# Phase transitions of the displacement type in crystals at very low temperatures

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The problem of the low-temperature phase transition in cubic ferroelectrics is solved within the framework of the logarithmic theory. It is shown that a second-order transition changes into a first-order transition if the interaction anisotropy and the anisotropy of the critical oscillation spectrum are taken into account. In the extreme isotropic case and at T = 0, the dielectric susceptibility  $\chi$  is proportional to  $(p = -p_c) \ln^{25/51} | p - p_c |$ , and the correction to the compressibility is proportional to  $\ln^{1/51} | p - p_c |$ . A phase transition line on the p - T plane is plotted and the behavior of the crystals at finite temperatures is considered. It is shown that in the case of an impurity crystal, the impurity corrections obey a power law; in the vicinity of the transition point there are more logarithmic contributions from the anharmonic interaction.

### **1. INTRODUCTION**

Phase transitions of the displacement type, i.e., transitions associated with instability to optical vibrations, occur as a rule at high temperatures  $T \stackrel{>}{\sim} \omega_D$ . In the works of the authors<sup>[1]</sup> and Rechester,<sup>[2]</sup> the case of a low-temperature transition ( $T_c \ll \omega_D$ ) was discussed within the framework of self-consistent field theory. The self-consistent field approximation for transitions of the displacement type has a wide range of applicability, thanks to the smallness of the anharmonic constants, and is inapplicable only in the immediate vicinity of the transition point, where allowance for large classical fluctuations of the order parameter becomes important. At very low temperatures, moreover, there is an intermediate region in which it is necessary to take into account the quantum character of the fluctuations;<sup>[2]</sup> in the extreme case of a transition at zero temperature (T<sub>c</sub> = 0), there is no region of classical fluctuations at all, only quantum fluctuations. In this quantum region, the contribution of the fluctuations to the thermodynamic quantities increases as one approaches the transition point, not according to a power law but in logarithmic fashion. Thanks to this circumstance, the singularities of the thermodynamic quantities when  $T_c = 0$  can be found accurately.<sup>[2]</sup>

The analysis in the work of Rechester<sup>[2]</sup> was carried out within the framework of a simplified model. In the present work, we discuss the singularities that a transition at very low temperatures in real materials would possess. Account is taken of the effect of the anisotropy of four-phonon interaction and of the anisotropy of the spectra of transverse optical vibrations on the thermodynamics of the transition. The dependence of  $T_c$  on the pressure at very low temperatures is obtained.

We know of only one example of a transition of the displacement type for which  $T_c = 0$ , namely the alloy SnTe-GeTe. For substances of this type, consideration of the fluctuations of the impurity locations on the thermodynamics of the phase transition becomes important. Such fluctuations are always classical, and the corrections associated with them are power-law functions. Therefore, even in the case of small impurity concentrations, it is necessary to take these corrections into account, along with the logarithmic terms that are

due to the anharmonic interaction. In the present work we calculate the first nonvanishing corrections associated with the scattering of phonons by the impurities.

# 2. ACCOUNT OF BRANCH DEGENERACY AND ANISOTROPY

We write down the Hamiltonian of the crystal in the form

$$H = \frac{1}{2} \sum_{j,\mathbf{k}} [\xi_{j\mathbf{k}} \xi_{j-\mathbf{k}} + \omega_j^2(\mathbf{k}) \xi_{j\mathbf{k}} \xi_{j-\mathbf{k}}]$$
(1)  
+ 
$$\sum_{\substack{\mathbf{k}_1 + \dots + \mathbf{k}_n = 0 \\ j_1,\dots,j_n}} V_{j_1 k_2 j_1 k_1}^{(4)} (\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) \xi_{j_1 k_1} \xi_{j_2 k_2} \xi_{j_3 k_3} \xi_{j_4 k_4} + H_{imp}.$$

The Hamiltonian (1), in contrast with the model Hamiltonian of Rechester, <sup>[2]</sup> takes into account the anisotropy of the anharmonic interaction and the presence of optical vibrations with different polarizations, and also the scattering of critical phonons by impurities. In the Hamiltonian (1), terms are missing that describe the striction interaction of the critical phonons with the acoustic phonons. It is difficult to take into account the striction not only from purely computational considerations, but also in principle (the equations of the theory contain, besides logarithmic integrals, also integration with respect to the rapidly changing variable  $k^2/(k^2 + \omega^2)$ . Therefore we shall consider striction everywhere in what follows only in the first nonvanishing approximation.

