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LETTERS

Spin-Wave Analysis of the Antiferromagnetic Plane Rotator Model on the Triangular Lattice —Symmetry Breaking in a Magnetic Field

Hikaru KAWAMURA

Department of Physics, College of General Education Osaka University, Toyonaka, Osaka 560

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Lowest-order spin-wave analysis is applied to the antiferromagnetic plane rotator model on the triangular lattice in order to study the low-temperature properties in the presence of magnetic fields. Equilibrium spin configuration in the zero-temperature limit is calculated as a function of the magnetic field. It is found that the thermal-fluctuation effect reduces a continuous degeneracy of the ground state to a discrete one at non-zero temperatures.

Recently there is a considerable interest in the phase transition and low-temperature properties of the antiferromagnetic plane rotator model on the two-dimensional triangular lattice.[1,2] The ground state of this model consists of spins on three sublattices forming 120° angles leading to a $\sqrt{3}\times\sqrt{3}$ periodicity (120° structure). Such type of ground state has a twofold discrete degeneracy as well as an XY-like continuous degeneracy. As a consequence, this system is expected to have two different mechanisms of phase transition, i.e., the Ising-type symmetry breaking mechanism and the Kosterlitz-Thouless mechanism[3] with the low-temperature phase characterized by the power-law-decaying spin correlation.

Miyashita and Shiba[1] investigated properties of phase transition and low-temperature phase of this model by use of Monte Carlo simulation, and they analyzed the data on the basis of the twofold degeneracy of the ground state and also of the spin-wave-like excitation for the case of zero magnetic field. Their results show that there actually exist two types of mechanisms of phase transition. Lee, Joannopoulos, Negele and Landau[2] studied the same system by use of Monte Carlo simulations including the case of a finite magnetic field. It has been shown that in the presence of an in-plane magnetic field $\boldsymbol{H}$ the ground state magnetizations per spin $\boldsymbol{S}_a$, $\boldsymbol{S}_b$ and $\boldsymbol{S}_c$ satisfy the relation $|\boldsymbol{S}_a|=|\boldsymbol{S}_b|=|\boldsymbol{S}_c|=1$ with

$$\boldsymbol{S}_a+\boldsymbol{S}_b+\boldsymbol{S}_c=\boldsymbol{H}/(3J), \quad (|\boldsymbol{H}|<9J) \qquad (1)$$

where J is the nearest-neighbor coupling. This relation indicates that even though the Hamiltonian has no continuous symmetry the ground state has a continuous degeneracy as in the case of zero magnetic field. In other words, the application of magnetic field does *not* dissolve a continuous degeneracy of the ground state. This should be contrasted to the cases of ferromagnets or antiferromagnets on bipartite lattices where the application of magnetic field reduces the symmetry of the ground state. It should be noticed, however, that even if the ground state has a continuous degeneracy it does not necessarily persist at non-zero temperatures. In fact, even in the zero-temperature limit, the most favorable spin configuration is determined not only by its energy but also by the density of states just above the ground state. It is thereby possible that in the presence of magnetic fields the continuous degeneracy of the ground state is not fully reflected in the actual symmetry of the low-temperature phase. It is the purpose of the present letter to apply the lowest-order spin-wave analysis to the antiferromagnetic plane rotator model on the triangular lattice in order to determine equilibrium spin configurations in the zero-temperature limit. It is found that by applying any non-zero magnetic field the continuous degeneracy of the ground state is dissolved due to the thermal-fluctuation effect. The obtained spin configurations are shown in Fig. 1.

We consider the Hamiltonian given by

$$\mathscr{H}=J\sum_{\langle ij\rangle}\boldsymbol{S}_i\cdot\boldsymbol{S}_j-\boldsymbol{H}\cdot\sum_i\boldsymbol{S}_i,\quad (J>0) \tag{2}$$

where $\boldsymbol{S}_i$ is a two-component unit vector $\boldsymbol{S}_i=(\cos\phi_i, \sin\phi_i)$, and the sum is taken over all nearest neighboring pairs. We assume that the magnetic field $\boldsymbol{H}$ is applied parallel to the x-axis, i.e., $\boldsymbol{H}=(H, 0)$. The ground-state spin configuration can be specified by the relations:

