Phase diagram of the two-dimensional antiferromagnetic *XY* model in an external magnetic field

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The phase diagram of two-dimensional (2*D*) planar antiferromagnets (*AF XY* model) in an external magnetic field contains in addition to the Berezinskiĭ–Kosterlitz–Thouless (BKT) transition lines the Ising type transition lines which are associated with the existence of discrete symmetry.

The systems examined here—an *AF* magnet with a square (*s*) or a regular triangular (*t*) lattice—are described by the Hamiltonian

$$\mathcal{H} = J \sum_{\mathbf{r},\mathbf{r}'} \mathbf{m}_{\mathbf{r}} \mathbf{m}_{\mathbf{r}'} - h \sum_{\mathbf{r}} \mathbf{m}_{\mathbf{r}} . \quad (1)$$

The two-component magnetic moment $\mathbf{m}_\mathbf{r}(m_\mathbf{r}^x,\ m_\mathbf{r}^y)$, situated at the site $\mathbf{r}$, has a unit length and interacts only with its nearest neighbors and with the magnetic field $\mathbf{h}$, which is also a two-component vector.

The main difference between the models "*AF XY* + field" with *s* and *t* lattices is that the ground state (GS) in the first one is doubly degenerate, whereas in the second one the continuous degeneracy remains, as in the absence of a field. The reason is that in the *t* lattice it is advantageous to form three magnetic sublattices instead of two, as in an *AF* magnet with the *s* lattice. We shall first analyze the *t* lattice and then return to the *s* lattice at the end of the paper.

Calculating the energy of the three-sublattice configuration, scaled to a single lattice site

$$E^{(0)} = -3J/2 + J(\mathbf{m}_1 + \mathbf{m}_2 + \mathbf{m}_3)^2/2 - \mathbf{h}(\mathbf{m}_1 + \mathbf{m}_2 + \mathbf{m}_3)/3 \quad (2)$$

and minimizing it, we obtain $E^{(0)} = -3J/2 - h^2/18J$. Here

$$\mathbf{m}_1 + \mathbf{m}_2 + \mathbf{m}_3 = \mathbf{h}/3J . \quad (3)$$

The orientation of $\mathbf{m}_j$ is fixed by the angle $\phi_j\,(j = 1, 2, 3)$, which is reckoned from the direction of the field. In these variables Eq. (3) represents a system of two equations with three unknowns, which leaves a continuous degree of freedom for the ground state. Figure 1 shows lines in the three-dimensional space (ϕ_1, ϕ_2, ϕ_3), which are the solutions of Eq. (3). In low fields, $0 < h < h_{c1} = 3J$, the space of degeneracy of the ground state consists of two lines. On one line $(B_1B_2B_3)$ the circulation in the triplet of vectors, $\mathbf{m}_1$, $\mathbf{m}_2$, $\mathbf{m}_3$, is equal to 2π, while on the other line $(A_1A_2A_3)$ the circulation is equal to -2π. At $h = h_{c1}$ the two lines degenerate into a single, self-intersecting line (see Fig. 1b). At $h_{c1} < h < h_{c2} = 9J$ the line becomes closed, and near a forbidden region for the ground state appears near the values $\phi = \pm\pi$. As the field is increased, the neighborhood becomes wider and occupies the entire $\vec{\phi}$ space at $h = h_{c2}$.

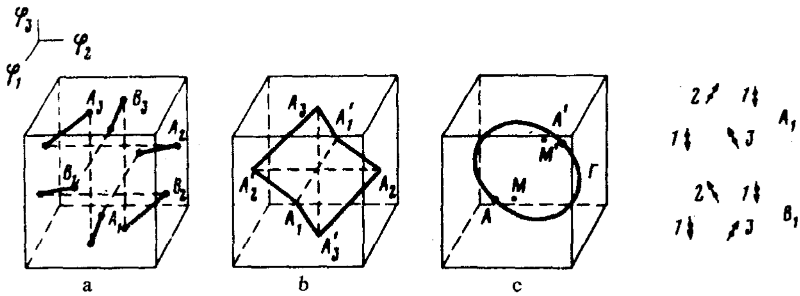

FIG. 1. Line of degeneracy of the ground state in the t lattice. Region of change of $\phi\,(-\pi,\pi)$. The broken lines connect the equivalent points. A fragment of the lattice corresponding to the points A_1 and B_1 is shown on the right.

