On the theory of phase transitions into inhomogeneous states

A. L. Korzhenevskiĭ

Leningrad Institute of Electrical Engineerng
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The possibility of the appearance of incommensurable superstructures as a result of the presence of non-Lifshitz-type gauge invariants in the crystal-free-energy expansion is investigated. Conditions for the occurrence of first- and second-order phase transitions into the inhomogeneous state are derived in terms of the values of the parameters of the thermodynamic potential. The shape of the phase diagram is established. The characteristics of the appearance of incommensurable phases in ferroelectric crystals are analyzed, and the existence domain and the structure of such phases in the ferroelectric perovskites are estimated with the aid of the available experimental data. The critical behavior in those cases in which the phase transitions into the homogeneous and inhomogeneous states are second-order transitions is studied with the aid of the renormalization-group technique, and it is shown that allowance for the fluctuations transforms these phase transitions into first-order transitions.

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INTRODUCTION

Much attention has recently been attracted by phase transitions into spatially modulated structures whose period varies with varying external conditions, and is not directly related to the crystal lattice constant. Such helical superstructures were first observed experimentally in magnetic substances.[1] Within the framework of the Landau theory, their appearance is a consequence of the presence in the free-energy expansion of invariants that are linear in the derivatives of the order-parameter components φ_1, i.e., invariants of the type

$$\sigma\left(\varphi_i\frac{\partial\varphi_j}{\partial x_k}-\varphi_j\frac{\partial\varphi_i}{\partial x_k}\right) \tag{1}$$

(Lifshitz invariants).[2] Let us note that an incommensurable structure (IS) arises in this case at any value of the coefficient σ attached to the invariant (1) (the value of which determines the magnitude of the IS period), i.e., the origin of the IS has a purely symmetry-related character. The characteristics of the phase transition for magnetic IS were first studied by Dzyaloshinskiĭ,[3] and, as applied to ferroelectrics (FE), by Levanyuk and Sannikov.[4]

At the same time the appearance of an IS is not necessarily connected with symmetry-related causes, and can arise at certain values of the parameters of the thermodynamic potential of the system. In this case there appears on the phase diagram a multicritical point separating the lines of phase transitions into the IS and the commensurable phase. The simplest example is the model proposed by Hornreich, Luban, and Strikman,[5] which can be described by a thermodynamic potential of the form

$$\Phi(\varphi)=a_2\varphi^2+a_4\varphi^4+\ldots+c_1(\nabla\varphi)^2+c_2(\nabla^2\varphi)^2+\ldots, \tag{2}$$

where the coefficient c_1 as a function of the external parameters (the pressure, concentration, etc.) can change its sign. The point on the phase diagram at which c_1 vanishes was named[5] the Lifshitz point (LP). Such multicritical LP can occur in the rare-earth alloys, e.g., in Gd_xY_{1-x}, Gd_xSc_{1-x}, liquid crystals (the point of intersection of the nematic–smectic-A–smectic-C phase transition lines), as well as in crystals that undergo structural transitions (see Ref. 6 for a review). A LP was quite recently detected experimentally in UAs.[7]

The LP, defined as points separating lines of phase transitions into different commensurable and incommensurable phases, have been classified by Aslanyan and Levanyuk.[8] They, in particular, demonstrate in their paper[8] the possibility of the existence of another type of LP as a result of the presence in the thermodynamic-potential expansion of third-order—in the order-parameter components—derivative invariants of the type

$$\varphi_i\varphi_j\frac{\partial\varphi_k}{\partial x_l}. \tag{3}$$

Such invariants occur in the expression for the free energy in those cases in which the nonsymmetric part of the cube of the order-parameter representation contains a vector representation. The purpose of the present paper is to investigate the nature of the phase transitions in systems whose symmetries admit of the existence of invariants of the type (3). To begin with, we shall consider within the framework of the Landau theory the properties of the phase transitions in crystals in which there are no dipole forces. We shall, as a result, construct a qualitative phase diagram. Then we shall analyze the characteristics of the phase transition in ferroelectric crystals, and estimate the temperature range in which the inhomogeneous phase exists in these crystals and the characteristic scale of the periodic structure of the phase. After this, we shall investigate the effect of the fluctuations on the properties of the phase transition with the aid of the renormalization-group (RG) technique.

DESCRIPTION WITHIN THE FRAMEWORK OF THE LANDAU THEORY

We begin the study of the properties of the phase transitions in systems that admit of the existence of invari-

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ants of the type (3) with the analysis of the simplest model describing the phase transition occurring in an "easy-plane" type of crystal, and characterized by a two-component vector order parameter $\varphi_x(\mathbf{r})$, $\varphi_y(\mathbf{r})$. Let us write the thermodynamic-potential density of this model in the form

$$\Phi=\Phi_0+{}^1/_2A(\varphi_x^2+\varphi_y^2)+{}^1/_2g[(\nabla\varphi_x)^2+(\nabla\varphi_y)^2]$$
$$+b(\varphi_x^3+\varphi_y^3)(\partial\varphi_x/\partial x+\partial\varphi_y/\partial y)+{}^1/_4u(\varphi_x^2+\varphi_y^2)^2+{}^1/_6d(\varphi_x^2+\varphi_y^2)^3. \quad (4)$$

We assume in the expression (4) that $A=\alpha(T-T_0)$, $g>0$, and $d>0$.

Let us show that at certain values of the coefficients in (4) the system will undergo a phase transition into an inhomogeneous state. For this purpose, we use, following Aslanyan and Levanyuk's suggestion,[8] the variational principle. Let us choose the trial functions for $\varphi_x(\mathbf{r})$ and $\varphi_y(\mathbf{r})$ in the form

$$\varphi_x=\rho\cos qx, \quad \varphi_y=\rho\sin tqx \quad (5)$$

and compute with them the value of Φ as a function of the parameters ρ, q, and t: $\Phi=\Phi_0+\frac{1}{2}A\rho^2+\frac{1}{4}(t^2+1)g\rho^2q^2+bq\rho^3\psi(t)+\frac{1}{4}u\rho^4\varphi(t)+\frac{1}{6}d\rho^6\gamma(t)$,

$$\varphi(t)=\frac{1}{4\pi}\left\{5\pi+\left[-\frac{1}{t}+\frac{1}{8t}\cos 4\pi t+\frac{t}{2(1-t^2)}\right]\sin 4\pi t\right\},$$
$$\psi(t)=\frac{\sin 2\pi t}{2\pi}\left[\frac{t^2-2}{t^2-4}+\frac{\sin 2\pi t}{1-4t^2}\right], \quad (6)$$
$$\gamma(t)=\frac{7}{4}-\frac{9\sin 2\pi t}{8\pi t}+\frac{\sin 4\pi t}{64\pi t}\left\{\frac{2\cos^2 4\pi t+31}{3}\right.$$
$$\left.+3\left[\frac{t^3+4t^2-t-16}{(1-t^2)(t^2-4)}+\frac{1-4t-4t^2}{1-4t^2}\cos 4\pi t\right]\right\}.$$

