Collinear Néel-type ordering in partially frustrated lattices

Uma Bhaumik and Indrani Bose
Department of Physics, Bose Institute, 93/1, Acharya Prafulla Chandra Road, Calcutta-700 009, India
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We consider two partially frustrated $S=\frac{1}{2}$ antiferromagnetic spin systems on the triangular and pentagonal lattices. In an elementary plaquette of the two lattices, one bond has exchange interaction strength α ($\alpha \leqslant 1$) whereas all other bonds have exchange interaction strength unity. We show that for α less than a critical value α_c, collinear Néel-type ordering is possible in the ground state. The ground-state energy and the excitation spectrum have been determined using linear spin-wave theory based on the Holstein-Primakoff transformation. [S0163-1829(98)04625-6]

Frustrated spin sytems show a tendency to be magnetically disordered. Frustration may occur due to the presence of further-neighbor interactions, besides the nearest-neighbor (NN) ones, as well as due to the topology of the underlying lattice. A well-known example of the latter is the triangular lattice. The ground state of the Ising antiferromagnet (AFM), defined on the triangular lattice, is highly degenerate with the entropy per site being a finite quantity. The Ising AFM thus does not order at any temperature. In this context, the question of interest is whether for a quantum-spin Hamiltonian long-range magnetic order can exist in the ground state. The quantum Heisenberg AFM (HAFM) has been widely studied on the triangular lattice[1–5] and there is now more or less a consensus that AFM long-range order (LRO) exists in the ground state. The ground state of the classical spin systems exhibits noncollinear 120° ordering. The ordering is partially destroyed but still exists once the quantum nature of the spins is taken into account.

Frustrated lattices, in general, exhibit noncollinear Néel-type magnetic order whereas nonfrustrated lattices like the square lattice exhibit collinear Néel-type order in the classical ground state. A partially frustrated lattice is obtained when not all the exchange interaction strengths along NN bonds have equal values. In this case, the classical ground state, in a particular parameter regime, exhibits collinear Néel-type ordering similar to that in the case of a nonfrustrated lattice. The ordering is not destroyed when quantum fluctuations are taken into account. Two examples of this will be given in this paper, namely, those of the triangular and the pentagonal lattices. The result for the classical ground state of the triangular lattice is already known.[6] In the so-called Row model, the strength of the unequal exchange interaction is α ($\alpha \leqslant 1$) whereas all other exchange interaction strengths have value unity (Fig. 1). For ($\alpha \leqslant \alpha_c$), the ground state has collinear order whereas for ($\alpha > \alpha_c$), noncollinear spiral ordering occurs. This ordering becomes the 120° ordering when $\alpha=1$. For $\alpha \leqslant \alpha_c$, we determine the excitation spectrum as well as the quantal correction to the ground-state energy using linear spin-wave (LSW) theory based on the Holstein-Primakoff (HP) transformation. We next consider the case of the partially frustrated pentagonal lattice. The Ising AFM has been previously studied on the pentagonal lattice[7,8] and the ground state has been found to be disordered. In this paper, we study the spin $S=\frac{1}{2}$ HAFM on the pentagonal lattice. The elementary plaquette of a pentagonal lattice is a pentagon and hence the lattice is topologically frustrated. We study the model in a limited parameter regime, namely, the one in which collinear Néel-type order exists in the ground state.

