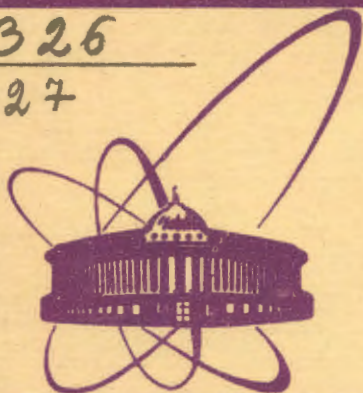


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**CHANGES OF ELASTIC CONSTANTS
IN STRUCTURAL PHASE TRANSITIONS.**

1.General Case

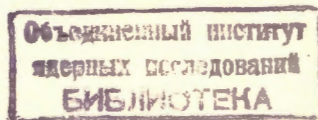
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IN STRUCTURAL PHASE TRANSITIONS.**

1.General Case



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Изменение упругих постоянных при структурном фазовом переходе. I. Общий случай

В рамках феноменологической теории рассмотрен тензор упругих постоянных в окрестности структурного фазового перехода. Выведено общее выражение для упругих постоянных.

Работа выполнена в Лаборатории теоретической физики, ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1979

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Changes of Elastic Constants in Structural Phase Transitions. I. General Case

The tensor of elastic constants in a vicinity of the structural phase transition is considered in the framework of the phenomenological theory. The general expression for the elastic constants is derived.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1979

INTRODUCTION

The behaviour of the elastic constants of a crystal in a vicinity of a structural phase transition point can successfully be described in the framework of the phenomenological theory of Landau and Lifshitz^{/1,2/}. The main idea of a reduction of the symmetry of a crystal by an active mode of definite wave vector and relevant irreducible representation involves also specific changes of the elastic constants. The kind of these changes depends upon the symmetry of the high and low symmetry phase and on the active wave vector and irreducible representation. In this respect, the phase transition can be divided into two groups, the equi-transitional phase transitions with an active mode in the centre of the Brillouin zone and phase transitions accompanied by an enlargement of the unit cell with the wave vectors out of the center of the Brillouin zone. The equi-transitional phase transitions can be again divided into non-elastic and elastic ones. In a non-elastic phase transition, if it is continuous, the eigenvalue conjugated to the active mode vanishes at the critical point. In the elastic phase transition critical expression of elastic constants vanishes at the critical point. This occurs either as a result of vanishing of the relevant expression of the elastic constants themselves or as a result of approaching to zero the eigenvalue conjugated to the normal mode of the same symmetry as the relevant elastic constant expression. In both cases a temperature behaviour of elastic constants is different. It is possible to classify the elastic constants tensor with respect to the kind of the structural phase transition without going into details of a particular behaviour of the order parameter. In^{/3/} examples of phase transitions have been elaborated in this way.

All elastic phase transitions have been listed by Aubry and Pick^{/4/} who have shown also that the soft modes which induce the elastic phase transitions are always Raman active in the high and low symmetry phases. If the soft mode in the high symmetry phase is not Raman active then the phase transition is non-elastic.

The tensor of the elastic constants changes also for the phase transitions associated with an enlargement of the unit cell, however then the variety of possible behaviours is reduced, namely the elastic constants are either not affected by the phase transition or exhibit only a jump. An example of such a behaviour is the R-corner structural phase transition in perovskites^{/5/}.

We start with writing the general free-energy expansion in terms of the order parameters or the active normal mode amplitudes and the deformation of the lattice. We obtain also a set of equations for the equilibrium values of the amplitudes of active normal mode and deformation. In the second part^{/6/} we derive the approximate form which describes the behaviour of the elastic constants in a vicinity of equi-translational phase transition induced by one-dimensional irreducible representation of the high symmetry group. The results are collected in two tables separately for non-elastic and elastic phase transitions. In addition we give a list of all elastic phase transitions, induced by one-, two- and three-dimensional irreducible representations, together with that combination of conventional elastic constants which tends to zero at the elastic phase transition point. In the second part we shortly discuss the elastic constants behaviour for the phase transitions with an active wave vector out of the center of the Brillouin zone. In this case the elastic phase transition cannot occur.

DEPENDENT VARIABLES

The free energy of the thermodynamical state of a crystal $F = F(T, \{V_i\}, \{X_\mu^{(m)}\})$ is a function of the temperature T and V_i ($i = 1, 2, \dots, 6$) the components of the symmetric deformation tensor. To study the stability of the system, it is convenient to introduce, apart of the independent variables T and V_i , a set of dependent variables $\{X_\mu^{(m)}\}$. Index m stays for the unit cell of the crystal and μ

stays both for a kind of atoms in the unit cell and for the type of variables. We specify below three types of such variables.