Differentiating then the expression for Φ with respect to ρ, q, and t, we obtain the following system of equations determining the minimum of Φ:

$$\frac{\partial\Phi}{\partial\rho}=\rho\left[A+\frac{1}{2}g(t^2+1)q^2+3b\psi(t)\rho q+u\varphi(t)\rho^2+d\gamma(t)\rho^4\right]=0,$$
$$\frac{\partial\Phi}{\partial q}=\rho^2\left[\frac{1}{2}g(t^2+1)q+b\psi(t)\rho\right]=0, \quad \frac{\partial\Phi}{\partial t}=0. \quad (7)$$

Assuming that $\rho_0\neq 0$, we find from the second equation of the system (7) that

$$\rho_0=\frac{-g(t^2+1)}{2b\psi(t)}q_0. \quad (8)$$

We can verify that the value t_0 corresponding to the minimum of Φ for the functions (5) is quite close to two ($t_0\approx 1.87$). In order to avoid unwieldy formulas, we shall hereafter set $t_0=2$, since this will be sufficient for our purpose [which is to show that the minimum of Φ, (4), is realized in an inhomogeneous state]. Substituting (8) into the first of the equations (7), we obtain for q_0^2 the following expression:

$$q_0^2=b^4(1-x)\left\{1-\left[1-\frac{100A\tilde{d}}{b^4(1-x)^2}\right]^{1/2}\right\}\Big/250\tilde{d}g^3, \quad \tilde{d}=\frac{53}{32}d, \quad (9)$$

where the dimensionless parameter

$$x=25ug/4b^2. \quad (10)$$

It is convenient to consider the $x>1$ case first. Then the expression (9) for $A\to 0$ ($T\to T_0$) assumes the form

$$q_0^2=A/5g(1-x). \quad (11)$$

It can be seen from (11) that, for $x>1$, an IS can arise only when $A\leq 0$. Substituting (8) and (11) into (6) (with $t_0=2$), we obtain the thermodynamic-potential value $\Phi_{IS}(\rho_0, q_0, t_0)$ for the inhomogeneous phase at $A\to 0$:

$$\Phi_{IS}(\rho_0, q_0, t_0)-\Phi_0=\frac{1}{4}\rho_0^2A=\frac{x}{5(1-x)}\frac{A^2}{u}. \quad (12)$$

Comparing this value of Φ_{IS} with the potential,

$$\Phi_c(q_0=0)-\Phi_0=-A^2/4u, \quad (13)$$

of the homogeneous phase, we find that, for $x<5$, $|\Phi_c(q_0=0)|<|\Phi_{IS}|$, and, consequently, the appearance of an IS at $A\leq 0$ is advantageous. Since on the segment $A=0$, $1<x<5$, as can be seen from (8) and (11), the IS appears continuously (without the order parameter's undergoing a jump), the phase transition into the IS is a second-order transition.

The point with the coordiantes $A=0$, $x=5$ turns out to be a LP at which two second-order phase transition lines separating the high-symmetry homogeneous phase from the homogeneous low-symmetry and inhomogeneous phases and another phase transition line lying between them converge (touch). The last line will most likely be a first-order phase transition line on which ρ_0, $q_0\neq 0$ (as in the case of a phase diagram having a LP of the type considered in Ref. 5), although we cannot prove this, since the expressions given in Ref. 5 for $\varphi_x(\mathbf{r})$ and $\varphi_y(\mathbf{r})$ are only trial functions and not at all exact values of the order-parameter components in the inhomogeneous phase.

For $x<1$ the phase transition line between the homogeneous high-symmetry and inhomogeneous phases is determined from the condition that their thermodynamic potentials be equal:

$$\Phi_{IS}(\rho_0, q_0, t_0)=\Phi_0, \quad (14)$$

from which we obtain an expression for the transition temperature:

$$T_c(x)=T_0+\alpha^{-1}A^*(x), \quad A^*(x)=3(1-x)b^4/400\tilde{d}g^3. \quad (15)$$

Substituting this expression into (9), we find the corresponding value of the IS wave vector $q_0(x)$ at the transition point ($T=T_c$):

$$q_0^2(T=T_c)=(1-x)b^4/500\tilde{d}g^3. \quad (16)$$

It is clear from (15) that, for the values of $x<1$, the phase transition into the inhomogeneous state occurs at temperatures $T_c(x)>T_0$. In their turn, as can be seen from (8) and (16), the IS-order-parameter components $\varphi_x(\mathbf{r})$ and $\varphi_y(\mathbf{r})$ have finite values at the transition point, and, consequently, this phase transition is a first-order transition. The point with the coordinates $A=0$, $x=1$, which separates the lines of first- and second-order phase transitions into the IS, thus turns out to be a tricritical point with unique properties. In particular, the character of the temperature dependence of the wave vector q_0 changes in its vicinity: as $A\to 0$, $x\to 1^{(-)}$, q_0^2 varies in proportion to $(T-T_0)^{1/2}$ [see (9)], and not to $T-T_0$, as in the formula (11) for $5>x>1$.

For $x<0$, a first-order transition into a homogeneous state is possible in the system. The corresponding critical temperature T_1, expressed in terms of the

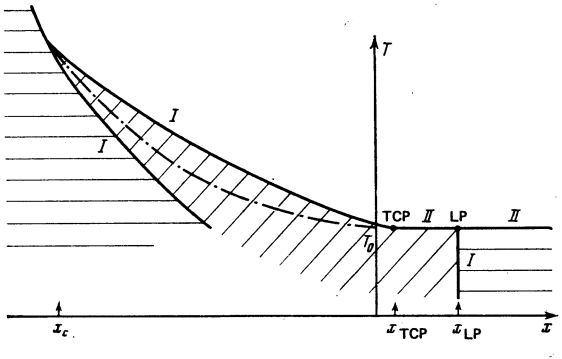

FIG. 1. Phase diagram for the model (4) in the temperature-dimensionless parameter x plane.

quantity A, is given by the well-known formula

$$A(T=T_1)=\frac{3}{16}\frac{u^2}{d}. \tag{17}$$

It can easily be verified, however, that a phase transition from the high-symmetry phase directly into a homogeneous low-symmetry phase is advantageous only at fairly large values of $|x|$; at low $|x|$ values the transition will, as before, be into the IS. It is easiest to determine the $|x_c|$ value at which the homogeneous phase begins to be energetically more advantageous than the inhomogeneous phase by equating the temperature values in (15) and (17). We then obtain $|x_c|\approx 33$. The boundary line between the homogeneous and inhomogeneous phase can be completely determined by equating the corresponding thermodynamic potentials.

Using all the above results, we arrive at the (T,x) phase diagram shown in Fig. 1. The letters TCP and LP in the figure indicate respectively a tricritical point and a bicritical LP, and x_{TCP} and x_{LP} are the values of the parameter x for these points. The Roman numbers I and II indicate the first- and second-order phase transition lines. The dot-dash parabola corresponds to the equation $\Phi_c=\Phi_0$ (for $x<0$), $x_c\approx -33$ is the value of x at which $T_c(x_c)=T_1$. The region hatched with thin horizontal lines is the existence domain of the homogeneous phase, while the obliquely hatched region represents the existence domain of the inhomogeneous phase.