The case that is most interesting for experiment will be investigated—the case of a cubic crystal in the symmetric phase. In such a crystal, the optical branch is triply degenerate in the polarization at  $\mathbf{k} = 0$ . For a ferroelectric crystal, because of the long-range dipoledipole interaction, the doubly degenerate branch of the transverse optical vibrations is critical. For  $\mathbf{k} \neq 0$ , the degeneracy is lifted because of the anisotropy. In the simplest case,  $\hat{\mathbf{v}} \ll \hat{\mathbf{s}} - \hat{\mathbf{a}}$  (see Appendix), the spectra take the form

$$\omega_{1,2}^{2} = \omega_{0}^{2} + s_{i}k^{2} + s_{a}k^{2}\Phi_{1,2}(n), \quad n = k/|k|.$$

It frequently turns out that  $s_0 \ll s_t$ .<sup>1)</sup> In this case one can regard the vibrations as degenerate and the Green's function of the transverse optical phonons can be written down in the form

$$G_{\alpha\beta}(\mathbf{k},\omega) = \frac{\delta_{\alpha\beta} - n_{\alpha}n_{\beta}}{\omega_{0}^{2} + s_{l}\mathbf{k}^{2} + \omega^{2}}$$

Moreover, the four-phonon anharmonic interaction  $b_{\alpha\beta\gamma\delta}$  has a complicated tensor structure, which leads to an intermingling of the phonon polarizations in the scattering. We consider the behavior of the crystal near the transition point with account of this circumstance, assuming  $s_a \ll s_t$ .

In the calculation of the graphs of perturbation theory for T = 0, a class of graphs can be separated for which the expansion parameter is not the small dimensionless constant of the four-phonon interaction  $\gamma = 3z^4b_{12}/2T^2s_t^{3/2}v_0^2$ , but the quantity

$$\gamma \ln \frac{\omega_D^2}{\max\{s_i \mathbf{k}^2, \omega_0^2\}}.$$

Near the transition point  $(\omega_0^2 \rightarrow 0)$  this parameter can turn out not to be small, and then it is necessary to sum the obtained infinite succession of terms of the perturbation-theory series. An examination of the graphs for the Green's function G(k) of the critical phonons shows<sup>[2,3]</sup> that the relevant corrections to the quantity  $G^{-1}(0)$  are of the order of  $[\gamma \ln (\omega_D^2/\omega_0^2)]^n$ . Corrections to  $G^{-1}(\mathbf{k}, \omega)$ , which depend on k and  $\omega$ , are proportional to  $\gamma \lfloor \gamma \ln (\omega_D^2/\omega_0^2) \rfloor^n$  and will not be taken into consideration. Therefore we can write down the Green's function in the form

$$G_{\alpha\beta}(\mathbf{k}, \omega) = \left(\delta_{\alpha\beta} - n_{\alpha}n_{\beta}\right) / \left(\Delta^2 + s_t \mathbf{k}^2 + \omega^2\right), \qquad (2)$$

where  $\Delta^2 = \omega_0^2 + \Sigma(\mathbf{k} = 0, \omega = 0)$ .

We consider the scattering amplitude of long-wave critical phonons by one another at T = 0. Summation of the principal graphs for the scattering amplitude leads to the well-known "parquet" equation,<sup>[4]</sup> which in our case is of the form

$$\Gamma_{\alpha\beta\gamma\delta}(k) = \gamma_{\alpha\beta\gamma\delta} - \int \frac{d^{4}q}{(2\pi)^{4}} G_{\mu\lambda}(q) G_{\nu\varphi}(q) [\Gamma_{\alpha\beta\mu\nu}(q) \Gamma_{\lambda\varphi\gamma\delta}(q) + \Gamma_{\alpha\beta\mu\nu}(q) \Gamma_{\lambda\beta\gamma\delta}(q) + \Gamma_{\alpha\beta\mu\nu}(q) \Gamma_{\lambda\varphi\gamma\delta}(q)].$$
(3)

The tensor structure of the scattering amplitude is determined by the equation

$$\Gamma_{\alpha\beta\gamma\delta} = \frac{1}{3}\Gamma_1(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) + \Gamma_2 g_{\alpha\beta\gamma\delta}, \qquad (4)$$

where  $g_{\alpha} \beta \gamma \delta = 1$  if  $\alpha = \beta = \gamma = \delta$ , and  $g_{\alpha} \beta \gamma \delta = 0$  in all the remaining cases. The amplitude  $\Gamma_2$  determines the degree of anisotropy of the anharmonic interaction of the phonons.

