Appearance of inhomogeneous states in systems with two order parameters

A. L. Korzhenevskiĭ

V. I. Ul'yanov (Lenin) Electrical Engineering Institute, Leningrad

(Submitted 16 February 1982)

Pis'ma Zh. Eksp. Teor. Fiz. **35**, No. 8, 315–318 (20 April 1982)

The possibility for the appearance of an inhomogeneous superstructure in a crystal due to the presence of anharmonic, linear with respect to gradients, interaction of two order parameters is investigated. It is shown that this interaction becomes effectively strong in a region with developed fluctuations and, in addition, a first-order phase transition into the inhomogeneous state will occur in the system.

PACS numbers: 61.50.Lt, 61.50.Em

It is customarily assumed that the appearance of an inhomogeneous phase (IP), within the scope of a phenomenological approach, is a result of the breakdown of Lifshitz's condition or is related to the presence of a frequency minimum of the soft mode $\omega(\mathbf{q})$ with a "random" value $\mathbf{q}=\mathbf{q}_0$.[1,2] The possibility of the appearance of IP due to non-Lifshitz gradient invariants (cubic with respect to the components of the order parameter) was pointed out in Ref. 3. The properties of phase transition in such IP were investigated in Refs. 4 and 5. In what follows, it will be shown that together with the cases listed above, IP can also appear in systems with two order parameters, whose interaction contains anharmonic terms that are linear with respect to the gradients.

As the simplest example of such a system, we shall examine a model of two coupled single-component fields $\phi(x)$ and $\psi(x)$, whose thermodynamic potential has the form

$$\Phi = \Phi_0 + \int dx \left[\frac{1}{2} r_1 \phi^2 + \frac{1}{2} r_2 \psi^2 + \frac{1}{2} g_1 (\nabla \phi)^2 + \frac{1}{2} g_2 (\nabla \psi)^2 + \frac{1}{4!} (u_0 \phi^4 + 2\lambda_0 \phi^2 \psi^2 + v_0 \psi^4) + \frac{1}{2} b_0 \phi^2 \frac{d\psi}{dz} \right]. \tag{1}$$

Here, r_1 and r_2 are smooth functions of the external parameters, which vanish on the phase transition lines with respect to the fields $\phi(x)$ and $\psi(x)$, respectively, and u_0, $v_0, \lambda_0 > 0, \lambda_0 < (u_0 v_0)^{1/2}$. The potential (1) describes, for example, the behavior of a crystal in which a structural phase transition occurs with a doubling of the spacing of the unit cell (in particular, antiferromagnetic) or a ferromagnetic phase transition, as well as a structural phase transition without a change in the unit cell volume.

It is already possible to verify within the scope of Landau's theory that near the point of intersection of phase transition lines $r_1 = r_2 \equiv r = 0$, formation of the IP becomes energetically favorable for sufficiently large values of the coefficient b_0. We shall use the variational principle, choosing the trial functions $\phi(x) = \rho \cos(qz)$, $\psi(x) = \rho \sin(2qz)$. Minimizing the potential (1) with these functions, we shall calculate the values of the variable parameters $\tilde{\rho}, \tilde{q}$

$$\tilde{q}^2 = \frac{-r}{(g_1 + 4g_2)(x-1)}, \quad \tilde{\rho} = \frac{-(g_1 + 4g_2)}{b_0} \tilde{q}, \tag{2}$$

where the dimensionless parameter $x = (g_1 + 4g_2)(u_0 + v_0 - \frac{4}{3}\lambda_0)/4 b_0^2$ and we shall obtain an expression for the potential of the inhomogeneous phase $\Phi_{IP}(\tilde{\rho}, \tilde{q})$

$$\Phi_{IP} - \Phi_0 = -\frac{(g_1 + 4g_2) r^2}{(x-1) b_0^2}. \tag{3}$$

Equating (3) to the potential of the homogeneous phase Φ_{HP}

$$\Phi_{HP} - \Phi_0 = -\frac{3(u_0 + v_0 - 2\lambda_0) r^2}{2(u_0 v_0 - \lambda_0^2)}, \tag{4}$$

we find that for $x = 1 + \delta^2, \delta^2 \ll 1$ a second-order phase transition to the IP occurs at the point of intersection of the lines $r = 0$. If the value of the parameter $x < 1$, then a first-order phase transition to the IP will occur for $r > 0$. The line of these phase transitions can be found by including in (1) terms of sixth order.[1)]