As we have already noted above, the phase diagram in Fig. 1 was constructed on the basis of calculations in which essential use was made of the explicit form of the trial functions (5), which do not describe the true structure of the inhomogeneous state. Therefore, it is necessary to ascertain which of the results obtained remain valid when exact expressions for the order-parameter components, $\varphi_x(\mathbf{r})$ and $\varphi_y(\mathbf{r})$, in the inhomogeneous phase are used. Firstly, it is clear that the existence domain of the IS can then only expand, and, consequently, the phase transition into the inhomogeneous state will, as before, be possible. Secondly, the assertion that this phase transition may be of first or second order is also apparently valid. In the case of the second-order transition the wave vectors describing the IS should vanish at[1] $T=T_c$, and the phase diagram should contain characteristic LP and TCP. Thus, it may be thought that all the main qualitative features of the diagram in Fig. 1 survive in a more exact solution of the problem within the framework of the Landau theory. But the numerical characteristics, in particular, the positions of the TCP and LP, will undoubtedly change, since the true values of their coordinates, x_{TCP} and x_{LP}, are clearly greater than the values indicated in Fig. 1.

Let us now show that phase transformations similar to those occurring in the model (4) are characteristic of other systems, the expression for whose thermodynamic potential contains terms of the type (3). Let us investigate, for example, the nature of the phase transitions occurring in cubic crystals with the group O_h, and characterized by an order parameter that transforms according to the three-dimensional irreducible (nonvector) representation F_{2u}. Let us write the thermodynamic potential corresponding to this representation in the form

$$\Phi=\Phi_0+\tfrac{1}{2}A(\eta_1^2+\eta_2^2+\eta_3^2)+\tfrac{1}{4}u(\eta_1^2+\eta_2^2+\eta_3^2)^2+\tfrac{1}{2}v(\eta_1^2\eta_2^2+\eta_1^2\eta_3^2+\eta_2^2\eta_3^2)$$
$$+\tfrac{1}{2}g[(\nabla\eta_1)^2+(\nabla\eta_2)^2+(\nabla\eta_3)^2]+\tfrac{1}{6}d(\eta_1^2+\eta_2^2+\eta_3^2)^3$$
$$+b\left[\eta_1^2\left(\frac{\partial\eta_2}{\partial z}+\frac{\partial\eta_3}{\partial y}\right)+\eta_2^2\left(\frac{\partial\eta_1}{\partial z}+\frac{\partial\eta_3}{\partial x}\right)+\eta_3^2\left(\frac{\partial\eta_1}{\partial y}+\frac{\partial\eta_2}{\partial x}\right)\right]. \tag{18}$$

For definiteness, we shall assume that $v>0$ in (18), so that in the absence of the third-order invariant the system will undergo a transition into the homogeneous phase with $\eta_1=\eta_2=0$, $\eta_3\neq 0$.

The analysis of the properties of the phase transition in the model (18) will literally be a repetition of the above-performed investigation of the model (4) if we take the trial function $\eta_1=0$ and for the functions $\eta_2(\mathbf{r})$ and $\eta_3(\mathbf{r})$ we use the expressions (5). All the changes amount to the replacement of u in the numerator of the expression for the dimensionless parameter x by the linear combination $u+\frac{1}{5}v$:

$$x\to x'=\frac{25}{4}\frac{(u+\frac{1}{5}v)}{b^2}g. \tag{19}$$

The (T,x') phase diagram then remains the same as the diagram for the model (4) shown in Fig. 1.

It must be noted that the case in which the phase transition is described by the irreducible representation F_{2u} was recently considered by Aslanyan and Levanyuk.[8 2)] To elucidate the nature of the phase transitions, they decided to use the variational method, but the representation chosen by them for the trial functions, which was in the form of a five-parameter family, turned out to be so complex that it was impossible to carry out the computations to the end, i.e., find the adjustable-parameter values corresponding to the minimum of the potential (18). As a consequence, they were not able to compute the thermodynamic potential of the inhomogeneous state and compare its magnitude with the value of the potential of the homogeneous phase. Therefore, they could only limit themselves to postulating the occurrence of a phase transition into the IS state as the temperature is lowered in the region $A>0$, a transition which, in their opinion, will be of first order because of the presence in (18) of a term that is cubic in the order-parameter components. As a result, they assert in

their paper[8] that the line of transitions into the homogeneous phase goes over into a line of first-order phase transitions into the IS phase, i.e., that there should intersect at the LP (whose coordinates were not determined) two first-order and one second-order phase transition lines. In order for such a LP to arise in the system, it was considered necessary to take into account in the expansion (18) third-order invariants (in the order-parameter components and their derivatives) of the type

$$\eta_i^2 \frac{\partial^3 \eta_j}{\partial x_k^3}. \tag{20}$$

In fact, as has been shown above, the LP is the point of intersection of one line of first-order phase transitions (from the homogeneous phase into the IS) and two second-order transition lines (see Fig. 1). The period of the resulting superstructure then becomes infinite not only at this point, but also at every point on the segment of the line of phase transitions into the IS state from the LP to the TCP [see (11) and (16)].

Allowance for the invariant (20) is not by any means a necessary condition either for the existence of a LP for the system, or the occurrence of a phase transition into the IS state [as follows from (11), it can generally be neglected in the vicinity of the line of second-order phase transitions into the IS state]. Thus, we see that the computation of the thermodynamic potential of the IS with the use of trial functions of the form (5) that do not even correspond to its minimum allowed us nevertheless to verify the validity of Aslanyan and Levanyuk's conjectures,[8] and obtain new results concerning the properties of the phase transition into the IS state.

The case in which the order parameter of the cubic crystal transforms according to an irreducible vector representation [the invariant (3) then has the form $\mathbf{P}^2 \operatorname{div} \mathbf{P}$ (Ref. 9)] can similarly be investigated. Since for systems with short-range interaction potentials this case does not differ significantly from the situation with the nonvector representation F_{2u}, we shall consider in the following section the case of a vector representation for the phase transitions in cubic FE, which, because of the presence of dipole forces, have their own characteristics.