Substituting Eqs. (2) and (4) in Eq. (3), carrying out integration of the vector  $\mathbf{q}$  over the angles and transforming to the logarithmic variables

$$x = \ln \frac{\omega_D^2}{\max\{k^2, \Delta^2\}}, \qquad y = \ln \frac{\omega_D^2}{q^2},$$

we obtain the following set of equations:

$$\Gamma_{1}(x) = \gamma_{1} - \frac{1}{15} \int_{0}^{x} dy [34\Gamma_{1}^{2}(y) + 24\Gamma_{1}(y)\Gamma_{2}(y) + 3\Gamma_{2}^{2}(y)], \quad (5)$$

$$\Gamma_{2}(x) = \gamma_{2} - \frac{1}{15} \int_{0}^{x} dy [3\Gamma_{2}^{2}(y) + 4\Gamma_{1}(y)\Gamma_{2}(y)];$$

$$\gamma_{1} = \frac{3z^{4}b_{12}}{2\pi^{2}s_{1}^{\prime\prime}v_{0}^{2}}, \quad \gamma_{2} = \frac{z^{4}(b_{11} - 3b_{12})}{2\pi^{2}s_{1}^{\prime\prime}v_{0}^{2}}.$$

Here  $b_{11}$  and  $b_{12}$  are the coefficients of the Landau expansion:<sup>[1]</sup>

$$F(\mathbf{P}) = \frac{2\pi}{C} (T^2 - T_c^2) \mathbf{P}^2 + 3b_{12} \sum_{\alpha \neq \beta} P_{\alpha}^2 P_{\beta}^2 + b_{11} \sum_{\alpha} P_{\alpha}^4.$$

In order that the transition under discussion be a secondorder transition, it is necessary that the term of the Landau expansion proportional to  $p^4$  be positive. This is satisfied if

$$\Gamma_1 + \Gamma_2 > 0, \quad \Gamma_1 + \frac{1}{3}\Gamma_2 > 0. \tag{6}$$

Differentiating Eq. (5) with respect to x, we obtain the set of differential equations

$$\Gamma_{i}'(x) = -i_{1i5} [34\Gamma_{i}^{2}(x) + 24\Gamma_{i}(x)\Gamma_{2}(x) + 3\Gamma_{2}^{2}(x)], \Gamma_{2}'(x) = -i_{1i5} [3\Gamma_{2}^{2}(x) + 4\Gamma_{i}(x)\Gamma_{2}(x)]$$
(7)

with initial conditions

$$\Gamma_1(0) = \gamma_1, \quad \Gamma_2(0) = \gamma_2. \tag{8}$$

The right sides of Eqs. (7) are homogeneous polynomials of second order relative to  $\Gamma_1$  and  $\Gamma_2$ . It is therefore natural to seek a solution in the form

$$\Gamma_1(x) = \Psi(x) \Gamma_2(x). \tag{9}$$

Differentiating (9) and using (7), we get

$$\Psi' = -\frac{1}{5}\Gamma_2(2\Psi^2 + \Psi + 1).$$
 (10)

On the other hand,

$$\Psi + \Gamma_{z} \frac{d\Psi}{d\Gamma_{z}} = \frac{34\Psi^{2} + 24\Psi + 3}{28\Psi + 21}.$$
 (11)

The solution of Eq. (11) is of the form

$$\Gamma_{2} = \gamma_{2} \left[ \frac{(4\Psi + 1)^{2} + 7}{(4/\lambda + 1)^{2} + 7} \right]^{\gamma_{2}} \exp\left[ \frac{4\sqrt{7}}{3} \left( \operatorname{arctg} \frac{4\Psi + 1}{\sqrt{7}} - \operatorname{arctg} \frac{4/\lambda + 1}{\sqrt{7}} \right) \right],$$
(12)

where  $\lambda = \gamma_2/\gamma_1$ . Substituting (12) in Eq. (10), we obtain a closed equation for  $\Psi$ :

$$\Psi' = f(\Psi) = -\frac{\gamma_2 \left[ (4\Psi + 1)^2 + 7 \right]^{\frac{1}{3}}}{40 \left[ (4/\lambda + 1)^2 + 7 \right]^{\frac{7}{3}}} \exp\left[ \frac{4\sqrt{7}}{3} \left( \arctan \frac{4\Psi + 1}{\sqrt{7}} - \arctan \frac{4/\lambda + 1}{\sqrt{7}} \right) \right].$$
(13)

The function  $\Psi(\mathbf{x}) = \Gamma_1(\mathbf{x})/\Gamma_2(\mathbf{x})$  is large when the anisotropic part of the amplitude is small in comparison with the isotropic part and vanishes in the extreme anisotropic case.