1. The deformation of the crystal can be divided into a homogeneous deformation of the Bravais lattice and additional displacement $s_i^{(m)}(\delta)$ of an atom δ in m -th unit cell. If $r_i^o(\delta^{(m)})$ will denote the equilibrium position of atom δ inside the underformed m -th unit cell and $r_i(\delta^{(m)})$ the position of the same atom in the same deformed unit cell, then the additional displacement to the homogeneous strain of the Bravais lattice can be written as the following dependent variable

$$s_i(\delta^{(m)}) = r_i(\delta^{(m)}) - r_i^o(\delta^{(m)}).$$

In molecular crystals when a group of atoms can be treated as a rigid molecule the $s_i(\delta^{(m)})$ represents the displacement of the center of mass of a given group.

2. Consider a molecular crystal. If the orientational potential acting on a given molecular group ($m\kappa$) is strong enough then this group has a definite equilibrium orientation $\alpha^o(\kappa^{(m)})$ in the underformed configuration. A deformation may twist the molecular group to $\alpha_i(\kappa^{(m)})$ orientation. For the dependent variable we can choose the difference

$$\Theta_i(\kappa^{(m)}) = \alpha_i(\kappa^{(m)}) - \alpha_i^o(\kappa^{(m)}).$$

3. It might happen that equivalent or even non-equivalent sites of an ideal crystal are not actually occupied by atoms. This situation might occur when the number of sites in the lattice for atoms of a given kind is in excess over the number of atoms. This concerns also the case of different static orientations occurring in molecular crystals. Another possibility is that equivalent sites in different unit cells can be occupied by different atoms. In both the cases the crystal can be specified by a probability of finding a specific atom or molecular group at a definite location or orientation with respect to the ideal lattice. We recognize this class of crystals as having the straightforward relation to an order-disorder phenomenon.

Let $\sigma(\frac{m}{\rho})$ and $\sigma^0(\frac{m}{\rho})$ be the probabilities of occupation of a site ($m\rho$) by a desired kind of atom or the probability of a given orientation of the molecular group in the deformed and underformed state, respectively. Then the relevant dependent variables can be chosen as

$$\Delta(\frac{m}{\rho}) = \sigma(\frac{m}{\rho}) - \sigma^0(\frac{m}{\rho}).$$

Generally, the set of the dependent variables consists of the following components

$$\{X(\frac{m}{\mu})\} = \{s_i(\frac{m}{\delta})\}, \{\Theta_i(\frac{m}{\kappa})\}, \{\Delta(\frac{m}{\rho})\},$$

where $\mu = (i, \delta, \kappa, \rho)$. We agree that these variables are chosen in such a way that in the underformed state their equilibrium values are equal to zero.

THE FREE-ENERGY EXPANSION

The equilibrium configuration of the system is achieved once the free energy reaches a minimum. Therefore at an equilibrium state the values of $\{X(\frac{m}{\mu})\}$ are adjusted so that the following set of equations is fulfilled

$$\frac{\partial F}{\partial V_i} \Big|_{\{V_i^0, X^0(\frac{m}{\mu})\}} = p_i, \quad \frac{\partial F}{\partial X(\frac{m}{\mu})} \Big|_{\{V_i^0, X^0(\frac{m}{\mu})\}} = 0, \quad (1)$$

where p_i are the components of the stress tensor and the symbol $\{V_i^0, X^0(\frac{m}{\mu})\}$ denotes the equilibrium values of the variables.

To assure that the system remains stable against any displacements $v_i = V_i - V_i^0$, $x(\frac{m}{\mu}) = X(\frac{m}{\mu}) - X^0(\frac{m}{\mu})$ the quadratic form

$$\delta^2 F = \frac{1}{2} \sum_{ik} \frac{\partial^2 F}{\partial V_i \partial V_k} v_i v_k + \sum_{i\mu} \frac{\partial^2 F}{\partial V_i \partial X(\frac{m}{\mu})} v_i x(\frac{m}{\mu}) + \frac{1}{2} \sum_{\substack{mn \\ \mu\nu}} \frac{\partial^2 F}{\partial X(\frac{m}{\mu}) \partial X(\frac{n}{\nu})} x(\frac{m}{\mu}) x(\frac{n}{\nu}) \geq 0$$

has to be positive definite^{17/}. Adding the condition T/C_V , where C_V is a heat capacity at a constant volume, we get the complete requirement that the system is stable against any displacement of the entropy, deformation, and $X(\frac{m}{\mu})$.