Consider a single triangular plaquette with three NN bonds. One of the bonds has exchange interaction strength α, the other two have exchange interaction strengths unity. The three spins sit at the three vertices and interact through NN interaction. If the spins are treated as classical vectors, it is easy to show that for $\alpha \leqslant \frac{1}{2}$, collinear Néel-type ordering is obtained in the ground state. Let 0, Q, Q' be the respective orientations of the spins with respect to the z axis. The first and third spins interact through exchange interaction of strength α. In the collinear state, $Q=\pi$ and $Q'=0$. For $\alpha > 0.5$, $Q'=2Q$ in the ground state with $Q=\cos^{-1}(-1/2\alpha)$, i.e., a spiral ordering is obtained. We first consider the Row model (Fig. 1) with $\alpha \leqslant \frac{1}{2}$. The sites belonging to alternate rows (shown by dashed lines) belong to one of the sublattices A or B. The interaction Hamiltonian is

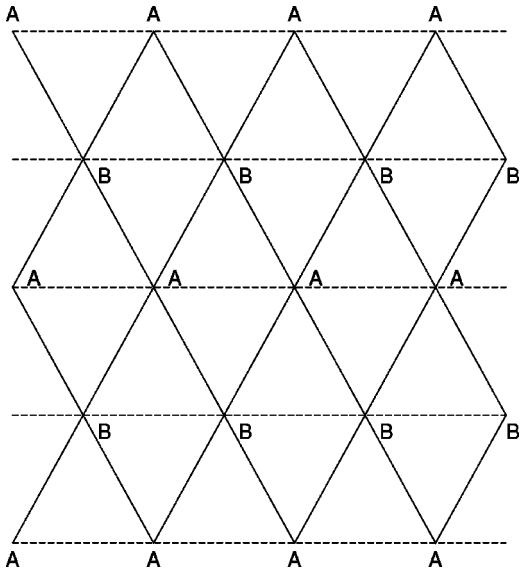

FIG. 1. The partially frustrated Row model defined on the triangular lattice. A and B denote the two sublattices. The dashed bonds have exchange interaction strength α ($\alpha \leqslant 1$), all other bonds (solid lines) have exchange interaction strength unity.

$$H=\sum_{i\in A,B,\boldsymbol{\delta}=\hat{a}_2\hat{a}_3}\mathbf{S_i}\cdot\mathbf{S_{i+\delta}}+\alpha\sum_{i\in A,B,\boldsymbol{\delta}=\hat{a}_1}\mathbf{S_i}\cdot\mathbf{S_{i+\delta}}, \quad (1)$$

$\hat{a}_1$, $\hat{a}_2$, $\hat{a}_3$ are the NN vectors in the horizontal and oblique directions, respectively. The spins on the A (B) sublattice are pointing up (down). This is the classical ground state. The foundation of spin-wave theory is the assumption that AFM LRO exists in the ground state and the amplitude of zero-point motion produced by quantum fluctuation about the classical ordered state is small. This assumption fails if quantal corrections diverge. The first step in the LSW theory is to transform the operators to the bosonic operators. The HP transformations connecting the spin operators to the bosonic operators a_j, b_j's are given in the lowest order by

$$S^{\dagger}_{A_j}=\sqrt{2s}a_j,$$

$$S^{\dagger}_{B_j}=\sqrt{2s}b^{\dagger}_j,$$

$$S^{z}_{A_j}=s-a^{\dagger}_j a_j,$$

$$-S^{z}_{B_j}=s-b^{\dagger}_j b_j, \quad (2)$$

where j denotes the lattice site and S is the magnitude of the spins. We will ultimately consider the case of $S=\frac{1}{2}$. $S^{\dagger}$, S^z are the spin raising operator and z component of the spin, respectively. One can similarly define the spin lowering operator S^{-}_j. We will not exhibit the different steps of LSW theory as these are standard.[9,10] The Hamiltonian (1) is expressed in terms of bosonic operators and then Fourier transformed. The Hamiltonian contains only quadratic operators and so can be diagonalized by the well-known Bogolyubov transformation. The diagonalized Hamiltonian is given by

$$H=NS(S+1)(2\alpha-4)+S\sum_k \omega_k+S\sum_k \omega_k(c^{\dagger}_k c_k+d^{\dagger}_k d_k), \quad (3)$$

where c_k, d_k are the new transformed operators and N is the total number of sites. The excitation spectrum ω_k is given by