Let us examine the effect of critical fluctuations on the appearance of the IP. Let the system be near the line $r_1 = 0$, where the field $\varphi(x)$ fluctuates strongly, while $\psi(x)$ is noncritical. We shall show that the gradient coupling between $\phi(x)$ and $\psi(x)$ can lead to instabilities relative to the formation of IP. As a guide, we note that the first fluctuation correction to the coefficient g_2 is negative and depends on r_1 in a singular manner: $\Delta g_2 \sim -b_0^2/\sqrt{r_i}$. In the region of strong fluctuations of the field $\phi(x)$, we cannot draw any conclusions as to the nature of the phase transition according to the form of one such correction, but it is necessary to take into account the contributions of other singular graphs for $r_1 \to 0$ as well. This can be done if we assume that the period of the IP that arises $L \gg r_c$, where r_c is the correlation length of $\phi(x)$. From this assumption, whose validity is demonstrated in what follows, it follows that the presence of the gradient coupling in (1) for $r_1 \to 0$ reduces to the substitution $r_1 \to \tilde{r}_1 = (r_1 + b_0\, d\psi/dz)$ and the singular part of the thermodynamic potential Φ_s can be represented as a homogeneous function of $\tilde{r}_1$[2),6]:

$$\Phi_s = -\frac{3}{2u_0^{1-2a}} |\widetilde{r}_1|^{2-a}. \tag{5}$$

The potential of the weakly fluctuating field ψ (x) assumes the form

$$\Phi = \Phi_0 + \int dx \left\{ -\frac{3}{2u_0^{1-2a}} \left| r_1 + b_0 \frac{d\psi}{dz} \right|^{2-a} + \frac{1}{2} r_2 \psi^2 + \frac{1}{4!} v_0 \psi^4 + \frac{1}{2} g_2 \left(\frac{d\psi}{dz} \right)^2 \right\}. \tag{6}$$

The equilibrium configuration of ψ (x), for which the functional (6) has a minimum value, can be found from Euler's equation:

$$\left(g_2 - \epsilon \left| r_1 + b_0 \frac{d\psi}{dz} \right|^{-a} \right) \frac{d^2\psi}{dz^2} - \left(r_2 + \frac{v_0}{6} \psi^2 \right) \psi = 0, \tag{7}$$

where $\epsilon = 3b_0^2(2-a)(1-a)/2u_0^{1-2a}$. In order to clarify the qualitative nature of its solutions, we shall introduce the variables $\psi(x) = x$ and $d\psi/dz = y$ and we shall write down the equation of the isocline:

$$\frac{dx}{dy} = \frac{y(g_2 - \epsilon |r_1 + b_0 y|^{-a})}{x\left(r_2 + \frac{v_0}{6} x^2 \right)}. \tag{8}$$

The variables in this equation separate and the general integral has the form

$$\left(r_2 + \frac{v_0}{12} x^2 \right) x^2 = g_2 y^2 - \frac{2\epsilon}{b_0^2} \left[\frac{|r_1 + b_0 y|^{2-a}}{(2-a)} \mp \frac{r_1 |r_1 + b_0 y|^{1-a}}{(1-a)} \right] + \frac{3r_1^{2-a}}{u_0^{1-2a}} + C \equiv \Theta(r_1, y, C), \tag{9}$$

where the $(\mp)$ signs correspond to the conditions $y \lessgtr -r_1/b_0$ and C is an integration constant. The graph of the function $\Theta(y)$ for $r_1 < (1-a)(\epsilon/g_2)^{1/a}/2(2-a)$ is presented in Fig. 1. The numbers 1, 2, and 3 correspond to the values $C_1 = 0, 0 < C_2 < C_3, \Theta(b_0 y = -r_1 + (\epsilon/g_2)^{1/a}, C_3) = 0$. It is evident from the figure that for $0 < C < C_3$ the trajectories in the (x,y) plane are closed and, therefore, Eq. (7) has periodic solutions. Numerical calculations show that as r_1 decreases the periods of these solutions increase and there exists a region of values of r_1 in which $L \gg r_c$. At the same time, the value of the potential (6) turns out to be less for them than for the solution describing the phase transition to the homogeneous phase. It follows from here that for some $r_1^* > 0$ a first-order phase transition to the IP will occur in the system. This conclusion is closely related to the divergence of the heat capacity ($a > 0$) for an effectively single-component fluctuation field, for example, a phase transition in a cubic crystal, compressed (stretched) along a single axis. At the same time, since the IP arises for finite $r_1 = r_1^*$, the divergence of the heat capacity is not a necessary condition and a sharp increase in the heat capacity of the system in the region $r_1 \gtrsim r_1^*$ is sufficient for the appearance of an IP.

