.558	1.270
0.45	0.804	2.731
0.49	1.591	15.21

It can be seen that B/S increases with J_2/J_1 more rapidly than A does, which shows that the frustrations result in a large spin fluctuation even for the large-S limit. So we expect that the linear CSW theory cannot give a correct phase diagram for the J_1-J_2 model.

In order to avoid the difficulty associated with CSW theory, we consider the MSW approach. For a small value of J_2/J_1, we assume that the lattice is divided into A and B sublattices. Instead of the Holstein-Primakoff (HP) transformation,[13] the Dyson-Maleev (DM) transformation[9,14,15] will be introduced:

$$S_i^- = a_i^\dagger , \quad S_i^+ = (2S - a_i^\dagger a_i) a_i , \quad S_i^z = S - a_i^\dagger a_i , \quad \text{for } i \in A , \tag{5}$$

$$S_j^- = -b_j , \quad S_j^+ = -b_j^\dagger (2S - b_j^\dagger b_j) , \quad S_j^z = -S + b_j^\dagger b_j , \quad \text{for } j \in B , \tag{6}$$

where the spin-wave operators a and b satisfy the bosonic commutation relations. In the DM transformation, the Hamiltonian (1) has no term higher than the fourth order, which opens the possibility of constructing a self-consistent spin-wave theory instead of the conventional $1/S$ expansion. Following a similar procedure as in Ref. (9), we obtain the staggered magnetization M_{01} and the ground-state energy E_{01} in the Néel state:

$$M_{01} = S + \frac{1}{2} - \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2k}{(2\pi)^2} \frac{1}{(1 - \eta_k^2 \gamma_k^2)^{1/2}} , \tag{7}$$

$$E_{01} = -2J_1 [g(\delta)]^2 + 2J_2 [f(\delta')]^2 , \tag{8}$$

with

$$\eta_k^{-1} = 1 - \frac{J_2}{J_1} \frac{f(\delta')}{g(\delta)} (1 - \gamma_k') , \tag{9}$$

$$g(\delta) = M_{01} + \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2k}{(2\pi)^2} \frac{\eta_k \gamma_k^2}{(1 - \eta_k^2 \gamma_k^2)^{1/2}} , \tag{10}$$

$$f(\delta') = M_{01} + \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2k}{(2\pi)^2} \frac{\gamma_k'}{(1 - \eta_k^2 \gamma_k^2)^{1/2}} . \tag{11}$$

For $J_2 = 0$, Eqs. (7) and (8) return to the results obtained by Takahashi for the 2D Heisenberg model without frustrations,[9] as expected.

As mentioned before, when the frustrations become large, the system decouples into two Néel sublattices with an energy independent of the angle θ between the corresponding staggered magnetizations in the classical limit. But the quantum fluctuations will select the special angle θ, and actually there are two states which are true minima in energy with respect to quantum corrections characterized by $\theta = 0, \pi$.[7,8] This results in dominant configurations having alternating rows (or columns) of spins up and down that we will call the collinear state. In this case, performing a DM transformation for spins, and applying the MSW approach, we obtain the staggered magnetization M_{02} and the ground-state energy E_{02} in the collinear state:

$$M_{02} = S + \frac{1}{2} - \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2k}{(2\pi)^2} \frac{B_k}{(B_k^2 - A_k^2)^{1/2}} , \tag{12}$$

$$E_{02} = -J_1 [g(\delta_x)]^2 + J_1 [f(\delta_y)]^2 - 2J_2 [g(\delta')]^2 , \tag{13}$$

with

$$A_k = \frac{g(\delta_x)}{f(\delta_y)} \cos k_x + \frac{2J_2}{J_1} \frac{g(\delta')}{f(\delta_y)} \gamma_k' , \tag{14}$$

$$B_k = \frac{g(\delta_x)}{f(\delta_y)} - 1 + \cos k_y + \frac{2J_2}{J_1} \frac{g(\delta')}{f(\delta_y)} , \tag{15}$$

$$f(\delta_y) = M_{02} + \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2k}{(2\pi)^2} \frac{B_k \cos k_y}{(B_k^2 - A_k^2)^{1/2}} , \tag{16}$$

$$g(\delta_x) = M_{02} + \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2k}{(2\pi)^2} \frac{A_k \cos k_x}{(B_k^2 - A_k^2)^{1/2}} , \tag{17}$$

$$g(\delta') = M_{02} + \frac{1}{2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2k}{(2\pi)^2} \frac{A_k \gamma_k'}{(B_k^2 - A_k^2)^{1/2}} . \tag{18}$$