$$\omega_k=\sqrt{\left(1-\alpha\,\sin^2\frac{\mathbf{k}\cdot\mathbf{a}_1}{2}\right)^2-\gamma_k^2}, \quad (4)$$

where

$$\gamma_k=\frac{1}{z}\sum_{\boldsymbol{\delta}=\hat{a}_2,\hat{a}_3}e^{i\mathbf{k}\cdot\delta} \quad (5)$$

and z, the number of NN's along the oblique directions, is 4. Figure 2 shows the excitation spectrum for $\alpha=0.3$ and $S=\frac{1}{2}$. The ground-state energy E_g [the sum of the first two terms in Eq. (3)] is given by $E_g=-0.6025$. One can verify that for $\alpha=0$, the excitation spectrum for the square lattice is recovered. As long as $\alpha<\frac{1}{2}$, ω_k is positive for all momentum wave vectors. This shows that the choice of the starting ground state is correct.

We next turn to the case of the pentagonal lattice. A cross section of the lattice is shown in Fig. 3. The lattice is a non-Bravais lattice and has two types of sites with coordination numbers 3 and 4, respectively. The NN exchange interaction strengths along the solid lines are given by α ($\alpha\leq 1$). Consider a single pentagonal plaquette. The classical ground state for different values of α can be determined by minimizing the exchange interaction energy with respect to the spin-orientation angles. For $\alpha<0.4$, one finds that the collinear Néel state is the ground state. The question is whether this order survives once the quantal fluctuations are taken into account. Again, we perform LSW theory to get an answer. Figure 3 shows the six sublattices (A_i, B_i, $i=1,2,3$) corresponding to the six inequivalent sites. The A (B) sublattices contain up (down) spins. The interaction Hamiltonian is given by

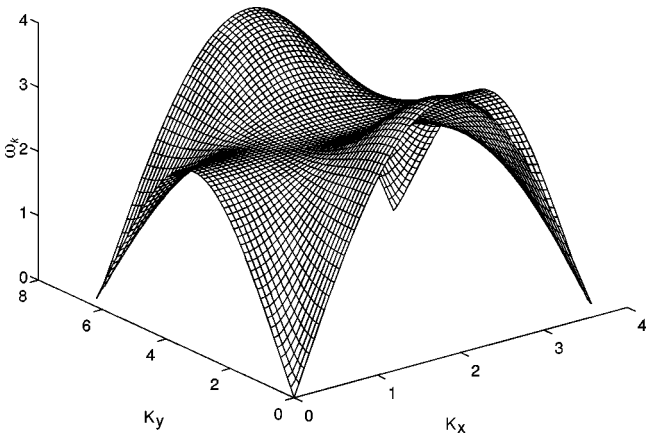

FIG. 2. Excitation spectrum of the Row Model for $\alpha=0.3$.

$$H=\sum_{\langle ij\rangle}J_{ij}\mathbf{S_i}\cdot\mathbf{S_j}, \quad (6)$$

where $<i\ j>$ denotes NN's and $J_{ij}=1$ for NN's shown by solid lines in Fig. 1. The NN vectors $\boldsymbol{\delta}_i$'s are given by

