First order transition in MnO and the renormalization group (scaling)

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It is shown that fluctuations near the phase-transition point in MnO, CoO, NiO, etc. convert the possible second-order transition into a first-order transition. The calculations are performed within the framework of the Wilson ϵ expansion with allowance for the real cubic symmetry of the crystal.

It was recently shown experimentally[1] that the antiferromagnetic transition in MnO is of first order. We shall show below that when the fluctuations are taken into account the transition of this type in MnO, CoO, FeO, NiO, etc. cannot be of second order for any value of the constants that enter in the theory. Although the calculations were performed by us only within the framework of the Wilson ϵ expansion, i.e., actually in a hypothetical four-dimensional space, we expect that the structure of the renormalization group will not change on going to three-dimensional space, and the qualitative conclusion concerning the character of the transition will remain in force.

The antiferromagnetic transition in MnO, and in CoO, FeO, and NiO, which are isomorphic to it, has been long known. These oxides have a cubic face-centered lattice with the transition-metal ions at the sites and centers of the faces. The transition results in an antiferromagnetic structure with two sublattices: the spins are the same in planes of the (111) type, perpendicular to the body diagonals [111] of the cube, and their signs alternate on going from one plane to the neighboring one. From the point of view of the Landau theory (see, e.g., [2]), structures of this type enter in a 12-dimensional representation of the group O_h^5, specified by four "vectors" $\mathbf{s}_1$, $\mathbf{s}_2$, $\mathbf{s}_3$, and $\mathbf{s}_4$. Under symmetry transformations from the O_h^5 group, including translations, the "vectors" $\mathbf{s}_i$ transform like[1)]

$$\begin{aligned} s_1 &\sim s_0 \cos\pi(x+y+z), & s_2 &\sim s_0 \cos\pi(-x+y+z), \\ s_3 &\sim s_0 \cos\pi(x-y+z), & s_4 &\sim s_0 \cos\pi(x+y-z). \end{aligned} \tag{1}$$

The two-sublattice structure in MnO, FeO, NiO, and CoO appears when only one of the "vectors" $\mathbf{s}_i$ differs from zero. In principle, however, more complicated structures are also possible, when all four "vectors" differ from zero.

The representation (1) is reducible. What are irreducible are the four- and six-dimensional representations. The former contain the projections s_{11}, s_{22}, s_{33}, and s_{44} of the vectors $\mathbf{s}_i$ on the corresponding diagonals of the cube ([111], [$\bar{1}$11], etc.), while the six-dimensional representation contains the remaining projections. The answer to the question whether the transition is determined by the reducible 12-dimensional representation (1) or by one of the irreducible ones depends on the relation between the exchange forces and the magnetic-anisotropy forces. At very weak anisotropy, only the exchange forces are significant, and the transition is determined by the entire representation (1), which is "irreducible" with respect to rotations of all spins through an arbitrary angle in the immobile lattice. At relatively large anisotropy, the transition is already determined by one of the irreducible representations. We consider here the simplest mathematical case, when the transition is described by a four-dimensional representation.

In our case, the most general symmetry-admitted expression for the energy in the Landau theory[2] is[2)] ($\eta_i \equiv s_{ii}$)

$$\Phi = -\frac{1}{2} r (\eta_1^2 + \eta_2^2 + \eta_3^2 + \eta_4^2) + \frac{1}{24} \gamma_1 (\eta_1^4 + \eta_2^4 + \eta_3^4 + \eta_4^4) + \frac{1}{4} \gamma_2 (\eta_1^2\eta_2^2 + \eta_1^2\eta_3^2 + \eta_1^2\eta_4^2 + \eta_2^2\eta_3^2 + \eta_2^2\eta_4^2 + \eta_3^2\eta_4^2) + \gamma_3 \eta_1\eta_2\eta_3\eta_4. \quad (2)$$