Let us expand the free energy around the point $V_i = 0$ and $X(\frac{m}{\mu}) = 0$ which corresponds to an underformed state. Then

$$\begin{aligned} F = & F(T, \{0\}, \{0\}) + \sum_i p_i V_i + \frac{1}{2} \sum_{ik} c_{ik} V_i V_k + \\ & + \sum_{i\mu} U_i(\frac{m}{\mu}) V_i X(\frac{m}{\mu}) + \frac{1}{2} \sum_{\substack{mn \\ \mu\nu}} D(\frac{m}{\mu} \frac{n}{\nu}) X(\frac{m}{\mu}) X(\frac{n}{\nu}) + \\ & + \frac{1}{2} \sum_{ik} \sum_{m\mu} K_{ik}(\frac{m}{\mu}) V_i V_k X(\frac{m}{\mu}) + \frac{1}{2} \sum_i \sum_{\substack{mn \\ \mu\nu}} L_i(\frac{m}{\mu} \frac{n}{\nu}) V_i X(\frac{m}{\mu}) X(\frac{n}{\nu}) + \\ & + \frac{1}{24} \sum_{\substack{m_1 m_2 m_3 m_4 \\ \mu_1 \mu_2 \mu_3 \mu_4}} B(\frac{m_1}{\mu_1} \frac{m_2}{\mu_2} \frac{m_3}{\mu_3} \frac{m_4}{\mu_4}) X(\frac{m_1}{\mu_1}) X(\frac{m_2}{\mu_2}) X(\frac{m_3}{\mu_3}) X(\frac{m_4}{\mu_4}) + \dots \end{aligned} \quad (2)$$

where the expansion coefficients are the second, third, and fourth derivatives of the free energy, taken at $V_i = 0$ and $X(\frac{m}{\mu}) = 0$. The symmetry of these coefficients being a

result of the order of differentiation has been already taken into account. In particular, c_{ik} are the bare isothermal elastic constants. The higher order terms have been neglected.

Let the system be at a static deformed state $\{V_i^0, X^\circ(\mu^m)\}$ and suppose this state is not very far from the underformed state $\{V_i^0\} = 0$ and $\{X^\circ(\mu^m)\} = 0$. Inserting into (2) $V_i = V_i^0 + v_i$ and $X(\mu^m) = X^\circ(\mu^m) + x(\mu^m)$ and rearranging the terms we get the expansion over accidental displacements v_i and $x(\mu^m)$ around the point $\{V_i^0, X^\circ(\mu^m)\}$. The expansion up to quadratic terms takes the form

$$\begin{aligned}
 F = & F(T, \{V_i^0\}, \{X^\circ(\mu^m)\}) + \sum_i p_i v_i + \\
 & + \frac{1}{2} \sum_{ik} [c_{ik} + \sum_{m\mu} K_{ik}(\mu^m) X^\circ(\mu^m)] v_i v_k + \\
 & + \sum_{im\mu} [U_i(\mu^m) + \sum_k K_{ik}(\mu^m) V_k^0 + \sum_{n\nu} L_i(\mu^m n) X^\circ(\nu^n)] v_i x(\mu^m) + \\
 & + \frac{1}{2} \sum_{\substack{mn \\ \mu\nu}} [D(\mu\nu) + \sum_i L_i(\mu\nu) V_i^0 + \\
 & + \frac{1}{2} \sum_{\substack{m_3 m_4 \\ \mu_3 \mu_4}} B(\mu\nu \mu_3 \mu_4) X^\circ(\mu_3^{m_3}) X^\circ(\mu_4^{m_4})] x(\mu^m) x(\nu^n) + \dots
 \end{aligned} \tag{3}$$