Thus we have a set of self-consistent equations (7)–(18) to determine the staggered magnetization M_0 and the ground-state energy E_0. If taking $f(\delta')/g(\delta) = g(\delta_x)/f(\delta_y) = g(\delta')/f(\delta_y) \equiv 1$, Eqs. (7) and (12) reduce back to the results of the linear CSW theory.[6,11,12] But $f(\delta')/g(\delta)$, $g(\delta_x)/f(\delta_y)$, and $g(\delta')/f(\delta_y)$ are all, in fact, different from unity and vary with J_2/J_1. We have tabulated these quantities numerically for a variety of values of J_2/J_1 in Table II. So, it is expected that our theory will give a very different result from the linear CSW approach. We have performed the self-consistent calculations for Eqs. (7)–(18), the results of the ground-state energy E_0, and the magnetization M_0 for $S = \frac{1}{2}$ are shown in Figs. 1 and 2, respectively. It is clear from Fig. 1 that the present result for E_0 is lower than that obtained from the CSW theory and very close to that given by the exact diagonalization for finite lattices.[7,8]

In Fig. 2, the results for the staggered magnetization with $S = \frac{1}{2}$ show that the Néel state is stable for small frustrations, while for large J_2/J_1 the large value of M_{02} tells us that the collinear state is actually the ground state

TABLE II. $f(\delta')/g(\delta)$, $g(\delta_x)/f(\delta_y)$, and $g(\delta')/f(\delta_y)$ as a function of J_2/J_1.

J_2/J_1	$f(\delta')/g(\delta)$	$g(\delta_x)/f(\delta_y)$	$g(\delta')/f(\delta_y)$
0.00	0.775		
0.10	0.761		
0.20	0.743		
0.30	0.722		
0.40	0.694		
0.50	0.661		
0.60	0.621	1.672	1.053
0.70		1.326	1.122
0.80		1.231	1.182
0.90		1.184	1.233
1.00		1.155	1.277

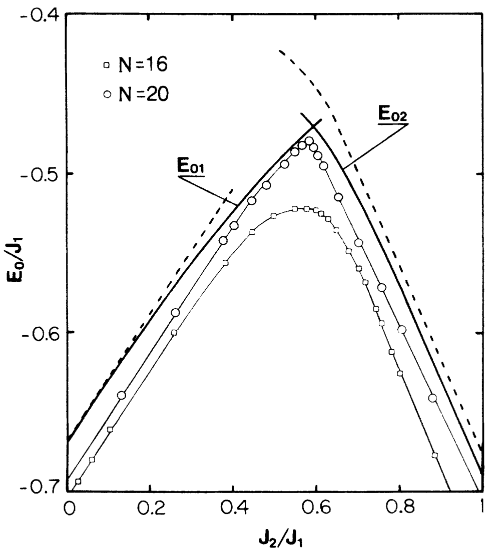

FIG. 1. Energy of the ground state vs J_2/J_1. The solid and the dashed lines are the results of the present theory and those of the linear CSW theory, respectively. The numerical results for the $N=16$ and 20 lattice from Ref. 8 are also shown for comparison.

of the system. Between $J_2/J_1 \approx 0.55$ and 0.62, there is a coexisting region of Néel and collinear orders (the shaded region in Fig. 2). Since these two states exclude each other (see Fig. 1), the ground state in that region should exhibit some kind of disorder (DO). There are many candidates for the ground state in that region. For example, the twisted state[16] is the most possible one. This state can be obtained from the Néel state by applying a uniform twist Q along some direction. According to the linear CSW theory, these states [including $Q=0$ (Néel state) and $Q=\pi$ (collinear state)] are all degenerate at $J_2/J_1=0.5$ and $S=\infty$, and only at that point do they form the ground state. But, our theory first predicts that there is a finite parameter region in the J_1-J_2 model even with $S=\frac{1}{2}$ where the ground state is the twisted state, which is in agreement with the numerical results that the twisted order parameter is strongly enhanced in the DO region.[7,8,12]