The fluctuations make expression (2) unsuitable near the immediate vicinity of the transition; it is valid only for the so-called region of the molecular field if the constants γ are small enough. Near the transition, the situation is described by a renormalization group (scaling). The structure of the renormalization group (RG) is very complicated and its connection with (2) can in fact not be established. The connection of the RG with the Landau energy becomes simple and explicit only in the so-called ϵ expansion of Wilson,[4] when we operate in fictitious space of dimensionality $4-\epsilon$ with $\epsilon \to 0$ and extrapolate the results to $\epsilon = 1$. In this case the RG equations are transformed into the equations of Gell-Mann and Low[5] of ordinary field theory. Moreover, in this case it is possible to calculate explicitly also the equation of state (i.e., Φ as a function of the order parameters η).[6,7]

In the linear approximation in ϵ, expression (2) remains in force for the energy, except that the charges γ_i in (2) begin themselves to depend on τ and η_i and are replaced by the invariant charges $\gamma_i(\xi)$, where

$$\xi \sim \frac{1}{\epsilon} \left[\left(\frac{\Lambda}{\max\{r, \eta^2\}} \right)^{\epsilon} - 1 \right], \quad (3)$$

where Λ is a cutoff parameter. With sufficient accuracy we can put $\epsilon = 0$ in (3), and we then have

$$\xi \sim \ln \frac{\Lambda}{\max(r, \eta^2)} \quad (3')$$

and formula (2) generalizes the result of Larkin and Khmel'nitskiĭ,[8] obtained for the simple case[3)] $\gamma_1 = 3\gamma_2$, $\gamma_3 = 0$.

The invariant charges $\gamma_i(\xi)$ satisfy the RG equations, which in our case take the form (cf.[8]):

$$-\frac{d\gamma_1}{d\xi} = 3\gamma_1^2 + 9\gamma_2^2, \quad -\frac{d\gamma_3}{d\xi} = 12\gamma_2\gamma_3, \quad -\frac{d\gamma_2}{d\xi} = 12\gamma_1\gamma_2 + 6\gamma_2^2 + 4\gamma_3^2. \quad (4)$$

Second-order transitions correspond to stationary points of the RG equations, near which $\gamma_i \sim 1/\xi$. At the transition point, ξ becomes infinite ($\tau \to 0$), and far from the transition region we have $\xi \to 0$ and we arrive at the "bare" charges $\gamma_i(0)$ in (2).

Wilson and Fisher,[9] however, considering a simple case of two fields ($\eta_3 = \eta_4 \equiv 0$ in (2)), have shown that at a definite ratio of the bare charges $\gamma_1(0)$ and $\gamma_2(0)$ the solution does not enter either of the two stationary points that are possible in this case as $\xi \to \infty$, and to the contrary, at the values of $\gamma_1(\xi_0)$ and $\gamma_2(\xi_0)$ reached for finite $\xi = \xi_0$ the fourth-order terms are no longer positive definite. It is clear that in this case there will occur a first-order transition (with logarithmic accuracy) at the point $\tau_0 \sim \eta_0^2$, determined by formulas (3) with $\xi = \xi_0$. The properties of the first-order phase transition in the case of two fields were recently calculated by Lyuksyutov and Pokrovskiĭ.[10]

The system (4) has four stationary points:

$$O: \gamma_1 = 1/3\xi, \quad \gamma_2 = \gamma_3 = 0,$$
$$A: \gamma_1 = 1/4\xi, \quad \gamma_2 = 1/12\xi, \quad \gamma_3 = 0,$$
$$B_\pm: \gamma_1 = \gamma_2 = \pm\gamma_3 = 1/12\xi.$$

The solid lines in the figure show the integral curves of the system in the variables $u = \gamma_2/\gamma_1$ and $v = \gamma_3/\gamma_1$. The coordinates of the cooresponding singular points are $O(0,0)$, $A(1/3,0)$, and $B_\pm(1, \pm 1)$.

