Cascade first-order phase transitions in quasi-one-dimensional antiferromagnets. Low-temperature analysis

G. V. Uĭmin

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR, Moscow

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It is shown that a cascade of magnetic phase transitions from the antiferromagnetic phase to a phase with magnetization corresponding to one-third the saturation magnetization should exist in some quasi-one-dimensional antiferromagnets.

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The existence of first-order cascade phase trainsitions ("fourth" ladder) has been clearly explained theoretically in the last two to three years. This phenomenon can be described by the Ising model with an interaction including neighbors other than nearest neighbors, which in the literature is referred to as the ANNNI model (axial next-nearest neighbor Ising model). The ANNNI model was analyzed in the self-consistent field approximation[1] with the help of the low-temperature expansion[2] and with the help of the high-temperature expansion.[3] All of these attempts were stimulated by the experimentally observed, very complex phase diagram of cerium antimonide CeSb (see Refs. 4–6). This substance is unique: the phase diagram in the T-H plane (T is the temperature, H is the magnetic field) contains 14 different magnetic phases and three cascades of first-order transitions. The theoretical interpretation of this friction assumes that the difference $J_1 - 2J_2$ is especially small, where J_1 and J_2 are exchange interaction constants of nearest and next-to-nearest magnetic atoms. In this paper, we examine a less special case of quasi-one-dimensional antiferromagnet in which the interaction along filaments decreases rapidly: $J_1 \gg J_2$.

The Hamiltonian of the model examined has the form

$$\mathcal{H} = - q^{-1} J_0 \sum_{l,\, \mathbf{r}, \mathbf{r}'} \sigma_{\mathbf{r},l} \sigma_{\mathbf{r}',l} + \frac{1}{2} \sum_{l,\mathbf{r}} (J_1 \sigma_{\mathbf{r},l} \sigma_{\mathbf{r},l+1} + J_2 \sigma_{\mathbf{r},l} \sigma_{\mathbf{r},l+2}) - H \sum_{l,\mathbf{r}} \sigma_{\mathbf{r},l}, \quad (1)$$

where $\sigma_{\mathbf{r},l}$ is the Ising variable ($\sigma = \pm 1$), assigned to the lattice site with coordinate $(\mathbf{r}, l)$. Summation within a plane is performed, for definiteness, over the nearest neighbor sites, whose number is equal to q. The ground state of the quasi-one-dimensional Ising magnet described by Hamiltonian (1) with positive J_0 and J_1 ($J_1 \gg J_0$) contains ferromagnetic planes, whose sequence of magnetization orientations is a function of the magnetic field H. The phase diagram in the plane of the exchange interaction constants J_1 and J_2 at $T = 0$ and fixed H is shown in Fig. 1. We shall be interested in the region of exchange constants J_1 and J_2 close to the point of existence of the three phases: ferromagnet (F), antiferromagnet (AF), and the $[2,\bar{1}\rangle$ phase. The phase $\langle 2,\bar{1}\rangle$ contains a periodic sequence of ferromagnetically ordered planes with the following magnetization sequence along filaments: $+ + -$.

It is clear from Fig. 1 that as the magnetic field increases at $T = 0$, the following sequence of magnetic phases arises: $AF - \langle 2,\bar{1}\rangle - F$. The phase degeneration curves

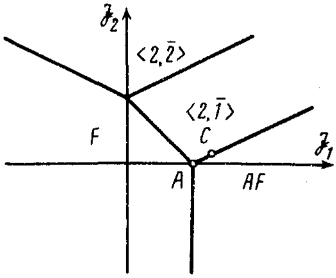

FIG. 1. Phase diagram for the model examined at $T=0$. As the magnetic field is varied, the phase degeneration curves are displaced parallel to themselves. The coordinate of the point A is $(H,0)$. The point C is a multiphase point. To the right or of it for $T\neq 0$ the curve splits into the sequence (3), and to the left it remains unsplit.

(PDC) are interesting. Along PDC $AF - \langle 2\bar{1}\rangle$, the ground state, consisting of an arbitrary sequence of blocks $A(++-)$ and $B(+-)$ is degenerate:

$$A^{n_1}B^{m_1}A^{n_2}B^{m_2}\ \dots\ . \qquad (2)$$

For $T\neq 0$ in the vicinity of the PDC indicated, the configuration energy (2) competes with the entropy contribution to the free energy determined by elementary excitations. We must distinguish two cases. In the first $J_0>J_2\gg T$, the low-lying excitations are related to flipping of a single spin in the following configurations along a filament (the Boltzmann weights of the excitations are enclosed in parentheses, while the circle encloses the flipped spin):

$$+\ +\ \ominus\ +\ +\left(w=\exp\left(-\frac{1}{T}(2J_0+6J_2)\right)=w_0w_2^3\right),$$

$$+\ +\ -\ +\ -\quad \text{or}\quad -\ +\ -\ +\ +\ (w=w_0w_2^2),$$

$$-\ +\ -\ +\ -\ \ (w=w_0w_2).$$

In the second case $(J_2>J_0\gg T)$, two-spin flipping along the chain is important:

$$-\ +\ \oplus\ \ominus\ +\ -\quad \text{or}\quad -\ +\ \ominus\ \oplus\ +\ -\ (w=w_0^2)\ .$$