We shall begin the construction of the phase diagram with the region corresponding to Fig. 1a. The system has a discrete Ising symmetry in addition to a continuous degeneracy which leads at $T\neq 0$ to the formation of the Berezinskiĭ phase (the so-called phase with a power-law order). The Ising variable is related to the local position of the system on the line $A_1A_2A_3$ or on the line $B_1B_2B_3$. The elements of this symmetry are ordered at low temperatures. This situation is fully consistent with the absence of long-range order for the spin variable, since the discrete symmetry is determined by the local arrangement of the moments.

In conformity with the two types of symmetry, the two types of topological excitations are also important. Excitations of the first type include the usual vortices, which at low temperatures bind together, forming neutral molecules that dissociate at the temperature of the BKT transition $T_{\rm BKT}$. Excitations of the second type are walls that separate two vacuum states corresponding to the lines $A_1A_2A_3$ and $B_1B_2B_3$. At the Ising disordering temperature T_I, the energy barrier between the points A_1 and B_1, A_2 and B_2, and A_3 and B_3 (Fig. 1a) vanishes. At $h=0$ the barrier vanishes at these points and the straight line $B_1B_2B_3$ can be reached from any point on the straight line $A_1A_2A_3$ directly without encountering a barrier. The numerical estimates in Ref. 1 show that at $h=0$ T_I must be less than $T_{\rm BKT}$. It was also concluded there that the Ising transition initiates the BKT transition at the point T_I, which should lead to a phase transition with a new universality class. However, as T_I is approached from below, the spin rigidity ρ_s, which directly determines $T_{\rm BKT}$ (ρ_s vanishes identically at $T=T_I$ and $h=0$) decreases. The BKT phase transition must therefore occur before the Ising transition, at least at $h=0$, which was confirmed numerically in Ref. 2.

We note that in the course of the I transition examined above the physical picture in Fig. 1a "transforms" to the one described in Fig. 1b. At $h=0$ this transformation corresponds to $T_I\sim J$—this is the energy ϵ of the wall per unit length. However, as $h\to h_{c1}$, the points A_1 and B_1 converge toward each other—the energy of the wall becomes small [$\epsilon\sim(h_{c1}-h)^{3/2}/J^{1/2}$], while its thickness l becomes large [$l\sim J^{1/2}/(h_{c1}-h)^{1/2}$]. We thus have

$$T_I(h)\sim\epsilon/\ln l\to 0 \quad \text{as} \quad h\to h_{c_1}. \tag{4}$$

The line of the I transitions separates the regions in which vortex excitations are

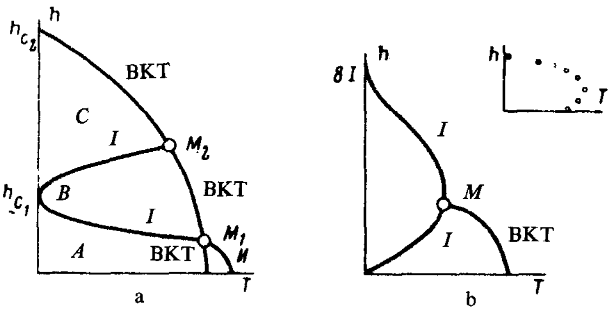

FIG. 2. Qualitative form of the phase diagram. (a) For the t lattice and (b) for the s lattice. M, M_1, and M_2 are multicritical points. A, B, and C are Berezinskiĭ phases with the topology of excitations corresponding to Figs. 1a–1c.