The character of the solution of Eq. (13) can be made clear qualitatively. For this purpose, we turn our attention to the fact that the function  $f(\Psi)$  is negative at  $\gamma_2 > 0$  and  $\Psi(x)$  decreases monotonically, going to  $-\infty$ at

$$x_0 = \int_{1/\lambda}^{-\infty} \frac{d\Psi}{f(\Psi)}.$$

This integral converges for finite  $\gamma_2$ , and is of the form  $x_0 \sim \gamma_2^{-17/3} \rightarrow \infty$  as  $\gamma_2 \rightarrow 0$ . As  $x \rightarrow x_0$ ,

$$\Psi(x) \sim (x-x_0)^{-\omega/\mu}, \quad \Gamma_2(x) \sim (x-x_0)^{-\omega/\mu}, \quad \Gamma_1(x) \sim (x-x_0)^{-1}.$$
 (14)

The formulas (14) should be interpreted as proof that as  $x \rightarrow x_0$  the amplitudes  $\Gamma_1$  and  $\Gamma_2$  cease to be small and it is impossible to use equations of the type of (5). Thus, thanks to the presence of the anisotropy, the interaction does not tend to zero upon approach to the transition point, but, on the contrary, increases, going over into the strong coupling regime. Upon decrease of the anisotropy, the region of strong coupling narrows and vanishes at the limit  $\gamma_2 = 0$ .

It must be noted that at

$$x^{*} < x < x_{0}, \quad x^{*} = \int_{1/\lambda}^{-\gamma_{h}} \frac{d\Psi}{f(\Psi)},$$

the stability consistions  $\Psi \ge -\frac{1}{3}$  and  $\Gamma_1 + \Gamma_2 \ge 0$  are violated. This converts the second-order transition into a first-order transition. The case  $\gamma_2 \le 0$  is considered similarly. For

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$$x \to x_0 = \int_{1/\lambda}^{\infty} \frac{d\Psi}{f(\Psi)}$$

 $\Psi(x) \sim (x_0 - x)^{-1/1}, \quad \Gamma_2(x) \sim -(x - x_0)^{-11/1}, \quad \Gamma_1(x) \sim (x - x_0)^{-1}.$ 

In this case, too, at

$$< x < x_0, \quad x^* = \int_{1/\lambda}^{-1} \frac{d\Psi}{f(\Psi)},$$

the stability conditions

x

 $\Psi < -1, \quad \Gamma_1 + \Gamma_2 > 0$ 

are violated.

# 3. ACCOUNT OF BRANCH DEGENERACY IN THE ISOTROPIC CASE

We consider the extreme isotropic case  $\gamma_2 = 0$ . Then

$$\Gamma_{i}(x) = \Gamma(x) = \frac{\gamma}{1 + \frac{3i}{15}\gamma x}, \quad \Gamma_{2}(x) = 0. \quad (15)$$

For the calculation of the susceptibility and compressibility, we find the effective three-prong diagram  $\mathcal{T}$ , which obeys the equation<sup>[5]</sup>

$$\mathcal{F}_{\alpha\beta}(k) = \delta_{\alpha\beta} + i Y_{\alpha\beta} - \int \frac{d^4 q}{(2\pi)^4} \mathcal{F}_{\mu\nu}(q) \Gamma_{\lambda\varphi\alpha\beta}(q) G_{\mu\lambda}(q) G_{\nu\varphi}(q).$$
(16)

Here  $Y_{\alpha\beta}$  is a summetric tensor with zero trace, |1| = 1.

Resolving the tensor  $\mathscr{T}_{\alpha\,\beta}$  into the irreducible components

$$\mathcal{T}_{\alpha\beta} = \mathcal{T}_{1}\delta_{\alpha\beta} + \mathcal{T}_{2}\mathbf{I}\mathbf{Y}_{\alpha\beta}$$

carrying out the integration in (16) over the angles, and transforming to logarithmic variables, we obtain the equations for  $\mathcal{T}_1$  and  $\mathcal{T}_2$ :

$$\mathcal{F}_{1}(x) = 1 - {}^{10}/_{0} \int_{0}^{x} dy \mathcal{F}_{1}(y) \Gamma(y), \quad \mathcal{F}_{2}(x) = 1 - {}^{14}/_{15} \int_{0}^{x} dy \mathcal{F}_{2}(y) \Gamma(y),$$

the solutions of which have the form

$$\mathcal{T}_{1}(x) = (1 + \frac{34}{15}\gamma x)^{-15} \gamma_{15}, \quad \mathcal{T}_{2}(x) = (1 + \frac{34}{15}\gamma x)^{-1} \gamma_{15}. \quad (17)$$

The polarization operators are calculated in similar fashion: [5]

$$\Pi_{1}(x) \sim \int_{0}^{1} dy \mathcal{F}_{1}^{2}(y) \sim \gamma^{-1} [(1 + \frac{34}{15} \gamma x)^{\frac{1}{3}} - 1],$$

$$\Pi_{2}(x) \sim \int_{0}^{\pi} dy \mathcal{F}_{2}^{2}(y) \sim \gamma^{-1} [(1 + \frac{34}{15} \gamma x)^{\frac{31}{3}} - 1].$$
(18)