It is evident from the list of excitations which are important in each case that in the second case thermal fluctuations can lead to the appearance of a structure of alternating A and B blocks: $ABAB\dots(\langle AB\rangle$ phase). In the first case, the entropy contribution from the alternation is suppressed by the corresponding contribution of pure states $AAA\dots$ and $BBB\dots$ (phases $\langle A\rangle$ and $\langle B\rangle$). Therefore, for $J_0>J_2$ the transition from $\langle A\rangle$ to $\langle B\rangle$ is a first-order transition without splitting.

In the next order for $J_2>J_0$ we must study the PDC $\langle A\rangle - \langle AB\rangle$ and $\langle AB\rangle - \langle B\rangle$. An intermediate phase $\langle A^2B\rangle$ forms near the first curve. There is no splitting on the second curve. In this case three-spin flipping along a filament is important:

$$-\ +\ \ominus\ \oplus\ \ominus\ +\ -\ \ (w\approx w_0^3)\ .$$

Excitations of this type block the appearance of intermediate phases of the type $\langle AB^2\rangle$.

These and all following orders can be analyzed rigorously by linear programming methods as in Refs. 2 and 3. For $J_2>J_0$ we obtain the following cascade of transitions:

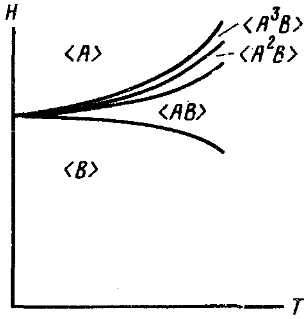

FIG. 2. Phase diagram in the T–H plane. The curves that bound the B and A phases in leading order are defined y the equations $H_B = H_c - 2Tw(T)$, $H_A = H_c + 3Tw(T)$ $(H_c = J_1 - 2J_2)$.

$$\langle B \rangle \longleftrightarrow \langle AB \rangle \longleftrightarrow \langle A^2B \rangle \longleftrightarrow \cdots \longleftrightarrow \langle A^nB \rangle \longleftrightarrow \cdots \longleftrightarrow \langle A \rangle. \tag{3}$$

The structure of the state $\langle A^nB \rangle$ is as follows:

$$\underbrace{+\,+\,-\,+\,+\,-\,\cdots\,+\,+\,-}_{n \text{ triplets}}\;+\,-$$

The value of the magnetization along this cascade varies according to the law:

$$M_n = \frac{n}{3n+2} \quad (n = 0, 1, 2, \ldots\ .) \tag{4}$$

The most intense Bragg reflection of the magnetic structure $\langle A^nB \rangle$ is related to the wave vector

$$k(n) = \frac{2\pi}{a}\,\frac{n+1}{3n+2} \tag{5}$$

(a is the magnetic lattice constant along a filament).

The phase diagram in the T-H plane is shown schematically in Fig. 2. By varying H with T constant, it is possible to traverse the entire ladder of phase transitions from the AF phase to the $\langle 2,\bar{1} \rangle$ phase. The value of the magnetization in this case varies according to (4), while the interval of magnetic fields ΔH_n, in which the phase $\langle A^nB \rangle$ is stable, is determined by the relation

$$\Delta H_n = (3n+2)Tw^n. \tag{6}$$

A multiphase point can be observed in quasi-one-dimensional antiferromagnets (point C in Fig. 1), since the ratio of J_0 and J_1 can be vaired by varying the pressure.

We should note a specific property of quasi-one-dimensionality. The PDC $AF - \langle 2,\bar{1}[$ $(\langle B \rangle - \langle A \rangle)$ was analyzed in Ref. 3 in the case of a layered quasi-two-dimensional structure $J_0 \gg J_1, J_2$. The result was the absence of splitting of this line. It was also shown in Ref. 3 that the PDC $\langle 2,\bar{1} \rangle - F$ is subjected to a very complicated splitting. In the quasi-one-dimensional case, this transition is a simple transition without splitting.

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