CONDITIONS FOR THE APPEARANCE OF IS IN FERROELECTRICS

It is convenient, in describing the phase transition in a system with the dipole interaction, to go over to the Fourier transform $\mathbf{P}(\mathbf{q})$ of the polarization field. Let us write the thermodynamic potential of a cubic FE in the form

$$\begin{aligned}\Phi=\Phi_0+\frac{1}{2}\mu\sum_{\substack{\mathbf{q}\\ \alpha,\beta=x,y,z}}&[\omega_t^2(\mathbf{q})n_\alpha n_\beta+\omega_t^2(\mathbf{q})(\delta_{\alpha\beta}-n_\alpha n_\beta)]P_\alpha(\mathbf{q})P_\beta(\mathbf{q})\\ +\sum_{\substack{\mathbf{q},\mathbf{q}',\mathbf{q}'',\mathbf{q}'''\\ \alpha,\beta=x,y,z}}&P_\alpha(\mathbf{q})P_\alpha(\mathbf{q}')P_\beta(\mathbf{q}'')P_\beta(\mathbf{q}''')\delta(\mathbf{q}+\mathbf{q}'+\mathbf{q}''+\mathbf{q}''')[(u+v)-v\delta_{\alpha\beta}]\\ +\frac{1}{6}d\sum_{\substack{\mathbf{q}_1,\dots,\mathbf{q}_6\\ \alpha,\beta=x,y,z}}&P_\alpha(\mathbf{q}_1)P_\alpha(\mathbf{q}_2)P_\beta(\mathbf{q}_3)P_\beta(\mathbf{q}_4)P_\gamma(\mathbf{q}_5)P_\gamma(\mathbf{q}_6)\delta\Big(\sum_{i=1}^{6}\mathbf{q}_i\Big)\\ +b\sum_{\substack{\mathbf{q},\mathbf{q}',\mathbf{q}''\\ \alpha,\beta=x,y,z}}&iq_\alpha P_\alpha(\mathbf{q})P_\beta(\mathbf{q}')P_\beta(\mathbf{q}'')\delta(\mathbf{q}+\mathbf{q}'+\mathbf{q}'').\end{aligned} \tag{21}$$

Here μ is the mass coefficient for the polarization oscillations and ω_l and ω_t are respectively the frequencies of the longitudinal and transverse branches.

The last term in (21) assumes a nonzero value (i.e., $\operatorname{div} \mathbf{P} \neq 0$) upon the appearance of an IS in the FE, and consequently acquires a longitudinal component after the polarization. Therefore, the difference between the longitudinal- and transverse-phonon spectra should be taken into consideration. At the same time, the anisotropy of the polarization-fluctuation spectrum can be neglected, and the corresponding term in (21) has been dropped. The sixth-order term has been included in (21), since phase transitions in the cubic FE are always first-order transitions and the fourth-order term is assumed to be negative. For definiteness, we shall assume that $u<0$, $v>0$, and that there occurs in the absence of the last term in (21) a phase transition from the cubic into the tetragonal phase[3)] (as in, for example, $KNbO_3$, $BaTiO_3$, and $PbTiO_3$).

In the case in question here of a phase transition in a FE, the formation of a longitudinal polarization wave is a necessary condition for the appearance of an IS. If the crystal were an ideal dielectric, then the appearance of a depolarization electric field would make the phase transition into the IS state energetically disadvantageous. Real FE, however, contain significant amounts of impurities, which transform even wide-band FE into semiconductors with characteristic Debye-screening-length (r_D) values of the order of[10] $10^{-6}-10^{-4}$ cm.[4)] Therefore, the dipole gap in the longitudinal-mode spectrum $\omega_l(\mathbf{q})$ vanishes, and, for $q \ll r_D^{-1}$, the difference between the longitudinal and transverse oscillations is insignificant.

The relation between $\omega_l(\mathbf{q})$ and $\omega_t(\mathbf{q})$ is given by the formula[11]

$$\varepsilon(\infty)\omega_l^2(\mathbf{q})=\omega_t^2(\mathbf{q})(1+q^2r_D^2)[1+q^2r_D^2/\varepsilon(0)]^{-1}, \tag{22}$$

where $\varepsilon(0)$ and $\varepsilon(\infty)$ are the values of the static and high-frequency dielectric constants respectively. The transverse-soft-mode spectrum $\omega_t(\mathbf{q})$ for $q \ll a^{-1}$ (a is the crystal-lattice constant) for cubic FE of the displacive type has the form[9]

$$\begin{aligned}&\omega_t^2(\mathbf{q})=4\pi(T-T_0)/\mu C+s_t q^2/\mu,\\ &\mu=4\pi/\lambda, \quad \lambda=4\pi z^2/v_c.\end{aligned} \tag{23}$$

Here C is the Curie–Weiss constant, z is the effective charge of the ferroelectric ion, v_c is the volume of the elementary cell, and s_t is a quantity of the order of the square of the velocity of sound in the crystal. In the case in which the FE is a good dielectric, we can assume that $r_D \to \infty$, and the formula (22) then goes over into the well-known Lyddane–Sachs–Teller relation for ionic crystals, written with allowance for one longitudinal, and one transverse, oscillation branch:

$$\omega_l^2/\omega_t^2=\varepsilon(0)/\varepsilon(\infty). \tag{24}$$

To determine the conditions for the appearance of an IS in a FE, we can use as trial functions for P_x and P_y the expression (5), which contains a longitudinal component P_z, and set P_z equal to zero. Then it follows from (21)–(23) that the situation is entirely similar to

the case of the phase transition described by the nonvector representation F_{2u}, but in place of the characteristic parameter x' there appears the parameter[5)] x'':

$$x''=\frac{25}{4}\frac{(u+{}^1/_3 v)}{b^2}\frac{d\omega_t^2(\mathbf{q})}{dq^2}\Big|_{q=q_0}. \tag{25}$$

If the period of the IS is fairly large and $q_0 r_D \ll 1$, then the difference between the parameters x' and x'' is insignificant, since on such large scales the dipole forces are screened. As to the formation of an IS with $q \gtrsim r_D^{-1}$ in a FE, it is highly improbable. Let us now estimate in order of magnitude the value of the parameter x'' for ordinary cubic FE. In the cgs system the nonlinearity coefficients u and v for FE of the displacive type are of the order of 10^{-12}. The quantity b has the value $a^3/z \sim 10^{-13}$. Let us note that the contribution to this coefficient that stems from the coupling between the critical-phonon and acoustic branches[6)] is of the same order of magnitude:

$$\Delta b \sim \frac{q v_0}{z}\frac{\tilde{v}}{\tilde{a}}, \tag{26}$$

where q is the electrostriction constant and $\tilde{a}$ is the constant of the acoustic spectrum. Assuming that $q_0 r_D^{-1} \ll 1$, we have

$$\frac{d\omega_t^2(\mathbf{q})}{dq^2} \sim \frac{s_t}{\mu} \sim 10^{-15}. \tag{27}$$

Thus, we obtain for the parameter x'' in a FE the value $x'' \sim -1$ [let us recall that the fourth-order term in (21) is negative for a FE]. Above we showed that the crystal undergoes a first-order phase transition into an IS state at values of $|x| < |x_c| \approx 33$ (see Fig. 1).