In order to analyze the critical behavior near the point of intersection of the lines $r_1 = r_2 = 0$, we shall use the renormalization group method. The system of the Gell-Mann-Low equations for the renormalized dimensionless charges b^2, u, v, λ has the form[3)]

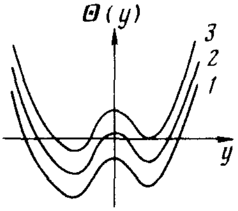

FIG. 1. Graph of the function $\Theta(y)$ for three different values of the integration constant.

$$\frac{db^2}{dt} = - b^2 + 3ub^2 - \frac{3}{2}b^4, \qquad \frac{d\lambda}{dt} = - \lambda + \frac{9}{2}\lambda^2 + \frac{1}{2}v^2,$$

$$\frac{du}{dt} = - u + \frac{9}{2}u^2 + \frac{1}{2}v^2 - \frac{3}{2}(3u + v)b^2 + \frac{9}{4}b^4, \tag{10}$$

$$\frac{dv}{dt} = - v + \frac{3}{2}(u + \lambda)v + 2v^2 - \frac{9}{4}\left(\lambda + \frac{v}{3}\right)b^2, \qquad t = - \frac{1}{2}\ln r_c .$$

For $b = 0$, these equations have a stable fixed point (FP) $u^* = v^* = \lambda^* = \frac{1}{5}$,[6,7] corresponding to an asymptotic increase in symmetry up to $O(2)$. When gradient coupling is included, the system (10) loses the stable FP. Numerical integration shows that the space of renormalized charges b, u, v, λ contains a region corresponding to generating values of the parameter $x \gg 1$, for which fluctuations increase the gradient coupling and cause the first-order phase transition to the IP. The existence of such a region can be discovered analytically by noting that near an Ising FP ($u = 2/9, \lambda = 0, v_{1,2} = 2/9, 0$) and $O(2)$ the ratio b^2/u increases for $r_c \to \infty$ as $r_c^{1/3}$ and $r_c^{2/5}$, respectively.

The results obtained above show that in solving the problem of the possibility of the appearance of an IP in crystals, which undergo several phase transitions, it is important to take into account gradient coupling of order parameters corresponding to different irreducible representations of the high-symmetry phase.

I thank S. A. Brazovskiĭ, S. L. Ginzburg, A. I. Sokolov, D. E. Khmel'nitskiĭ, and B. N. Shalaev for useful discussions of the problems examined in this paper.

[1)]The corresponding equations are completely analogous to those obtained in Ref. 5 describing a phase transition to IP in cubic ferroelectrics.
[2)]For simplicity, the term $\lambda_0 \phi^2 \psi^2$ was omitted in expressions (5) and (6), since a fluctuation phase transition to a non-Landau homogeneous phase is impossible ($\lambda_0 < (u_0 v_0)^{1/2}$)[6] and taking this term into account does not qualitatively affect the structure of the state diagram.
[3)]The normalization factor is equal to $(24\pi)^{-1}$, for example, $u = (24\pi)^{-1} r_c^{1/2} u(q_i = 0, r_c)$.

1. I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. **46**, 1420 (1964); **47**, 992 (1964) [Sov. Phys. JETP **19**, 960 (1964); **20**, 665 (1965)].
2. R. A. Cowley and A. D. Bruce, J. Phys. C **11**, 3577 (1978).
3. T. A. Aslanyan and A. P. Levanyuk, Fiz. Tverd. Tela **20**, 804 (1978) [Sov. Phys. Solid State **20**, 466 (1978)].
4. E. B. Loginov, Kristallografiya **24**, 1109 (1979) [**24**, 637 (1979)].

5. A. L. Korzhenevskiĭ, Zh. Eksp. Teor. Fiz. **81**, 1071 (1981) [Sov. Phys. JETP **54**, 568 (1981)].
6. I. F. Lyuksyutov, V. L. Pokrovskiĭ, and D. E. Khmel'nitskiĭ, Zh. Eksp. Teor. Fiz. **69**, 1817 (1975) [Sov. Phys. JETP **42**, 923 (1975)].
7. D. R. Nelson, J. M. Kosterlitz, and M. E. Fisher, Phys. Rev. Lett. **33**, 813 (1974).

Translated by M. E. Alferieff
Edited by S. J. Amoretty