In the zero-temperature case under consideration, the transition can occur, for example, upon change of pressure, since the limiting frequency  $\omega_0$  depends on the pressure according to the formula<sup>[1]</sup>

$$\omega_0^2(p) = \omega_0^2(0) + \sigma p,$$

$$\sigma = \frac{2z^2}{3K\nu_0} (3q_{12} + 2q_{44} + q_0).$$
(19)

The transition takes place at  $p = p_c$ , when  $\Delta^2(\omega_0^2)$  vanishes. Using the Ward identity

$$\partial G^{-1} / \partial \omega_0^2 = \mathcal{T}_1$$

and Eq. (17), we obtain

$$\Delta^{2} = G^{-1}(0) = \sigma(p - p_{c}) \left[ 1 + \frac{34}{15} \gamma \ln \frac{\omega_{p}^{2}}{\sigma(p - p_{c})} \right]^{-16/\mu}$$
(20)

The dielectric susceptibility at zero temperature is determined as a function of the pressure by the relation

$$\chi_{\alpha\beta}(p-p_c) = \delta_{\alpha\beta} \frac{\lambda}{4\pi\Delta^2} = \delta_{\alpha\beta} \frac{\lambda}{4\pi\sigma(p-p_c)} \left[ 1 + \frac{34}{15} \gamma \ln \frac{\omega_p}{\sigma(p-p_c)} \right]^{\pi/s_c}$$
(21)

The fluctuation corrections to the modulus of hydrostatic compression 1/K and to the shear modulus  $1/\mu$ are proportional <sup>[2,5]</sup> to the respective polarization operators  $\Pi_1$  and  $\Pi_2$ :

$$\frac{1}{K} - \frac{1}{K_0} \infty \frac{1}{\gamma} \left[ \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_D^2}{\sigma(p - p_c)} \right)^{1/\mu} - 1 \right], \\ \frac{1}{\mu} - \frac{1}{\mu_0} \infty \frac{1}{\gamma} \left[ \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_D^2}{\sigma(p - p_c)} \right)^{1/\mu} - 1 \right].$$
(22)

The dependence of the spontaneous moment P on  $p - p_C$  in the unsymmetric phase is given by the expression <sup>[2,3]</sup>

$$\mathbf{P}^{2} = -\frac{\lambda}{32\pi^{2}s_{t}^{s_{t}^{s}}}\frac{\Delta^{2}}{\Gamma} = \frac{\lambda}{32\pi^{2}s_{t}^{s_{t}^{s}}}\frac{\sigma |p-p_{c}|}{\gamma} \left[1 + \frac{34}{15}\gamma \ln \frac{\omega_{D}^{2}}{\sigma |p-p_{c}|}\right]^{s_{t}^{s}/s}.$$
(23)

Thus, even in the isotropic case, allowance for the multi-component character of the order parameter strongly affects the form of the singularities of the thermodynamic functions. Thus, in the first of the formulas of (22) we get  $\ln^{1/51} |p - p_c|$  as against  $\ln^{1/3} |p - p_c|$ , which was obtained by Rechester.<sup>[2]</sup> It is also interesting that the multicomponent character, which is connected with the double degeneracy of the transverse optical branch, reduces neither to the four-dimensional model of Heisenberg nor to the four-dimensional model of plane rotators.<sup>[3]</sup>

# 4. THERMODYNAMICS NEAR THE PHASE TRANSITION LINE

The previous preceding analysis pertained to the case of a pressure transition in an isotropic crystal at T = 0. We now consider the region of lower  $(\gamma \ln (\omega_D^2/T^2) \gtrsim 1)$  but finite temperatures. At finite temperatures, all the integrals over the frequencies should be replaced by Matsubara sums. A typical expression which we must compute is of the form

$$J = T \sum_{\substack{n \\ n}} \int \frac{d^{3}k}{(2\pi)^{3}} \frac{1}{(\omega_{n}^{2} + \Delta_{0}^{2} + s_{l}k^{2})^{2}}$$

In the region  $T \gg \Delta_0$  it is necessary to separate in this sum a term with n = 0, corresponding to classical fluctuations, and the remaining sum must be replaced by an integral. As a result we get

$$J(T, \Delta_{0}) = \begin{cases} \frac{1}{8\pi s_{t}^{*'}} \left(\frac{T}{\Delta_{0}} + \frac{1}{2\pi} \ln \frac{\omega_{D}^{2}}{T^{2}}\right) & T \gg \Delta_{0} \\ \frac{1}{32\pi^{2} s_{t}^{*'}} \ln \frac{\omega_{D}^{2}}{\Delta_{0}^{2}} + \frac{1}{64} \left[\frac{2T}{\pi^{3} s_{t}^{3} \Delta_{0}}\right]^{*''} \exp\left(-\frac{\Delta_{0}}{T}\right), & T \ll \Delta_{0} \end{cases}$$
(24)

The region of small T and not too small  $\Delta_0$  will be considered (such that the power-law term in Eq. (24) can be neglected in comparison with the logarithmic term.

