First-order phase transitions in systems with cubic anisotropy

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It is shown that the change of the symmetry in a system with strong cubic anisotropy occurs via a first-order transition. A phase diagram with three critical points is constructed.

The classical theoretical example of a first-order phase transition is the change of the crystal modification. Real transitions between crystal modifications are accompanied by jumps of the thermodynamic quantities, although these jumps are sometimes very small. One of the possible causes of the instability of the crystal and the appearance of a first-order phase transition, namely the interaction between optical and acoustic lattice vibrations, was investigated by Larkin and Pikin.[1]

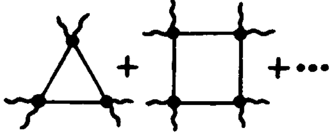

FIG. 1. Examples of ring diagrams.

It is shown in this paper that another cause of jumps in transitions from the tetragonal or hexagonal symmetry to the rhombic or monoclinic symmetry may be strong anisotropy.

Assume for the sake of argument that the initial symmetry was tetragonal. We consider a transition in which one of the cell atoms goes over into the asymmetrical position. By virtue of the initial symmetry, there exists four equivalent positions that are obtained from one another by rotation about the C_4 axis. We introduce the parameters ϕ_1 and ϕ_2, which characterize the long-range order in the arrangment of the asymmetrical atoms. Thus, for example, $\phi_1=1$ and $\phi_2=0$ corresponds to identical disposition of the asymmetrical atoms in all the cell, $\phi_1=-1$ and $\phi_2=0$ differs from the preceding disposition by rotation through π, and $\phi_1=0$ and $\phi_2=1$ differs by rotation through $\pi/2$ about the C_4 axis. According to Landau, [2] the system in question is described by the thermodynamic potential

$$\Phi = \int d^d X \{ (\nabla\phi_1)^2 + (\nabla\phi_2)^2 + r(\phi_1^2+\phi_2^2) + \lambda_1(\phi_1^4+\phi_2^4) + \lambda_2\phi_1^2\phi_2^2 \}. \quad (1)$$

The stability region of the system described by the potential (1) is determined by the inequality $\lambda_1 > 0$, $-2 \leq y_0 < \infty$, where $y_0=\lambda_2/\lambda_1$. The potential Φ is invariant with respect to the transformation

$$\phi_{1,2} \to \frac{\phi_1 \pm \phi_2}{\sqrt{2}}, \qquad y_0 \to \frac{6-y_0}{1+y_0/2} \quad (2)$$

which transforms the regions $-2<y_0<2$ and $2<y_0<\infty$ into each other. In the self-consistent-field approximation, a second-order phase transition occurs at $-2<y_0<2$ on the line $\tau=0$ between the symmetrical phase $\phi_1=\phi_2=0$ (phase I) and the asymmetrical phase $\phi_1=\pm\phi_2\neq 0$ (phase II). In the region $y_0>2$ we have in the asymmetrical phase $\phi_1\neq 0$ and $\phi_2=0$ or vice versa (phase III). Consequently there should exist a first-order phase-transition line between phases II and III. By virtue of the symmetry of (2), this is the line $y_0=2$. It turns out that there are two other first-order phase transitions on the phase diagram of the system described by the potential (1) in the (y_0, τ) plane.

A system of two coupled scalar fields with potential (1) was investigated by Wilson and Fisher[3] by a recurrence-relation system for a space with dimensionality $d=4-\epsilon$. It turned out that the solution of the recurrence equations (immobile point) exists only in the region $0\leq y_0\leq 6$. In this region, the renormalized interaction constants Λ_1 and Λ_2 tend to fixed values with increasing scale, so that the ratio $y=\Lambda_2/\Lambda_1$ is equal to 2 in the limit. The potential (1) becomes isotropic with respect to rotation in the (ϕ_1,ϕ_2) plane. We consider the regions $-2<y_0<0$ and $y_0>6$. The transformation (2) transforms them into each other, so that it suffices to consider the region $-2<y_0<0$.