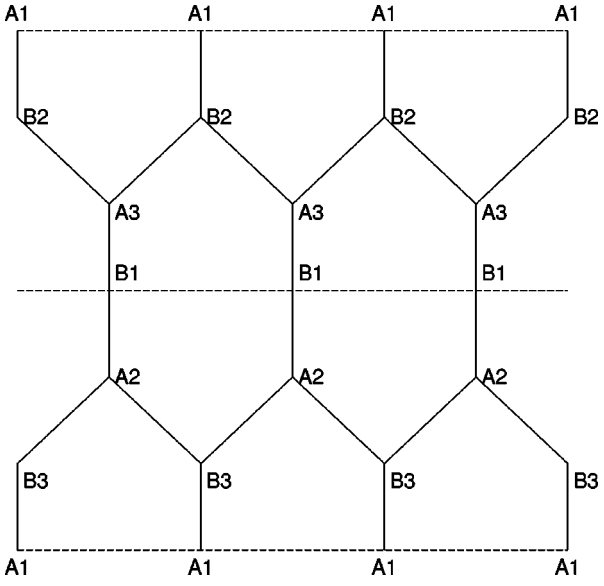

FIG. 3. The partially frustrated pentagonal lattice. The six sublattices are A_i and B_i ($i=1,2,3$). The dashed bonds have exchange interaction strength α ($\alpha<1$), all other bonds (solid lines) have exchange interaction strength unity.

$$\boldsymbol{\delta}_1=\hat{x},$$

$$\boldsymbol{\delta}_2=\hat{y},$$

$$\boldsymbol{\delta}_3=\frac{1}{2}\,\hat{x}+\frac{\sqrt{3}}{2}\,\hat{y},$$

$$\boldsymbol{\delta}_4=-\frac{1}{2}\,\hat{x}+\frac{\sqrt{3}}{2}\,\hat{y} \tag{7}$$

and similarly for the vectors in the reverse directions. The HP transformations connecting the spin operators to bosonic operators a_i and b_i are given by Eq. (2). Each of the six kinds of HP bosons forms a rectangular sublattice with dimension $(1,4+\sqrt{3})$. After Fourier transformation, the Hamiltonian (6) becomes

$$H=H_0+H_1,$$

where

$$H_0=NS(S+1)(-8+2\alpha), \tag{8}$$

$$H_1=S\sum_k\ \psi_k^\dagger M_k\psi, \tag{9}$$

$$\psi_k^\dagger=(a_{1k}^\dagger a_{2k}^\dagger a_{3k}^\dagger b_{1k} b_{2k} b_{3k}), \tag{10}$$

$$M_k=\begin{bmatrix} Z_{1k} & Z_{2k} \\ Z_{2k}^\dagger & Z_{1k}\end{bmatrix},$$

$$Z_{1k}=\begin{bmatrix} 2-4\alpha\,\sin^2\dfrac{\mathbf{k}\cdot\boldsymbol{\delta}_1}{2} & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3\end{bmatrix},$$

$$Z_{2k}=\begin{bmatrix} 0 & x_1^\star & x_2 \\ x_1 & 0 & x^\star \\ x_2^\star & x & 0\end{bmatrix},$$

$$x_1=e^{i\mathbf{k}\cdot\boldsymbol{\delta}_1},\quad x_2=e^{i\mathbf{k}\cdot\boldsymbol{\delta}_2},\quad x=e^{i\mathbf{k}\cdot\boldsymbol{\delta}_3}+e^{i\mathbf{k}\cdot\boldsymbol{\delta}_4}, \tag{11}$$

and N is the total number of sites. Following Jolicoeur and Le Guillou,[5] we consider the generalized Bogolyubov transformation matrix T as follows:

$$\begin{bmatrix}\alpha(k)\\ \beta(k)\end{bmatrix}=T\begin{bmatrix} a(k)\\ b^\dagger(k)\end{bmatrix}, \tag{12}$$

where $\alpha(k)$ is the column vector with three components $\alpha_n(k)$ $(n=1,2,3)$ and similarly for $\beta^\dagger(k)$. In order to satisfy the bosonic commutation relations, T has to satisfy