In order to find those values of the Debye length r_D at which this result is valid, let us determine the spatial period, $\lambda_0 = 2\pi/q_0$, of the IS for $|x''| \sim 1$. The formula (16) for q_0 can be rewritten in the form

$$q_0^2 = \frac{1-x}{8x^2}\frac{3u^2}{16d}\frac{s_t}{\mu}, \tag{28}$$

where we have separated the dimensionless combination $3u^2/16d$, which can be expressed in terms of experimentally known quantities:

$$\frac{3u^2}{16d} = \frac{4\pi}{C}(T_1 - T_0) \approx 10^{-3}. \tag{29}$$

Since $s_t/\mu \sim a^2$, we obtain for the IS period for $|x''| \sim 1$ the estimate

$$\lambda_0 \approx (10^2 - 10^3)a \sim 10^{-5} - 10^{-4}\ \text{cm}. \tag{30}$$

We see that the quantity λ_0 is roughly of the same order of magnitude as the normal screening-length values for FE. Therefore, it may be inferred that the question of the appearance of an IS in cubic FE does not have a universal answer: the appearance of IS is possible in low-resistance FE with strong internal screening, but apparently impossible in high-resistance FE. Above we treated r_D as a phenomenological parameter, and used the experimental values for it, since the theoretical computation of the screening length in a FE, in which the charged-defect concentration is certainly not low, is a separate complex problem.[7)]

Since the period λ_0 increases as the parameter x'' increases, it is more likely that IS will be observed in FE subjected to hydrostatic compression. Indeed, the fact that in the "free" crystal the phase transition is of first order and the nonlinearity coefficient $u < 0$ is primarily due to electrostriction. At the same time, for the "clamped" crystal $u > 0$ (see, for example, Ref. 9) and according to estimates $x'' \gtrsim 1$. If for a given FE the coefficient u changes its sign at pressures normally used in experiment (up to 10 kbar), then the IS can be observed. The width ΔT of the temperature domain of existence of the IS will then be determined by the inequality $r_D^{-1} > q_0(T)$, which, for $x'' \sim 1$, can be written in the form

$$q_0 \approx \left[\frac{4\pi(\Delta T)}{5a^2 C}\right]^{1/2} < r_D^{-1}. \tag{31}$$

For $r_D \sim 10^{-5}$ we obtain for the temperature range ΔT a value of the order of several degrees.

Let us note that Aslanyan and Levanyuk[12] investigated the problem of the existence of IS in FE of the type $BaTiO_3$, and obtained for ΔT a value of the order of hundredths of a degree. As a consequence, they concluded that the inhomogeneous phase that arises during the second-order phase transitions in FE can hardly be observed. Although the estimate for ΔT was derived by another method, the main cause of so large a disagreement with our result lies in the fact that the superstructure wave vector q_0 is estimated in Ref. 12 on the basis of general arguments to be

$$q_0 \sim a^{-1}[(T - T_0)/T_0]^{1/2},$$

whereas it follows from the above-presented calculation that q_0 is given by the formula (11), in the denominator of which stands the Curie–Weiss constant C instead of T_0. Since, because of the presence of a small parameter, FE of the displacive type are characterized by large C values, and $T_c/C \sim (3-8)\times 10^{-3}$ (Ref. 9), it is the neglect of this fact that led to the two-to-three orders of magnitude underestimation of the temperature domain of existence of the IS in Ref. 12.

EFFECT OF FLUCTUATIONS ON THE NATURE OF THE PHASE TRANSITIONS

The phenomenological theory constructed in the preceding sections shows that in the systems (4), (18), and (21) the phase transitions into both the homogeneous and inhomogeneous phases at $x > 1$ are second-order transitions. Therefore, the effect of the fluctuations should be taken into account in the description of their properties. As is well known, to solve this problem, we should go over from the thermodynamic potential to an effective Hamiltonian corresponding to the given system.[13] For a cubic crystal, the phase transition in which is described by a vector order parameter, the effective Hamiltonian can be written in the form

$$\mathcal{H}_{\text{eff}} = \frac{1}{2}\sum_{\alpha,\beta=1}^{3}\sum_{\mathbf{q}}\Big\{[(r_0+q^2)\delta_{\alpha\beta}+h_0 q_\alpha q_\beta]P_\alpha(\mathbf{q})P_\beta(-\mathbf{q}) + \frac{1}{12}\sum_{\mathbf{q}+\mathbf{q}'+\mathbf{q}''+\mathbf{q}'''=0}[v_0+(u_0-v_0)\delta_{\alpha\beta}]P_\alpha(\mathbf{q})P_\alpha(\mathbf{q}')P_\beta(\mathbf{q}'')P_\beta(\mathbf{q}''') + \frac{1}{3}b_0\sum_{\mathbf{q}'} iq_\alpha P_\alpha(\mathbf{q})P_\beta(\mathbf{q}')P_\beta(-\mathbf{q}-\mathbf{q}')\Big\}. \tag{32}$$

Here $P_\alpha(\mathbf{q})$ is the vector order-parameter field, $n_\alpha = q_\alpha/q$, and b_0, u_0, and v_0 are bare coupling constants ($u_0 > 0$, $v_0 > -u_0$). The "bare mass" r_0 is a linear function of the distance to the phase-transition line in the phase diagram. The presence of the constant $h_0 (h_0 > -1)$ reflects the nondegeneracy of the spectra of the longitudinal and transverse order-parameter fluctuations. Another quadratic—in $\mathbf{q}$—anisotropic invariant, $P(\mathbf{q})$, has been dropped in (32), since its consideration is unimportant for us.

As the system approaches the second-order phase transition line, the parameters of the basic Hamiltonian (32) vary, and the thermodynamic behavior is determined by their renormalized (temperature-dependent) values. In order to elucidate the distinctive features of the fluctuation theory for the Hamiltonian (32), let us first consider within the framework of perturbation theory the form of the correlation corrections to the bare values of the coefficients in (32). Here we can, for simplicity, take the free Green function $G^{(0)}_{\alpha\beta}$ to be isotropic:

$$G^{(0)}_{\alpha\beta} = \delta_{\alpha\beta}/(\tau + q^2). \tag{33}$$

In first order perturbation theory, the diagrammatic representation for the fluctuation corrections to the bare values of b_0 and $u_0(v_0)$ is given by the single-loop diagrams shown respectively in Figs. 2a and 2b. A wavy line going out of a third-order vertex is associated with the factor iq_α. Besides those shown in Fig. 2, there are other single-loop diagrams with a different wavy-line "topology," but it is not difficult to verify that all of them cancel out, and do not make a contribution to the values of the coupling constants. The integrals $I_i^{(n)}$ corresponding to the n-angle diagrams with internal wavy lines in Fig. 2 have the form

$$I_1^{(3)} = \frac{1}{(2\pi)^d}\int d^dq \frac{q_\alpha^2}{(\tau+q^2)^3},$$
$$I_2^{(4)} = \frac{1}{(2\pi)^d}\int d^dq \frac{q_\alpha^4}{(\tau+q^2)^4}, \tag{34}$$
$$I_3^{(4)} = \frac{1}{(2\pi)^d}\int d^dq \frac{q_\alpha^2 q_\beta^2}{(\tau+q^2)^4} \quad (\alpha \neq \beta).$$

It follows from (34) that the fluctuation corrections vary with temperature like $\tau^{(4-d)/2}$ both for the third- and fourth-order vertices; therefore, the highest critical dimensionality for our problem is $d_c = 4$. This result allows us to apply the ε-expansion method ($\varepsilon = 4 - d$), with the aid of which we can obtain asymptotically exact results for $\varepsilon \to 0$. Nevertheless, below we shall not use the ε expansion; rather we shall perform the calculations by the RG method directly for three-dimensional space. This computational scheme is preferred for two reasons: first, there is always the usual difficulty in the ε-expansion method of extrapolating the results to the $\varepsilon = 1$ value, a process which results in the loss of the asymptotic exactness of the theory; secondly, and this is even more important, the choice of this analytic continuation in our problem is itself nonunique, since it is necessary to set the dimensionality of the field $P_\alpha(\mathbf{q})$ equal to that of the space. At the same time, it is known from the solutions to the problem of the phase transition in cubic crystals[14] and the problem of the nematic–isotropic liquid transition occurring near an isolated point[15] that the two analytic-continuation procedures lead to qualitatively different results.