The phase-transition line is determined by the expression

$$\Delta^{2}(T_{c}) = \Delta_{0}^{2} + \Sigma (k = 0; T_{c}) - \Sigma (k = 0; T = 0) = 0.$$
 (25)

Therefore, to determine the phase-transition line it is necessary to calculate the temperature contribution  $\delta\Sigma(T) = \Sigma(T) - \Sigma(0)$  to the phonon self-energy. The change in the self energy is connected with the change in the exact Green's functions by the relation<sup>[6]</sup>

$$\frac{\delta\Sigma(k)}{\delta G(q)} = \frac{1}{2} \tilde{\Gamma}(k,q), \qquad (26)$$

where  $\hat{\Gamma}(k, q)$  is the sum of four-prong graphs, that are irreducible over the two-particle section separating the momenta k, k and q, q.

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When using Eq. (26), it is necessary to keep in mind that the exact Green's function itself contains a dependence on  $\delta\Sigma$ . The equation obtained for  $\delta\Sigma^{[2]}$  is therefore equivalent to the well-known equation<sup>[7]</sup> for the total amplitude  $\Gamma$  in terms of the irreducible amplitude  $\widetilde{\Gamma}$ . The final result takes the form

$$\delta\Sigma(k=0,T) = \frac{80}{3} \pi^2 s_t^{3/2} \Gamma(x) \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \left[ T \sum_{\substack{\mathbf{o} \\ \mathbf{n}}} -\int \frac{d\omega}{2\pi} \right] G(q; T=0),$$

$$x = \ln \frac{\omega_D^2}{\max\left\{ \Delta_{\mathbf{o}}^2, T^2 \right\}}.$$
(27)

The expression (27) can also be obtained by variation of the self-energy  $\Sigma$  with respect to the Green's function at T = 0. Therefore the answer contains only the difference between the sum over the frequencies and the integral of this Green's function:

$$\begin{bmatrix} T \sum_{a,n} -\int \frac{d\omega}{2\pi} \end{bmatrix} \int \frac{d^{3}\mathbf{q}}{(2\pi)^{3}} G(q; T=0)$$

$$= \frac{1}{(2\pi)^{3}} \int \frac{d^{3}\mathbf{q}}{2(\Delta_{0}^{2} + s_{i}\mathbf{q}^{2})^{\frac{1}{2}}} \left[ \operatorname{cth} \frac{(\Delta_{0}^{2} + s_{i}\mathbf{q}^{2})^{\frac{1}{2}}}{2T} - 1 \right].$$
(28)

Finally, we have

$$\delta \Sigma(T) = \begin{cases} \frac{20}{9} \pi^2 \frac{\gamma T^2}{1 + {}^{34}/{}_{15}\gamma \ln(\omega_p{}^2/T^2)}, & T \gg \Delta_0 \\ \frac{20}{3} \sqrt{2\pi} \frac{\gamma \Delta^{3h} T^{3/2}}{1 + {}^{34}/{}_{15}\gamma \ln(\omega_p{}^2/\Delta_0{}^2)} \exp\left(-\frac{\Delta_0}{T}\right), & T \ll \Delta_0 \end{cases}$$
(29)

Using Eq. (25) and the well-known dependence (20) of  $\Delta_0^2$  on the pressure, and recalling that  $T_C \gg \Delta_0$  when  $\gamma \ll 1$ , we find the phase transition curve on the p-T plane:

$$T_{c}^{2} = \frac{9\sigma}{20\pi^{2}\gamma}(p_{c}-p)\left[1 + \frac{34}{15}\gamma \ln \frac{\omega_{p}^{2}}{\sigma|p-p_{c}|}\right]^{3t/s}.$$
 (30)

In obtaining Eq. (30), we have neglected small quantities of the order  $\gamma \ln \gamma$ .