$$T^{-1}=\eta T\eta, \tag{13}$$

where

$$\eta=\begin{bmatrix} I & 0\\ 0 & -I\end{bmatrix}, \tag{14}$$

and I is the 3×3 identity matrix. Finally we have

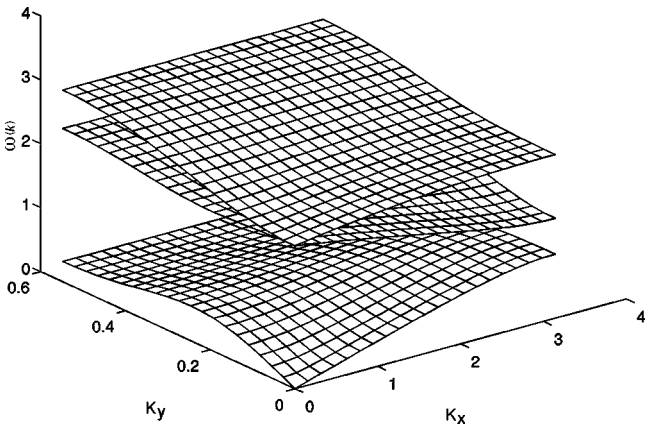

FIG. 4. Excitation spectra for the pentagonal lattice for $\alpha=0.27$.

$$H_1=S\sum_k\ [\alpha^\dagger(k)\beta(k)]\,\eta T[\eta M_k]T^{-1}\begin{bmatrix}\alpha(k)\\ \beta^\dagger(k)\end{bmatrix}. \tag{15}$$

To diagonalize H_1 a suitable choice for T is

$$T^{-1}=(v^1v^2v^3w^1w^2w^3), \tag{16}$$

where v^n and w^n are the eigenvectors of ηM_k, with corresponding eigenvalues $(\omega_n,-\omega_n)$. The eigenvalues of ηM_k occur in pairs with $\omega_n>0$. The matrix ηM_k can be diagonalized numerically. We obtain three excitation spectra each of which is doubly degenerate corresponding to the two sublattices A_i,B_i. The diagonalized Hamiltonian has the form

$$H=H_0+S\sum_{n=1}^{3}\ \omega_n(\alpha_n^\dagger\alpha_n+\beta_n^\dagger\beta_n), \tag{17}$$

$$H_0=NS(S+1)(-8+2\alpha)+S\sum_{n=1}^{3}\ \omega_n. \tag{18}$$

Figure 4 shows the three excitation spectra for $\alpha=0.27$ and $S=\frac{1}{2}$. The positivity of the spectra shows that the collinear Néel state with quantum corrections is still the ground state. For α beyond the critical value $\alpha_c\approx0.32$ this is no longer so. The ground-state energy E_g is given by Eq. (18) and has the value $E_g=-0.4835$ for $\alpha=0.27$.

For both the triangular and pentagonal lattices, there is a critical value α_c of α below which the classical ground state has collinear Néel-type order. As shown by LSW theory, the order is maintained, albeit with quantum corrections, when the quantum nature of the spins is taken into account. Let us now consider the case $\alpha>\alpha_c$. For the triangular lattice, as mentioned before, the ground state shows spiral ordering. For the pentagonal lattice, however, the problem is more difficult. Consider the case $\alpha=1$. Calculations for an elementary plaquette show that in the classical ground state the difference in the successive spin orientation angles is 144°. Unlike the case of the triangular lattice, the spin arrangement of a single pentagon cannot be repeated for the whole lattice. The determination of the classical ground-state structure thus becomes computationally more difficult. The parameter region $\alpha>\alpha_c$ for the pentagonal lattice has not been studied as yet. The value of α_c can be taken as a measure of frustration in a spin system. The values for the square, triangular, and

pentagonal lattices are $\alpha_c = 1$, 0.5, and ~ 0.32, respectively. Thus the pentagonal lattice appears to be more frustrated than the triangular lattice. Several studies have been undertaken in the recent past to understand the effect of topological frustration on ground-state properties. In two dimensions, the most studied cases are those of the triangular and *kagomé* lattices. Frustration, in general, leads to more disorder in the ground state. The interest in spin-disordered states has arisen in connection with high-temperature superconductivity. The pentagonal lattice is another topologically frustrated lattice which has not been studied so far in the context of quantum spin systems. The present study constitutes a small beginning which will hopefully lead to more exhaustive studies in the future.

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