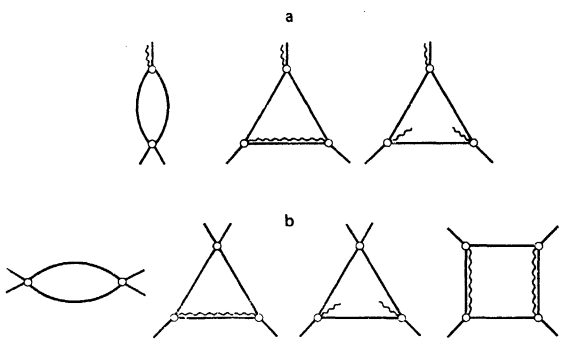

FIG. 2. Single-loop diagrams contributing to the renormalization of the third-order (a) and fourth-order (b) vertices.

Let us now proceed to the derivation of the RG equations for the Hamiltonian (32) in the region of highly developed fluctuations, choosing as the independent variable $\varkappa$, the reciprocal correlation length. The critical behavior of the system is determined by the temperature dependences of the third- and fourth-order vertex functions $\Gamma_3(\mathbf{q}, \mathbf{q}', \mathbf{q}'', \varkappa)$ and $\Gamma_4^{(u,v)}(\mathbf{q}, \mathbf{q}', \mathbf{q}'', \mathbf{q}''', \varkappa)$ respectively. Above we established within the framework of the phenomenological approach developed there that a transition on the line of second-order phase transitions into either the homogeneous phase or the inhomogeneous state is characterized by the wave vector $\mathbf{q}_0 = 0$. Consequently, to describe the properties of these phase transitions, we need to investigate the asymptotic forms of the vertex functions $\Gamma_n(\mathbf{q}_i, \varkappa)$ for small $\mathbf{q}_i$. The renormalized coupling constants u_R and v_R can be introduced in the process in the usual fashion:

$$u_R(\varkappa) = \Gamma_4^{(u)}(\mathbf{q}_i = 0, \varkappa),$$
$$v_R(\varkappa) = \Gamma_4^{(v)}(\mathbf{q}_i = 0, \varkappa),$$

and the renormalized charge $b_R(\varkappa)$ for the third-order vertex can be defined by the equation

$$\tfrac{1}{3} b_R(\varkappa)\,(q_{1\alpha}\delta_{\beta\gamma} + q_{2\beta}\delta_{\alpha\gamma} + q_{3\gamma}\delta_{\alpha\beta})$$
$$= \lim \Gamma_3^{\alpha\beta\gamma}(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \varkappa), \quad q_i/\varkappa \to 0. \tag{35}$$

In the first approximation in the charges, the renormalized Green function separates into a longitudinal, and a transverse, part:

$$G_{\alpha\beta}(\mathbf{q}, \varkappa) = \frac{\delta_{\alpha\beta} - n_\alpha n_\beta}{\varkappa^2 + q^2} + \frac{n_\alpha n_\beta}{\varkappa^2 + (1+h_R)q^2}, \tag{36}$$

where h_R is the renormalized value of h_0.

Let us note that the presence of the third-order vertex $\Gamma_3(q_i, \varkappa)$ leads to the renormalization of h_0 and the coefficient attached to q^2 in (32) even in the first approximation; therefore, the system of RG equations for the renormalized charges $u_R(\varkappa)$, $v_R(\varkappa)$, and $b_R(\varkappa)$ should be supplemented by the corresponding propagator equations. This is, however, not necessary in the case of large bare values of h_0. In fact, a direct verification shows that, as $h_0 \to \infty$, only the transverse part of the Green function, with which the third-order vertex $\Gamma_3(q_i, \varkappa)$ does not interact, makes a critical contribution

to the diagrams, and therefore the propagator is not renormalized in the first approximation. The system of RG equations for the renormalized charges then gets significantly simplified, since the charge $b_R(\varkappa)$ will not enter into the equations for $u_R(\varkappa)$ and $v_R(\varkappa)$ (since the diagrams containing wavy lines drop out) and its temperature dependence is entirely determined by the evolution of $u_R(\varkappa)$ and $v_R(\varkappa)$.

Using the Ward identity for the bare Green function:

$$\frac{\partial G^{(0)}_{\alpha\beta}}{\partial r_0}=-G^{(0)}_{\alpha\gamma}G^{(0)}_{\gamma\beta}, \tag{37}$$

we obtain the appropriate system of RG equations in the single-loop approximation:

$$\begin{aligned}
\frac{db_R^2}{d\varkappa^2}&=\frac{b_R^2}{2\varkappa^2}(K_1+2K_2)\left(u_R+\frac{2}{3}v_R\right),\\
\frac{du_R}{d\varkappa^2}&=\frac{1}{2\varkappa^2}\left[\left(-\frac{3}{2}K_1u_R+2K_2v_R\right)u_R+\frac{1}{3}(K_1+K_2)v_R^2\right],\\
\frac{dv_R}{d\varkappa^2}&=\frac{1}{2\varkappa^2}\left[\frac{3}{2}K_2u_R^2+(K_1+K_2)u_Rv_R+\frac{1}{6}(K_1+7K_2+4K_3)\right],
\end{aligned} \tag{38}$$

where we have denoted by K_1, K_2, and K_3 the integrals

$$\begin{aligned}
K_1(\varkappa)&=\frac{1}{(2\pi)^3}\int G_{\alpha\alpha}^2(\mathbf{q})\,d\mathbf{q},\quad K_2(\varkappa)=\frac{1}{(2\pi)^3}\int G_{\alpha\beta}^2(\mathbf{q})\,d\mathbf{q},\\
K_3(\varkappa)&=\frac{1}{(2\pi)^3}\int G_{\alpha\alpha}(\mathbf{q})G_{\beta\beta}(\mathbf{q})\,d\mathbf{q},\\
K_1&=8K_2=\frac{4}{3}K_3=\frac{1}{15\pi\varkappa}.
\end{aligned} \tag{39}$$

The system of RG equations describes, in particular, the critical behavior of cubic FE, since for them the value $h_0\sim r_D^2/a^2\gg 1$, and the small corrections of the order of $1/h_0$ can be neglected. The last two equations in (38) have, for the above-indicated reasons, the same form as the RG equations for cubic ferromagnets in the dipole region (see, for example, Ref. 16). As is well known, the latter have only one nontrivial (Heisenberg) fixed point (FP), which is unstable, and the solutions run off beyond the stability limits $u_0=0$, $v_0=-u_0$. It therefore follows that the critical fluctuations in a system described by the Hamiltonian (32) leads, when $h_0\gg 1$, to the transformation of the second-order transitions into first-order transitions. As a result, the TCP disappears, while the bicritical LP becomes a tricritical point. These are the main qualitative changes that occur in the phase diagram obtained in the phenomenological theory (Fig. 1) when the fluctuations are taken into account. The phases' existence domains themselves do not, apparently, change much.