The non-analytic character of  $T_c$  as a function of  $p - p_c$  leads to the result that the formulas for the thermodynamic quantities, as functions of  $p - p_c$  at T = 0 and as functions of T for  $p = p_c$ , contain various powers of the logarithms. Thus, for example,

$$\chi(T) = \frac{C}{4\pi (T^2 - T_c^2)} \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_D^2}{T_c^2} \right), \quad T > T_c, \quad (31)$$

and the "half-law" is satisfied, i.e., the susceptibility below the transition is one-half the value in the symmetric phase for the same values of  $|T^2 - T_c^2|$ .<sup>[3]</sup> The spontaneous moment as  $T_c^2 - T^2 \rightarrow +0$  falls off as

$$\mathbf{P}^{2} = \frac{5}{18} \frac{\lambda}{4\pi s_{t}^{3/2}} (T_{c}^{2} - T^{2}).$$
 (32)

The specific heat and the thermal expansion at low temperatures ( $\omega_D \gg T > T_c \gg \Delta_0$ ) are expressed in terms of the spectrum of quasiparticles at T = 0. By a method similar to that set forth in<sup>[6]</sup>, we get the following expression for the entropy per unit volume:

$$\frac{S(p,T)}{V} = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left[ \frac{\omega(\mathbf{k})}{T} n_{\omega(k)} - \ln(1 - e^{-\omega(k)/T}) \right],$$

$$n_{\omega} = (e^{\omega/T} - 1)^{-1}, \quad \omega^2(\mathbf{k}) = \Delta_0^2(p) + s_i \mathbf{k}^2.$$
(33)

Differentiating the entropy with respect to the temperature, we get for the specific heat C

$$C = \frac{2\pi^2}{15} \left( a_t^{-3/4} + 2a_t^{-3/4} + 2s_t^{-3/2} \right) T^3 V.$$
 (34)

The first two terms correspond here to the Debye contribution to the specific heat of the acoustical phonons, which was not included in (33), and the last term corresponds to the contribution of the critical phonons. If no transition occurs down to T = 0, then the contribution of the critical oscillations at  $T \ll \Delta_0$  contains the factor exp(= $\Delta_0/T$ ). If the transition takes place at finite temperatures, then there is an additional contribution to the specific heat below the transition point, associated with the temperature dependence of the polarization P(T). Therefore there is a jump in the specific heat at the transition point:

$$\Delta C = \left(\frac{10\pi}{9}\right)^2 \frac{VT_c^3}{s_i^{3/2}}, \frac{\gamma}{1 + {}^{34}/_{15}\gamma \ln\left(\omega_D^2/T_c^2\right)},$$

which falls off to zero as  $T_C \rightarrow 0$ . Below the transition point, when  $T \ll |\Delta_0|$ , the main contribution to the specific heat of the nonsymmetric phase is made by the Debye term, while the exponentially small contribution of the critical phonons can be neglected.

The thermal expansion coefficient  $\alpha$  can be obtained from (33) if we use the thermodynamic identity

$$(\partial V / \partial T)_p = -(\partial S / \partial p)_T.$$

As a result

$$\alpha(T) = \frac{1}{V} \frac{\partial V}{\partial T} = \frac{\sigma T}{12s^{3/2}} \left[ 1 + \frac{34}{15} \gamma \ln \frac{\omega_D^2}{\sigma(p - p_c)} \right]^{-\pi/s}.$$
 (35)

For  $T \gg \Delta_0$ , the numerical term is the principal one, and for  $T \ll \Delta_0$ , the thermal expansion is determined by the Debye term,<sup>[8]</sup> which is proportional to  $T^3$ . For  $p = p_c$ , the coefficient in the term of (35) that is linear in T vanishes. Therefore, for  $\Delta_0 = 0$  and  $T \rightarrow T_c$  $= 0^{[8]}$ 

$$\alpha(T) \sim T^3, \quad C_p - C_v \sim T^7.$$

As is seen from the above formulas, the quantum fluctuations do not change the results qualitatively at finite temperatures; these results were obtained in the self-consistent field approximation, and their account leads only to the additional temperature dependence of the phenomenological constants of the Landau expansion. The latter now takes the form

$$F(T, \mathbf{P}) = F(T_c) + \frac{2\pi}{C} \frac{(T^2 - T_c^2)}{1 + \frac{34}{15\gamma} \ln(\omega_D^2/T_c^2)} \mathbf{P}^1 + \frac{3b_{12}}{1 + \frac{34}{15\gamma} \ln(\omega_D^2/T_c^2)} \mathbf{P}^4.$$
(36)

Such a situation is connected with the ignoring of the classical fluctuations of the thermodynamic quantities, which are important in the immediate vicinity of the transition. The relative value of the classical terms has the order of  $\gamma T_C /\Delta(T)$ , i.e., with allowance for (25) and (29), is of the order

$$\frac{3}{2\pi} \left[ \frac{\gamma T_{\circ}}{10(T-T_{\circ})} \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_D^2}{T_{\circ}^2} \right) \right]^{1/2}$$

Thus the thermodynamic functions may have singularities, but the coefficient in front of the anomalous part, i.e., the specific heat, depends itself on  $T_c$  and vanishes when  $T_c = 0$ .