$$\cos\theta^a+\cos\theta^b+\cos\theta^c=\min(h, 3), \tag{3}$$

$$\sin\theta^a+\sin\theta^b+\sin\theta^c=0, \tag{4}$$

where $\theta^a-\theta^c$ are the angles representing the sublattice-magnetization vectors $\boldsymbol{S}_a-\boldsymbol{S}_c$, and h is a reduced magnetic field equal to $h\equiv H/(3J)$. From eq. (3), one can easily see that the ground-state magnetization per spin is equal to $h/3$ in the case $h\le 3$ and it saturates in the case $h\ge 3$. The ground-state energy is given by

$$E_0/(JN)=\begin{cases}-\dfrac{3}{2}-\dfrac{h^2}{2}, & (h\le 3)\\ 3-3h. & (h\ge 3)\end{cases} \tag{5}$$

In the following, we shall calculate the low-temperature expression of the free energy within the lowest-order spin-wave approximation focusing our attention on the case $h\le 3$. For each spin $\boldsymbol{S}_i=(\cos\phi_i, \sin\phi_i)$ belonging to the α-sublattice (α is a, b or c), we introduce a deviation angle ψ_i^α by $\phi_i=\theta^\alpha+\psi_i^\alpha$. Substituting this relation into (2) and expanding it up to the second order in ψ_i^α, we get

$$\begin{aligned}\mathscr{H}&=E_0+\mathscr{H}_{\text{s.w.}},\\ \mathscr{H}_{\text{s.w.}}&=\cos(\theta^a-\theta^b)\sum_{\langle ij\rangle}\psi_i^a\psi_j^b+\cos(\theta^b-\theta^c)\sum_{\langle jk\rangle}\psi_j^b\psi_k^c+\cos(\theta^c-\theta^a)\sum_{\langle ki\rangle}\psi_k^c\psi_i^a\\ &\quad+\frac{3}{2}\Big[\sum_i(\psi_i^a)^2+\sum_j(\psi_j^b)^2+\sum_k(\psi_k^c)^2\Big].\end{aligned} \tag{6}$$

After the Fourier transformation, the spin-wave part of the Hamiltonian can be written in the matrix form:

$$\mathscr{H}_{\text{s.w.}}=\sum_{\boldsymbol{q}}\psi_{\boldsymbol{q}}^+A_{\boldsymbol{q}}\psi_{\boldsymbol{q}}, \tag{7}$$

where the summation runs over all $N/3$ wave vectors associated with a sublattice. The column vector $\psi_{\boldsymbol{q}}$ and the hermite matrix $A_{\boldsymbol{q}}$ is defined by

$$\psi_{\boldsymbol{q}}=\begin{pmatrix}\psi_{\boldsymbol{q}}^a\\ \psi_{\boldsymbol{q}}^b\\ \psi_{\boldsymbol{q}}^c\end{pmatrix},\quad A_k=\begin{pmatrix}\frac{3}{2} & \frac{x}{2}\varepsilon_{\boldsymbol{q}} & \frac{z}{2}\varepsilon_{\boldsymbol{q}}\\ \frac{x}{2}\varepsilon_{\boldsymbol{q}}^* & \frac{3}{2} & \frac{y}{2}\varepsilon_{\boldsymbol{q}}\\ \frac{z}{2}\varepsilon_{\boldsymbol{q}}^* & \frac{y}{2}\varepsilon_{\boldsymbol{q}}^* & \frac{3}{2}\end{pmatrix}, \tag{8}$$

where $x\equiv\cos(\theta^a-\theta^b)$, $y\equiv\cos(\theta^b-\theta^c)$, $z=\cos(\theta^c-\theta^a)$, and $\psi_{\boldsymbol{q}}^\alpha$ is the Fourier transform of ψ_i^α. The complex quantity $\varepsilon_{\boldsymbol{q}}$ is defined by

$$\varepsilon_{\boldsymbol{q}}=\exp\left(i\frac{q_x+\sqrt{3}q_y}{2}\right)+\exp\left(i\frac{q_x-\sqrt{3}q_y}{2}\right)+\exp(-iq_x). \tag{9}$$