To corroborate this conclusion, let us estimate the rate of evolution of the parameter x'' in the critical region for the case in which the effective crystallographic anisotropy is small: $(u_R-v_R)/u_R\ll 1$. Substituting into the first of the equations (38) the expressions for $u_R(\varkappa)$ and $v_R(\varkappa)$ corresponding to the singular Heisenberg solution:

$$u_R^*(\varkappa)=\frac{120}{17}\pi\varkappa,\quad v_R^*=0,$$

we obtain for the charge $b_R(\varkappa)$ the following power dependence:

$$b_R(\varkappa)\sim\varkappa^{25/51}. \tag{40}$$

From this we find for the parameter $x''\sim u_R/b_R^2$ the expression

$$x''(\varkappa)\sim\varkappa^{1/51}\approx\tau^{0.01}. \tag{41}$$

It can be seen from (41) that x'' depends very weakly on temperature. Similar computations for isotropic FE of the "easy-plane" type yield for x'' the dependence

$$x''(\varkappa)\sim\varkappa^{1/9}\approx\tau^{0.06}. \tag{42}$$

Similar slow variations of parameters with temperature are quite often encountered in the theory of critical phenomena. For example, the isotropic-to-anisotropic critical behavior crossover rates for cubic and tetragonal crystals in the dipole region are given respectively by the expressions $\varkappa^{-3/17}$ (Ref. 14) and $\varkappa^{-1/3}$ (Ref. 17).

Having analyzed the case in which $h_0\gg 1$, let us now investigate the critical behavior of a system with the Hamiltonian (32) for[8] $|h_0|\ll 1$. We encounter the following difficulty here: we can easily verify with the aid of perturbation theory that the renormalizations of the longitudinal and transverse parts of the Green function are different, e.g., for $h_0=0$ the fluctuation correction to the square of the "velocity" of the longitudinal wave is three times greater in absolute value than the correction for the transverse wave. It therefore follows that, strictly speaking, we should, in constructing the RG equations, introduce two different scale factors, one for the longitudinal, and the other for the transverse, fluctuations. This not only very much complicates all the calculations, it makes the system of RG equations itself very unwieldy. At the same time, it can be verified that the numerical values of the coefficients of the expansions of the Gell-Mann–Low functions in the RG equations for the renormalized charges b_R, u_R, and v_R change little when allowance is made for the renormalization of the momentum dependence of the propagator. Therefore, it seems natural to assume that the qualitative results obtained with the use of the isotropic Green function ($h_R=0$) remain valid in the more exact computations.

In the isotropic-correlator approximation the RG equations for $b_R(\varkappa)$, $u_R(\varkappa)$, and $v_R(\varkappa)$ have the following form:

$$\begin{aligned}
\frac{db_R^2}{d\varkappa^2}&=\frac{1}{2\varkappa^2}\left[\left(u_R+\frac{2}{3}v_R\right)\mathcal{G}_1b_R^2-\frac{8}{9}\mathcal{G}_2b_R^4\right],\\
\frac{du_R}{d\varkappa^2}&=\frac{1}{2\varkappa^2}\left[\left(\frac{3}{2}u_R^2+\frac{1}{3}v_R^2\right)\mathcal{G}_1-\frac{4}{3}\left(u_R+\frac{1}{3}v_R\right)\right.\\
&\quad\left.\times\mathcal{G}_2b_R^2+\frac{4}{27}(\mathcal{G}_3+\mathcal{G}_4)b_R^4\right],\\
\frac{dv_R}{d\varkappa^2}&=\frac{1}{2\varkappa^2}\left[\left(u_R+\frac{5}{6}v_R\right)\mathcal{G}_1v_R-\frac{2}{3}\left(u_R+\frac{5}{3}v_R\right)\right.\\
&\quad\left.\times\mathcal{G}_2b_R^2+\frac{2}{27}(\mathcal{G}_3+5\mathcal{G}_4)b_R^4\right],\\
\mathcal{G}_1&=4\mathcal{G}_2=8\mathcal{G}_3=24\mathcal{G}_4=(8\pi\varkappa)^{-1}.
\end{aligned} \tag{43}$$

For the purpose of investigating the nature of the solutions of the systems (43), it is convenient to go over to the dimensionless charges $\tilde b$, $\tilde u$, and $\tilde v$:

$$b_R^2=24\pi\varkappa\tilde b,\ v_R=24\pi\varkappa\tilde v,\ u_R=24\pi\varkappa\tilde u.$$

After the substitution of the values of $\mathcal{G}_i$, the RG equations in the new variables assume the form

$$\begin{aligned}
\frac{d\tilde{b}}{dt} &= -\tilde{b}+(3\tilde{u}+2\tilde{v})\tilde{b}-\frac{2}{3}\tilde{b}^2,\\
\frac{d\tilde{u}}{dt} &= -\tilde{u}+\frac{9}{2}\tilde{u}^2+\tilde{v}^2-\left(\tilde{u}+\frac{1}{3}\tilde{v}\right)\tilde{b}+\frac{2}{27}\tilde{b}^2,\\
\frac{d\tilde{v}}{dt} &= -\tilde{v}+\left(3\tilde{u}+\frac{5}{2}\tilde{v}\right)\tilde{v}-\frac{1}{2}\left(\tilde{u}+\frac{5}{3}\tilde{v}\right)\tilde{b}+\frac{2}{27}\tilde{b}^2, \quad t=\ln\varkappa.
\end{aligned} \tag{44}$$

It is well known that, for $\tilde{b}=0$, the system (44) has three nontrivial FP: Ising ($\tilde{u}_I^*=\frac{2}{9}$, $\tilde{v}_I^*=0$), cubic ($\tilde{u}_c^*=\frac{4}{21}$, $\tilde{v}_c^*=\frac{2}{9}$), and Heisenberg ($\tilde{u}_H^*=\tilde{v}_H^*=\frac{2}{11}$) FP, only the last one being stable in the $\tilde{u}$–$\tilde{v}$ plane. For $\tilde{b}\neq 0$, this FP is, as can easily be verified by linearizing the equations (44) in $\tilde{b}$, also unstable ($\tilde{b}\sim\varkappa^{-1/11}$). Besides the FP lying in the $\tilde{u}$–$\tilde{v}$ plane, the system (44) possesses four other FP with the coordinates

$$\begin{aligned}
&\tilde{u}^*_{(1,2)}=\tilde{v}^*_{(1,2)}=-1\pm\sqrt{3}/2, \quad \tilde{b}^*_{(1,2)}=3/2(5\tilde{u}^*_{(1,2)}-1),\\
&\tilde{u}^*_{(3,4)}=1/9, \quad \tilde{v}^*_{(3,4)}=1/3(1\pm\sqrt{-3}/2), \quad \tilde{b}^*_{(3,4)}=(3\tilde{v}^*_{(3,4)}-1),
\end{aligned} \tag{45}$$

of which only the FP with

$$\tilde{u}^*=\tilde{v}^*=-1+\sqrt{3}/2, \quad \tilde{b}=3/2(5\tilde{u}^*-1)$$

corresponds to real values of the coupling constants. Calculations show that the FP is also unstable in the three-dimensional space of the charges $\tilde{b}$, $\tilde{u}$, and $\tilde{v}$. Thus, Eqs. (44) have no stable FP; consequently, only first-order phase transitions can occur in a system described by the effective Hamiltonian (32).