The equilibrium values of V_i^0 and $X^\circ(\mu^m)$ can be obtained from the equilibrium equations (1) written now as

$$\begin{aligned}
 \sum_k c_{ik} V_k^0 + \sum_{m\mu} [U_i(\mu^m) + \sum_k K_{ik}(\mu^m) V_k^0] X^\circ(\mu^m) + \\
 + \frac{1}{2} \sum_{\substack{mn \\ \mu\nu}} L_i(\mu^m n) X^\circ(\mu^m) X^\circ(\nu^n) = -p_i \quad \text{for } i=1,2,\dots,6 \\
 \sum_i [U_i(\mu^m) + \frac{1}{2} \sum_k K_{ik}(\mu^m) V_k^0] V_i^0 + \sum_{n\nu} [D(\mu\nu) + \sum_i L_i(\mu\nu) V_i^0 + \\
 + \frac{1}{6} \sum_{\substack{m_3 m_4 \\ \mu_3 \mu_4}} B(\mu\nu \mu_3 \mu_4) X^\circ(\mu_3^{m_3}) X^\circ(\mu_4^{m_4})] X^\circ(\nu^n) = 0 \\
 \text{for all } (m, \mu). \tag{4}
 \end{aligned}$$

Notice, that $V_i^0 = 0$ and $X^\circ(\mu^m) = 0$ is a trivial solution of the above set.

Consider the underformed configuration. At the instability point the system becomes unstable with respect to one normal mode. To treat this situation in detail, it is necessary to consider the following eigenvalue problem of the second derivatives of the free energy

$$\sum_{n\nu} D(\mu\nu) \exp[-i\vec{k}(\vec{R}(m) - \vec{R}(n))] e_\nu(\vec{k}, j) = \lambda_{\vec{k}, j} e_\mu(\vec{k}, j). \tag{5}$$

The eigenvalues and eigenvectors can be classified by the wave vectors \vec{k} from the first Brillouin zone and the branches j of normal modes, since the crystal possesses a periodic lattice. The eigenvectors are, in general, complex and orthonormal. Any nonhomogeneity of the system, static $X^\circ(\mu^m)$ or dynamic $x(\mu^m)$ can be expressed in terms of the introduced eigenvectors. Thus

$$X^\circ(\mu^m) = \sum_{\vec{k}, j} e_\mu(\vec{k}, j) \exp[i\vec{k}\vec{R}(m)] Q_{\vec{k}, j} \tag{6}$$

and

$$x_{\mu}^{(m)} = \sum_{\vec{k}, j} e_{\mu}(\vec{k}, j) \exp[i \vec{k} \vec{R}(m)] Q_{\vec{k}, j} \quad (7)$$

In a peculiar case the eigenvectors $e_{\mu}(\vec{k}, j)$ are the polarization vectors of phonons. In another simple case they characterize a contribution of one concentration plane wave (\vec{k}, j) into modulation of either a homogeneous distribution of atoms in the lattice or a homogeneous orientation of molecular groups. Generally, they are a mixture of all existing steps of freedom. We have also

$$e_{\mu}(-\vec{k}, j) = e_{\mu}^*(\vec{k}, j)$$

and

$$Q_{-\vec{k}, j} = Q_{\vec{k}, j}^*$$

The matrix of bare elastic constants can be also diagonalized. The relevant eigenvalue problem is

$$\sum_k c_{ik} \sigma_k(a) = c_a \sigma_i(a) \quad \text{for } a = 1, 2, \dots, 6. \quad (8)$$

The reducible representation of the six-component deformation vector can be written as a direct sum of the irreducible representations $\Gamma_a \oplus \Gamma_b \oplus \dots$. The six-component eigenvector $\vec{\sigma}(a)$ transforms according to one of the irreducible representation Γ_a . The eigenvectors $\sigma_i(a)$ are real and orthonormal. Again any V_i° static or v_i dynamic deformations can be expressed in terms of eigenvectors and corresponding normal amplitudes of the deformation, namely

$$\begin{aligned} V_i^{\circ} &= \sum_a \sigma_i(a) S_a \\ v_i &= \sum_a \sigma_i(a) s_a \end{aligned} \quad (9)$$

As a rule, the system becomes unstable with respect to a particular critical mode. In the homogeneous crystals the critical mode corresponds to a particular star of the

wave vectors $\{\vec{k}_c\}$ and irreducible representation of the little group of $\{\vec{k}_c\}$ which components are numbered by the index of the branches $\{j_c\}$ of normal modes. For one-dimensional irreducible representation $j_c = 1$, for two and three-dimensional one $j_c = 1, 2$ and $1, 2, 3$, respectively. The $\lambda_{\vec{k}_c, j_c}^{\vec{k}_c}$ for all \vec{k}_c and j_c are equal. The magnitudes of the displacements $X^{\circ}(\mu)$ are given by the amplitude $Q_{\vec{k}_c, j_c}$ of the active normal mode

$$X^{\circ}(\mu) = \sum_{\vec{k}_c, j_c} e_{\mu}(\vec{k}_c, j_c) \exp[i \vec{k}_c \vec{R}(m)] Q_{\vec{k}_c, j_c}$$