Within this approximation, the free energy is calculated as

$$F\simeq E_0+Nk_{\text{B}}T\ln\left(2\sqrt{\frac{\pi}{k_{\text{B}}T}}\right)+\frac{k_{\text{B}}T}{2}\sum_{\boldsymbol{q}}\ln(\det A_{\boldsymbol{q}}), \tag{10}$$

where $\det A_{\boldsymbol{q}}$ is given by

$$\det A_{\boldsymbol{q}}=\frac{27}{8}+\frac{xyz}{8}|\varepsilon_{\boldsymbol{q}}|^2(\varepsilon_{\boldsymbol{q}}+\varepsilon_{\boldsymbol{q}}^*)-\frac{3}{8}(x^2+y^2+z^2)|\varepsilon_{\boldsymbol{q}}|^2$$

$$=\frac{3(9-|\varepsilon_q|^2)}{8}+\frac{|\varepsilon_q|^2(6-\varepsilon_q-\varepsilon_q^*)}{64(1+h^2)}[(1-h^2)^3+16h^3\cos\theta^a\cos\theta^b\cos\theta^c]. \tag{11}$$

In deriving (11), we have used the relations (3) and (4). Now the problem is reduced to minimizing $\cos\theta^a\cos\theta^b\cos\theta^c$ under the restrictions (3) and (4). This problem can be solved leading to the following solutions:

I) $0<h\leq 1$

$$\theta^a=-\pi,\quad \theta^b=\cos^{-1}\frac{1+h}{2},\quad \theta^c=-\theta^b, \tag{12}$$

II) $1\leq h\leq 3$

$$\theta^a=\cos^{-1}\frac{h^2-3}{2h},\quad \theta^b=\theta^c=-\cos^{-1}\frac{h^2+3}{4h}. \tag{13}$$

These solutions represent the equilibrium spin configurations in the zero-temperature limit. The results are shown in Fig. 1(a) and (b). With increasing the magnetic field, the spin configuration changes continuously without spin flop except across the zero field. The free energy can be calculated by substituting (12) or (13) into (10) and (11). These results, which are expected to be exact in the zero-temperature limit, indicates that the continuous degeneracy of the ground state is dissolved by the temperature effect in the presence of magnetic fields. The remaining degeneracy is only a discrete one which will determine the nature of the phase transition taking place at higher temperature.[2)]

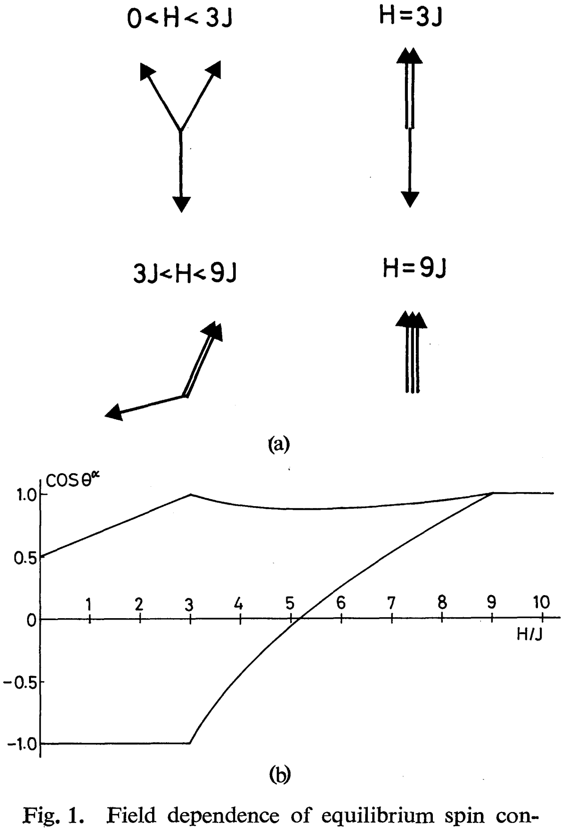

Fig. 1. Field dependence of equilibrium spin configurations in the zero-temperature limit. Three arrows in Fig. (a) represent the directions of spins on three sublattices, respectively. The magnetic field is applied in the upward direction.