In the case of four-dimensional space, the renormalized vertices Λ_1 and Λ_2 are determined by the equations of the renormalization group, [4] which are of the following form in first-order approximation:

$$\frac{d\Lambda_1}{d\xi} = -36\Lambda_1^2 - \Lambda_2^2 \qquad \Lambda_1\Big|_{\xi=0} = \lambda_1$$
$$\frac{d\Lambda_2}{d\xi} = -24\Lambda_1\Lambda_2 - 8\Lambda_2^2 \qquad \Lambda_2\Big|_{\xi=0} = \lambda_2 . \quad (3)$$

Here $\xi=\min\{\ln(1/p), \ln(1/\sqrt{\tau})\}$, and p is the momentum. The explicit solution of (3) is too complicated to write out here. It is important that at $y_0<0$ the function $y(\xi)$ decreases monotonically and becomes equal to $-\infty$ at a certain finite ξ_0. This means that y reaches the limit of the stability region $y=-2$ at another value ξ_1 that depends on y_0. In the case of weak coupling, the stability limit $\xi_1(y_0)$ differs little from the phase-equilibrium curve. The Hamiltonian (1) is then unstable, and it is necessary to take into account anharmonicities of higher order than fourth. Analysis shows that the main contribution is made by ring diagrams[1)] (Fig. 1). At $y_0<0$, symmetrical phase I and phase II can be in equilibrium. Knowing this, we can easily sum the ring diagrams. Replacing λ_1 and λ_2 by their renormalized values and discarding the gradient terms, we obtain the potential of the condensate:

$$\Phi = 2r\phi^2 + (2+y)\Lambda_1\phi^4 + 16\frac{\Lambda_1}{\pi^2}\phi^4 \ln\frac{16\Lambda_1\phi^2}{r} . \quad (4)$$

The equilibrium value of ϕ is obtained from the condition that Φ be a minimum. $\Phi=0$ on the equilibrium curve. The equations $\Phi=0$ and $\partial\Phi/\partial\phi=0$ determine the equilibrium value of y and the equilibrium curve in the (y_0, τ) plane.

At $y_0>6$ phase III appears, by virtue of the invariance with respect to transformation (2) in first-order phase transitions. It is interesting that the phase diagram has three tricritical points at $y_0=0$, 2, and 6 (Fig. 2).

The results can be easily continued also to a space with dimension $d=4-\epsilon$. For the condensate we obtain on the equilibrium curve

$$\phi = \text{const}\cdot r^{\frac{1}{2}+\frac{\epsilon}{4}} |y_0|^{-3-\frac{3}{4}\epsilon} \quad |y_0| << 1 .$$

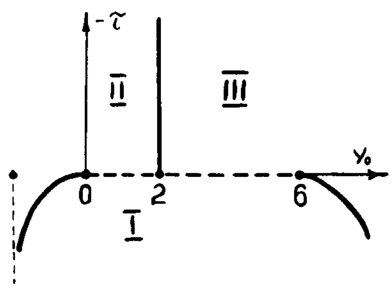

FIG. 2. Phase diagram of states.

The equation of the equilibrium curve near the tricritical point $\tau = y_0 = 0$ takes at $y_0 < 0$ the form

$$\tau = \left(1 + \text{const}\cdot\frac{\epsilon}{|y_0|^3}\right)^{-\frac{2}{\epsilon}} . \tag{5}$$

The formation of superstructures in alloys with initial T_d symmetry, forming a body-centered cubic lattice, is described by the same potential (1).[2] Our results apply therefore also to this case.

In real systems, the phase diagrams in a plane are topologically equivalent to the diagram of Fig. 2, if strong anisotropy can be obtained by varying the temperature and the pressure. The form of the equilibrium curve and the heat of transition, which is proportional to ϕ^2 on the transition curve, remain constant near the tricritical point (τ and y_0 are regular functions of P and T).

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[1)]For analogous summation in the case of scalar electrodynamics see[5].

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