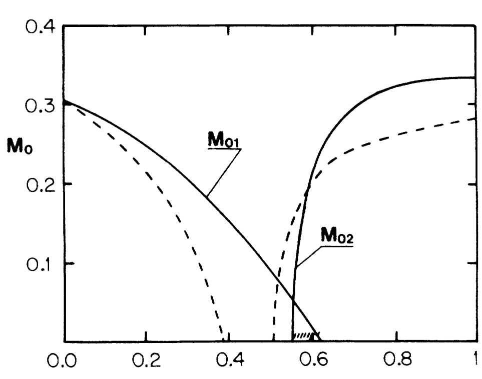

FIG. 2. Staggered magnetization vs J_2/J_1. The solid and the dashed lines corresponding to the results of the present theory and those of the linear CSW theory, respectively.

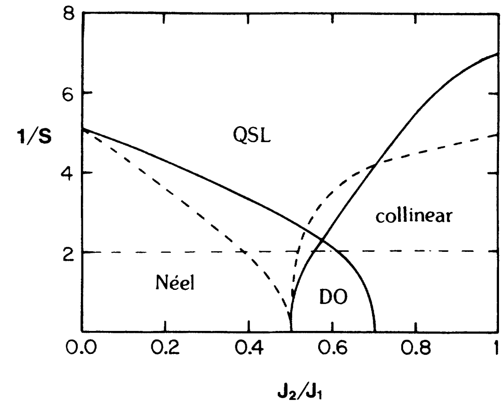

FIG. 3. Phase diagram of the considered model. The two lines, along which the staggered magnetization is vanishing, are shown. The solid and the dashed lines corresponding to the present theory and the linear CSW theory, respectively. The range of physical spin value is indicated by a dot-dashed line.

It should be pointed out that the present theory predicts almost exactly the same region ($J_2/J_1 \approx 0.55$–0.62) as that in numerical calculations[7,8,12] where the Néel state is changed to the collinear state. The quantitative agreement between the present results and the numerical conclusions is surprisingly good. We also show the results of the linear CSW theory[6] (the dotted line in Fig. 2) that indicate the ground state in the region between $J_2/J_1 \approx 0.38$–0.51 is nonmagnetic or a QSL state. Obviously, this conclusion is inconsistent with our and other numerical results.

For completeness, we also present a phase diagram for the J_1-J_2 model. The present MSW theory predicts a vanishing order parameter along those two solid lines in the $1/S$ vs J_2/J_1 as shown in Fig. 3. Based on this result, it is reasonable to speculate that there exists a critical value of the spin $S=S_c(J_2/J_1)$ below which the staggered magnetization vanishes. Unfortunately, S_c is less than the lowest physically accessible value $S=\frac{1}{2}$ to obtain a nonmagnetic QSL ground state within the J_1-J_2 model. This result is also consistent with the numerical calculations[8,12] that no evidence of chiral order,[17] which is believed to exist in the QSL state in the J_1-J_2 model with $S=\frac{1}{2}$, has been found.

In conclusion, we have given a new phase diagram for the frustrated Heisenberg model by using the MSW approach. For small J_2 we found that the ground state is Néel-like while the collinear state is more stable for large J_2. The change from one state to the other occurs at $J_2/J_1=0.55$ and 0.62 which is consistent with the numerical results.[7,8,12] In the intermediate region we found a DO state which is different than the nonmagnetic QSL state. The most possible candidate for the ground state in the DO region is the twisted state. The presence of a finite DO region in the J_1-J_2 model with $S=\frac{1}{2}$ is a result that the spin fluctuations are arbitrarily large due to the softened spin-wave modes in that region. An investigation with other analytical or numerical methods would be necessary to characterize the true ground state in the DO region.

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