As is apparent from (11), the entropy term favors the configuration in which spins on two sublattices are parallel and spins on one sublattice is antiparallel with the applied field. In this ferrimagnetic configuration, $\cos\theta^a\cos\theta^b\cos\theta^c$ takes its possible minimum value equal to minus unity. Though such configuration is compatible with the energy minimization conditions (3) and (4) only at $h=1$, one can expect that at *finite* temperatures the ferrimagnetic state might be stabilized over a finite range of magnetic fields due to the entropy effect. In fact, appearance of the stable ferrimagnetic state at finite temperatures is observed in the neighborhood of $h=1$ in Monte Carlo simulation by Lee *et al.*[2),*]

The spin-wave dispersion consists of three branches. In the long-wavelength limit $q\to 0$, they have the following asymptotic forms:

I) $0<h\leq 1$

$$\varepsilon_{\mathrm{I}}/J\sim\frac{3}{8}q^2, \tag{14}$$

$$\varepsilon_{\mathrm{II}}/J\sim\frac{3}{4}(3+2h+h^2), \tag{15}$$

$$\varepsilon_{\mathrm{III}}/J\sim\frac{3}{4}(3-2h-h^2), \tag{16}$$

II) $1\leq h\leq 3$

$$\varepsilon_{\mathrm{I}}/J\sim\frac{3}{8}q^2, \tag{17}$$

* *Note added in proof*: Experimentally, the appearance of the stable ferrimagnetic state means the appearance of the 1/3 plateau in the magnetization curve. We note that this phenomenon has been observed in C_6Eu by H. Suematsu, K. Ohmatsu, K. Sugiyama, T. Sakakibara, M. Motokawa and M. Date: Solid State Commun. **40** (1981) 241.

$$\varepsilon_{\mathrm{II}}/J \sim \frac{3}{4}[3+\sqrt{1+(h^2-5)^2/2}], \tag{18}$$

$$\varepsilon_{\mathrm{III}}/J \sim \frac{3}{4}[3-\sqrt{1+(h^2-5)^2/2}]. \tag{19}$$

Among these three branches, one branch is always gapless (Goldstone mode) which reflects the continuous degeneracy of the ground state. Physically speaking, this Goldstone mode corresponds to the long-wavelength rotation of the 120° structure. The spinwave stiffness constant of the Goldstone mode is field-independent. On the other hand, other two branches are "optical modes" with finite gaps which correspond to internal distortion of the 120° structure. Especially in zero-field, the energy of this gap is equal to $9J/4$ which is considerably larger than the transition temperature of this model $k_BT_C \simeq 0.5\,J$.[1,2] From this observation, one can expect that the 120° structure gives a fairly good short-range description of the model even around the transition point.

In the case $h \geq 3$, all spins are completely polarized in the ground state. The spin-wave dispersion has only one branch with a finite gap:

$$\varepsilon_{\boldsymbol{q}} \simeq \frac{3h}{2} - \frac{3}{4}q^2. \tag{20}$$

Though we hitherto concentrate our discussions on the purely two-dimensional triangular lattice, we note that similar arguments can readily be extended with slight modifications to the three-dimensional hexagonal (or stacked-triangular) lattice system with an interplane coupling of arbitrary sign and strength. In particular, equilibrium spin configurations in the zero-temperature limit obtained in (12) and (13) are the same even in the presence of an interplane coupling.

We finally refer to the two-dimensional classical *Heisenberg* antiferromagnet on the triangular lattice.[4] It can be shown that the ground state of the Heisenberg model is also specified by the relation (1) as in the case of the plane rotator. (In the Heisenberg case, $\boldsymbol{S}_a - \boldsymbol{S}_c$ are the three-component unit vectors.) This fact means hat the ground state in the presence of magnetic fields has the same degree of continuous degeneracy with the zero-field case. The present results of the spin-wave calculation for the plane rotator model suggest, however, that this continuous degeneracy of the ground state of the Heisenberg model is dissolved at non-zero temperature and the actual symmetry of the low-temperature phase is lower than the symmetry of the ground state. In fact, results of a Monte Carlo simulation show that the H-T phase diagram of this model has a rich structure. Details of this Monte Carlo simulation will be reported elsewhere.[5]

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