determined by the topology in Figs. 1a and 1b. Thus, in the case a, the vortex corresponds to the circuit $A_1A_2A_3A_1$ or $B_1B_2B_3B_1$ with a total circulation of $\pm 6\pi$ in all three sublattices. In the case b, in addition to the circuits mentioned above, there is also the circuit $A_1A'_2(A_2)A'_1(A_1)$, which corresponds to a vortex with fixed $\phi_3 = 0$ and $\phi_1 = \phi_2 - \pi$ and with a total circulation of $\pm 4\pi$. The vortices equivalent to the one examined above are obtained by interchanging sublattices. Above the line of the I transitions, the BKT transition is therefore realized as a result of the competition between several types of vortices. There is no conflict here: The rigorous conclusion that a BKT transition occurs before the Ising transition is valid at $h = 0$. If $h \neq 0$, we see that ρ_s on the line of I transitions does not vanish identically. A multicritical point M_1 at which the I and BKT transition lines converge must therefore exist (see Fig. 2a). Furthermore, the type of BKT transition changes after passing through this point.

We shall now examine the neighborhood of $h = h_{c2}$. The topology in this case can be explained in Fig. 1c. The space of degeneracy is the closed contour Γ, which accounts for the unavoidable vortex-type topological singularity (although with zero circulation!). The temperature of the BKT transition goes down to zero in the limit $h \to h_{c_2}$ as

$$T_{\text{BKT}} \sim h_{c_2} - h.$$

As the field decreases from h_{c_2} to h_{c_1}, the contour Γ approaches the boundary of the cube and its trajectory becomes similar to the one illustrated in Fig. 1b. It is possible to move between the two states A and A' (Fig. 1c), which in the limit $h \to h_{c_1}$ go into A_1 and A'_1 (Fig. 1b), without encountering a barrier along the contour Γ. There exists a temperature at which the direct transition $A \rightleftarrows A'$ through the point $M(\phi_1 = \pi, \phi_2 = \phi_3 = 0)$ also occurs without encountering a barrier. In this case the contour Γ becomes equivalent to the contour in Fig. 1b. The transition itself is an Ising type transition, and its temperature is given by an expression analogous to (4).

The considerations presented above are summarized by the phase diagram in Fig. 2a.

Let us finally consider the same problem for the s lattice. In contrast to the case examined above, there are two sublattices and the space of degeneracy of the ground

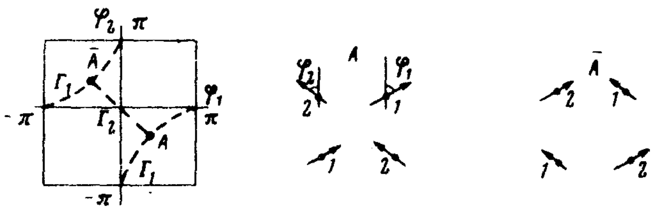

FIG. 3. A and $\bar{A}$ are points of degeneracy of the ground state in the s lattice. Right: fragments of the lattice corresponding to them.

state consists of two points in the (ϕ_1, ϕ_2) plane (Fig. 3). The main Ising-type excitations are walls, which above a certain temperature remove the barrier between the states A and $\bar{A}$ (Fig. 3). The barrier is removed along the contour Γ_1 in weak fields and along the contour Γ_2 in strong fields. In the first case, vortex excitations can appear in the isotropic phase, whereas in the second case they are forbidden. The phase diagram is shown in Fig. 2b. The top part of the figure shows the result of a numerical calculation,[1] which evidently reproduces only the I-transition line. According to our understanding, the line must hit the origin. It is difficult to observe this in a numerical simulation, since the walls in this region become wide $(l \sim I/h)$ and can become comparable to the dimensions of the system.

The theoretical magnetic systems examined here are not unique, and we hope that soon our ideas, expressed in Fig. 2, will be confirmed experimentally.

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