We can similarly investigate the critical behavior of cubic crystals, the phase transition in which corresponds to the nonvector order-parameter representation F_{2u}. We shall not write out the effective Hamiltonian for this case, since it is evidently connected with the expression for the thermodynamic potential (18); rather let us give at once the corresponding system of RG equations for the renormalized charges[9]:

$$\begin{aligned}
\frac{db_R^2}{d\varkappa^2} &= \frac{b_R^2}{2\varkappa^2}\left(\mathcal{G}_1 u_R-\frac{4}{9}\mathcal{G}_2 b_R^2\right),\\
\frac{du_R}{d\varkappa^2} &= \frac{1}{2\varkappa^2}\left[\left(\frac{3}{2}u_R^2+\frac{1}{3}v_R^2\right)\mathcal{G}_1-\frac{4}{3}\left(u_R+\frac{1}{3}v_R\right)\right.\\
&\left.\times\mathcal{G}_2 b_R^2+\frac{4}{27}(\mathcal{G}_3+\mathcal{G}_4)b_R^4\right]\\
\frac{dv_R}{d\varkappa^2} &= \frac{1}{2\varkappa^2}\left[\left(u_R+\frac{5}{6}v_R\right)\mathcal{G}_1 v_R\right.\\
&\left.-\frac{2}{3}(u_R+v_R)\mathcal{G}_2 b_R^2+\frac{2}{9}(\mathcal{G}_3+\mathcal{G}_4)b_R^4\right].
\end{aligned} \tag{46}$$

Going over, as in (43), to the dimensionless charges, we obtain

$$\begin{aligned}
\frac{d\tilde{b}}{dt} &= \tilde{b}\left(-1+3\tilde{u}-\frac{1}{3}\tilde{b}\right),\\
\frac{d\tilde{u}}{dt} &= -\tilde{u}+\frac{9}{2}\tilde{u}^2+\tilde{v}^2-\left(\tilde{u}+\frac{1}{3}\tilde{v}\right)\tilde{b}+\frac{2}{27}\tilde{b}^2,\\
\frac{d\tilde{v}}{dt} &= -\tilde{v}+\left(3\tilde{u}+\frac{5}{2}\tilde{v}\right)\tilde{v}-\frac{1}{2}(\tilde{u}+\tilde{v})\tilde{b}+\frac{1}{9}\tilde{b}^2.
\end{aligned} \tag{47}$$

In the $\tilde{b}=0$ plane the system (47) of course processes the same FP as the system (44). Besides them, there are, for $\tilde{b}\neq 0$, two other FP with real coordinate values: ($\tilde{u}^*=\frac{2}{3}$, $\tilde{v}^*=0$, $\tilde{b}^*=3$), ($\tilde{u}^*\approx 0.5$, $\tilde{v}^*\approx 0.23$, $\tilde{b}^*\approx 1.5$). All the FP of the system (47) turn out to be unstable; consequently, as in the case of the vector representation, only first-order phase transitions are possible. Let us note that the conversion of second-order phase transitions into first-order transitions in the fluctuation region is generally characteristic of problems in which the number of important invariant charges is greater than two, and we can even adduce some general arguments to support the regularity of this circumstance.[18,19] Therefore, it is also natural to expect the occurrence of only first-order phase transitions in those cases in which the symmetry of the system admits of the existence of not just one (as was the case above),[10] but several independent invariants of the type (3).

CONCLUSION

Let us briefly discuss possible experiments in which the appearance of the above predicted long-period superstructure can be detected. It follows from the performed analysis that the condition for the existence of the superstructure is the definite limitedness of the value of the modulus of the dimensionless parameter x. Since this parameter is proportional to the magnitudes of the coefficients describing the anharmonic fourth-order interaction, the value of x will be small for phase transitions occurring in the vicinity of a TCP. Therefore, it seems to be expedient to carry out the experimental search for IS primarily in those crystals whose phase diagrams contain TCP. Since according to the estimates made above, the period of an IS near a TCP turns out to be long, and can be longer than the wavelength of light, the superstructure can apparently be observed by the appearance of Bragg peaks in the elastic scattering of light. In the case of smaller values of the superstructure period, the traditional techniques of small-angle neutron scattering and x-ray structural analysis can be used to detect the IS. In this case it is natural to regard the dependence of the superstructure period on the external parameters [see (9) and (11)] as a characteristic indication of a transition into the IS state.

As we have seen, the conditions for the appearance of IS in cubic FE are more rigid than the conditions for the occurrence of phase transitions for which the dipole interaction does not play a distinct role. Nevertheless, the appearance of IS under these conditions is possible, especially in the vicinity of a TCP. Since the appearance of polarization is usually accompanied by an abrupt change in the forbidden-band width and, consequently, by a long-wave shift of the fundamental-absorption edge, it is possible in this case to observe IS in transmitted light of wavelength close to the fundamental absorption edge. Even if the phase transition in the FE occurs at a point not too close to a TCP, the appearance of an IS in the crystal's surface region, where a layer with a high carrier concentration is formed, seems to be possible.[10]

On the whole, the formation of IS of the above-investigated type is possible in a fairly broad class of crystals; therefore, their experimental detection is quite probable.

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[1)]This condition is a necessary condition for the transition into the IS state to be continuous.

[2)]They investigated the situation in which in the absence of terms of the type (3) the phase transition is of second order.

[3)]The case of the transition into the orthorhombic phase, when $u>0$, $v<-u$ (as in GeTe or $CsGeCl_3$), can be investigated in an entirely similar fashion.

[4)]Let us note that a pure $BaTiO_3$ crystal with the forbidden-band width $\Delta E = 3.2$ eV would have at room temperature $r_D \approx 10$ m.

[5)]We have, for simplicity, chosen the value $t_0 = 2$.

[6)]This coupling is described by a term of the type $\tilde{v}(\partial P_i/\partial x_j + \partial P_j/\partial x_i)u_{ij}$ in the thermodynamic potential. For the coefficients $\tilde{v}$, $\tilde{a}$, q, and s_t we use the values given in Ref. 9.

[7)]The complexity is due to the substantial disordering of FE crystals, which contain, in contrast to doped semiconductors with small impurities, deep-lying impurity levels with an unknown band structure.

[8)]For the values of $h_0 \sim 1$ the critical behavior will be described by the crossover regime between these two cases.

[9)]Let us note that, in comparison with the case of the vector representation, there appear additional diagrams with internal wavy lines.

[10)]An example may be the easy-plane-type tetragonal crystal with a vector order parameter, for which the thermodynamic-potential expansion contains three such invariants.

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