A characteristic feature of the RG equations (4) is

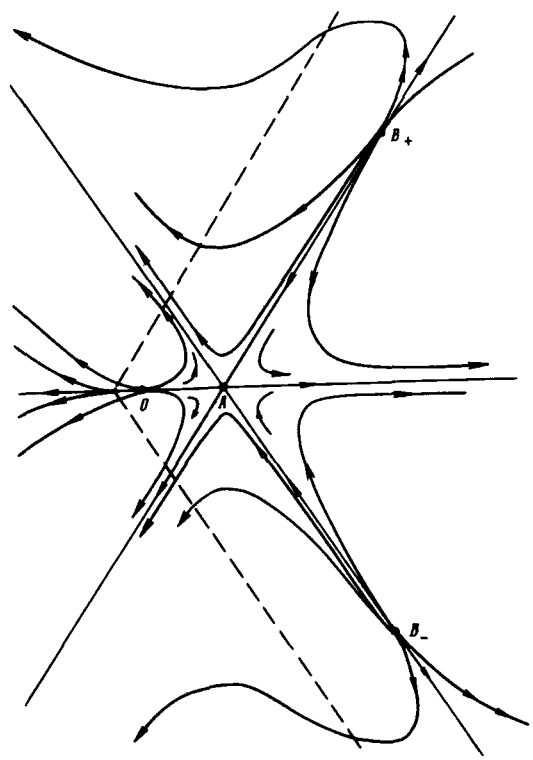

FIG. 1.

that the charge γ_1 can only decrease with increasing ξ. It is clear, on the other hand, that at $\gamma_1 < 0$ the fourth-order terms lose their positive-definite property, and therefore it is meaningful to consider only the positive bare charge $\gamma_1(0)$ and remain in the region $0 < \gamma_1(\xi) < \gamma_1(0)$. The direction of motion along the trajectories with growth is shown by the arrows. We see that a second-order transition is never possible, since the point A is generally unstable, and the trajectories from the stable points O and $B_\pm$ are always outgoing.

It remains to describe the region where the fourth-order terms in (2) are positive definite. It is located to the right of the angle made up by the intersection of the dashed lines (their equations are $1 + 9u - 6|v| = 0$). The first-order transition occurs either at the points of intersection of the trajectory with the dashed line, or else as a result of the departure of the trajectories to the right to infinity (this corresponds to vanishing of γ_1). Recognizing further that the dashed lines are parallel to the separatrices $AB_\pm$ (their equations are $1 + 3u \pm 2v = 0$), we can draw the following final conclusions:

1) From the region lying to the right inside the angle B_+AB_- made up by the separatrices there proceeds a first-order transition when the invariant charge $\gamma_1(\xi)$ vanishes at a certain point ξ_0. The state produced at the transition point is one in which only one of the four parameters η_i differs from zero, i.e., precisely the state observed in the experiment.

2) From the region lying in the chevron made up by the dashed lines and the separatrices B_+AB_-, i.e., from the region of the bare constants, there proceeds a first order transition when, at finite $\xi = \xi_0$ the combination of the invariant charges $\gamma_1(\xi) + 9\gamma_2(\xi) - 6|\gamma_3(\xi)|$ vanishes. At the transition point there is formed a complicated magnetic structure in which all four parameters η_i are equal in absolute magnitude. This structure, it appears, has not yet been observed.

The transition temperature τ_0 and the order parameter η_0 are determined with logarithmic accuracy by formula (3), i.e., $\eta_0^2 \sim \tau_0 \sim \Lambda \exp(-\xi_0)$. To determine ξ_0 it is necessary to integrate numerically the system (4). This will be described elsewhere.

In the case of small anisotropy, when only exchange forces are significant and all 12 components of the "vectors" enter in the problem, the expression for the energy and the RG equations are much more complicated. This situation will be described in another place. We note here that only first-order transitions are possible there, too, since the trajectories, as in the case considered here, are outgoing from all the stable stationary points of the RG with increasing ξ.

[1)] Formulas (1) must be understood (cf.[2]) to mean that the arguments of the cosines are transformed in accordance with the transformations of the coordinates (the edge of the cube is equal to unity), and S_0 (which realizes the so-called "small" transformation) is transformed only in rotation like an axial vector.

[2)] An energy in this form was considered by Lifshitz[3] in his work on transition in ordered alloys, and therefore our results are suitable also for that problem.

[3)] The quantity τ [in (2)] is also replaced by $\tau\mathcal{T}(\xi)$, where the function $\mathcal{T}$ itself is determined from the invariant charges $\gamma(\xi)$ (cf.[8]), but to determine the phase-transition line with logarithmic accuracy this substitution is inessential.

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