Now, on the basis of the expansions (6,7) and (9), the free energy (3) can be reformulated and expressed in terms of the amplitudes of normal modes and deformations. It can also be confined to the wave vectors from the critical star $\{\vec{k}_c\}$ and branches $\{j_c\}$ from the relevant irreducible representation. With the aim of the familiar procedure of completing the square we rearrange the expansion of the free energy and get eventually

$$\begin{aligned} F &= F(T, \{S_a\}, \{Q_{\vec{k}_c, j_c}\}) + \sum_a p_a s_a + \\ &+ \frac{1}{2} \sum_{\alpha\beta} [c_{\alpha} \delta_{\alpha\beta} + \sum_{j_c} K_{\alpha\beta}(\vec{k}_c, j_c) Q_{\vec{k}_c, j_c} - \\ &- \sum_{\vec{k}_c, j_c} \sum_{\vec{k}'_c, j'_c} N_{\alpha}(\vec{k}_c, j_c) M(\vec{k}_c, \vec{k}'_c) N_{\beta}(\vec{k}'_c, j'_c)] s_{\alpha} s_{\beta} + \\ &+ \frac{1}{2} \sum_{\vec{k}_c, j_c} \sum_{\vec{k}'_c, j'_c} R(\vec{k}_c, \vec{k}'_c) t_{\vec{k}_c, j_c} t_{\vec{k}'_c, j'_c} + \dots \end{aligned} \quad (10)$$

where

$$N_a(\vec{k}, j) = U_a(\vec{k}, j) + \sum_{\beta} K_{a\beta}(\vec{k}, j) S_{\beta} + \sum_{j'} L_a(\vec{k}, j, j') Q_{\vec{k}, j'} \quad (11)$$

$$R\left(\begin{matrix} \vec{k} & \vec{k}' \\ j & j' \end{matrix}\right) = \lambda_{\vec{k}, j} \delta_{\vec{k}, \vec{k}'} \delta_{j, j'} + \delta_{\vec{k}, \vec{k}'} \sum_{\alpha} L_{\alpha}(\vec{k}, j, j') S_{\alpha} + \frac{1}{2} \sum_{\substack{\vec{k}_1, \vec{k}_2 \\ j_1, j_2}} B\left(\begin{matrix} \vec{k} & \vec{k}' & \vec{k}_1 & \vec{k}_2 \\ j & j' & j_1 & j_2 \end{matrix}\right) \delta(\vec{k} + \vec{k}' + \vec{k}_1 + \vec{k}_2) Q_{\vec{k}_1, j_1} Q_{\vec{k}_2, j_2} \quad (12)$$

and

$$P_a = \sum_i \sigma_i(a) P_i$$

$$U_a(\vec{k}, j) = \delta_{\vec{k}, 0} \sum_{i\mu} U_i(\mu) e_{\mu}(\vec{k}, j) \sigma_i(a)$$

$$K_{a\beta}(\vec{k}, j) = \delta_{\vec{k}, 0} \sum_{ik\mu} K_{ik}(\mu) e_{\mu}(\vec{k}, j) \sigma_i(a) \sigma_k(\beta)$$

$$L_a(\vec{k}, j, j') = \sum_i \sum_{\mu\nu} \sigma_i(a) e_{\mu}(\vec{k}, j) \sum_n L_i(\mu, \nu) \times \exp[i\vec{k}(\vec{R}(m) + \vec{R}(n))] e_{\nu}(\vec{k}, j') \quad (13)$$

and

$$t_{\vec{k}_c, j_c} = q_{\vec{k}_c, j_c} + \sum_{\alpha} \sum_{\vec{k}'_c, j'_c} M\left(\begin{matrix} \vec{k}_c & \vec{k}'_c \\ j_c & j'_c \end{matrix}\right) N_{\alpha}(\vec{k}'_c, j'_c) S_{\alpha}$$

and

$$\sum_{\vec{k}'_c, j'_c} M\left(\begin{matrix} \vec{k} & \vec{k}'_c \\ j & j'_c \end{matrix}\right) R\left(\begin{matrix} \vec{k}'_c & \vec{k}'' \\ j & j'' \end{matrix}\right) = \delta_{\vec{k}, \vec{k}''} \delta_{j, j''} \quad (14)$$

The equilibrium value of the amplitudes S_{α} and $Q_{\vec{k}_c, j_c}$ can be found from the equilibrium equations (4) which now take the form

$$p_{\alpha} + c_{\alpha} S_{\alpha} + \sum_{\vec{k}_c, j_c} U_{\alpha}(\vec{k}_c, j_c) Q_{\vec{k}_c, j_c} + \sum_{\beta} \sum_{j_c} K_{\alpha\beta}(\vec{k}_c, j_c) Q_{\vec{k}_c, j_c} S_{\beta} + \frac{1}{2} \sum_{\vec{k}_c, j_c, j'_c} L_{\alpha}(\vec{k}_c, j_c, j'_c) Q_{\vec{k}_c, j_c} Q_{\vec{k}'_c, j'_c} = 0 \quad (15)$$

for $\alpha = 1, 2, \dots, 6$.

$$\sum_{\alpha} U_{\alpha}(\vec{k}_c, j_c) S_{\alpha} + \frac{1}{2} \sum_{\alpha\beta} K_{\alpha\beta}(\vec{k}_c, j_c) S_{\alpha} S_{\beta} +$$

$$+ \sum_{\vec{k}'_c, j'_c} \left[\frac{2}{3} \lambda_{\vec{k}_c, j_c} \delta_{\vec{k}_c, \vec{k}'_c} \delta_{j_c, j'_c} + \right.$$

$$\left. + \frac{2}{3} \delta_{\vec{k}_c, \vec{k}'_c} \sum_{\alpha} L_{\alpha}(\vec{k}_c, j_c, j'_c) S_{\alpha} + \frac{1}{3} R\left(\begin{matrix} \vec{k}_c & \vec{k}'_c \\ j_c & j'_c \end{matrix}\right) \right] Q_{\vec{k}'_c, j'_c} = 0. \quad (16)$$

To find the effective elastic constants \tilde{c}_{ik} we take the second derivative of the free energy with respect to the deformation. So

$$\tilde{c}_{ik} = \sum_{\alpha\beta} \sigma_i(a) c_{\alpha\beta} \sigma_k(\beta), \quad (17)$$

where

$$c_{\alpha\beta} = c_{\alpha} \delta_{\alpha\beta} + \sum_{j_c} K_{\alpha\beta}(\vec{k}_c, j_c) Q_{\vec{k}_c, j_c}$$

$$- \sum_{\vec{k}_c, j_c} \sum_{\vec{k}'_c, j'_c} N_a(\vec{k}_c, j_c) M \begin{pmatrix} \vec{k}_c & \vec{k}'_c \\ j_c & j'_c \end{pmatrix} N_\beta(\vec{k}'_c, j'_c). \quad (18)$$

Consider a crystal in an undeformed state and call it a high symmetry phase. In this state the static normal amplitudes of deformation and the normal mode amplitudes vanish, i.e., $S_a = 0$ ($a = 1, 2, \dots, 6$) and all $Q_{\vec{k}_c, j_c} = 0$. Under such circumstances the expansion of the free energy becomes much simpler, namely

$$F = F(T, \{0\}, \{0\}) + \sum_a p_a s_a + \\ + \frac{1}{2} \sum_a [c_a - \delta_{\vec{k}_c, 0} \frac{\sum_{j_c} [U_a(0, j_c)]^2}{\lambda_{\vec{k}_c, j_c}}] (s_a)^2 + \\ + \frac{1}{2} \lambda_{\vec{k}_c, j_c} \sum_{\vec{k}_c, j_c} (t_{\vec{k}_c, j_c})^2 + \dots \quad (19)$$

It might happen that the change of external conditions leads to an instability point where either $\lambda_{\vec{k}_c, j_c}$ vanishes for a particular mode (\vec{k}_c, j_c) or the effective elastic constant coefficient vanishes. Then generally speaking, the system deforms to a new phase of lower symmetry. The point of reconstruction of the crystal is called the phase transition point. It might occur that the instability point of the low symmetry phase coincides with the instability point of the high symmetry phase, then the phase transition is continuous. The expansion of the free energy (10) corresponds to that case. A majority of phase transitions is of the discontinuous type (first order), however, usually the departure from the continuity is not severe. Anyway, the reduction of the symmetry from the high symmetry phase to the low one is properly taken into account by a freezing of an active normal mode. This allows us to classify the change of elastic constants across the phase transition.

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