### 5. ACCOUNT OF SCATTERING BY IMPURITIES

The scattering of phonons by impurities takes place because the mass of the impurity differs from the mass of the atom of the matrix, and the impurity atoms and the matrix interact differently than the atoms of the pure substance. The difference in the masses leads to a difference in the kinetic energy and therefore the associated scattering is proportional to the square of the phonon frequency  $\omega^2$ . In the static limit ( $\omega = 0$ ) the scattering as a whole is due to the difference in the force constants. For the case discussed below, of the scattering of longwave critical phonons, the scattering amplitude can be assumed to be independent of the momenta. Therefore, the impurity part of the Hamiltonian is of the form  $^{[\mathfrak{s},\mathfrak{g}]}$ 

$$H_{i_{mp}} = \frac{1}{2} \zeta \sum_{\mathbf{k},\mathbf{k}'} [\langle \omega^2 \rangle - \omega^2(\mathbf{k}) - \omega^2(\mathbf{k}')] \xi_{\mathbf{k}} \xi_{\mathbf{k}'} \frac{1}{N} \sum_{a} e^{i(\mathbf{k}+\mathbf{k}')\mathbf{R}_a}.$$
 (37)

Here  $\langle \omega^2 \rangle \sim \omega_D^2$  is the mean squared frequency over the unperturbed spectrum. The dimensionless amplitude  $\xi$  is assumed small for simplicity ( $\xi \ll 1$ ) and only the first nonvanishing  $\xi$  terms will be taken into account.

By calculating the corresponding quantities for fixed positions of the impurities and then averaging the result over all possible positions, we can arrive at the standard impurity diagram technique.<sup>[6]</sup> Typical diagrams for the Green's function are shown below.



The contribution of graph a to the self-energy  $\Sigma$  is proportional to  $n\zeta$  (n is the impurity concentration) and leads to a shift in the transition point. The contribution of graph c, which is proportional to  $n\zeta^2$ , can be neglected along with the contribution of graph b:

$$\Sigma^{\flat}(\mathbf{k},\omega) = n\zeta^{2}v_{\flat}\int \frac{d^{2}\mathbf{k}'}{(2\pi)^{2}} [\langle \omega^{2} \rangle - \omega^{2}(\mathbf{k}) - \omega^{2}(\mathbf{k}')]^{2}G(\mathbf{k}',\omega).$$
(38)

The region of large k' is important in the interval, and we can assume  $\omega_0 = 0$  in the calculation of the principal term. Such a term is not dependent on  $\omega_0$ , just as the contribution of graph a, and leads only to a displacement of the transition point. The dependence on  $\omega_0$  is expressed by the graph for the three-prong amplitude:



It is then seen that allowance for impurities leads to terms that increase as  $\omega_0 \rightarrow 0$  according to a power law. The vicinity of the phase transition point will be considered, in which these terms are small and there is no necessity of taking into account the more complicated graphs of type d.

The correlation corrections due to the impurities are proportional to n and are small at small concentrations. However, because of their power-law growth, these corrections turn out, sufficiently close to the transition point, to be comparable with the logarithmic contribution of the anharmonic interaction. The scattering by the impurities is an effect of the harmonic approximation. Therefore, the smallness of the impurity corrections is due only with the smallness of the concentration and, perhaps, with the numerical smallness of the amplitude  $\zeta$ . The corrections from the interaction of the phonons with one another, which are proportional to  $\gamma \ln (\omega_D^2/\omega_0^2)$ , contain the small constant  $\gamma$  of the anharmonic interaction. Therefore, if the impurity concentration is not too small, then the contribution of the impurity corrections becomes equal to the logarithmic contribution even at  $\gamma \ln (\omega_D^2/\omega_0^2) \ll 1$ . Then the region of applicability of the logarithmic formulas considered above is completely absent. In the case of small concentrations, there is a region of applicability of these formulas, but in the immediate vicinity of the

transition point the impurity terms again turn out to be important. We shall show how to compute the first impurity corrections without assuming smallness of the anharmonic terms.

For example, we consider the graphs for the threeprong diagram  $\mathcal{F}_1$ . Inserting dashed lines in the parquet diagram, we can establish the fact that those graphs give the highest power of the logarithm in which the dashes connect lines with close momenta. Moreover, in the case in which the dashes connect external lines, the power of the logarithm is one unit higher than in all the other cases. Therefore, we have for the impurity correction to the three-prong diagram



Similarly, the scattering amplitude is

$$\Gamma = \frac{\gamma}{1 + {}^{34}/_{15}\gamma \ln(\omega_{D}^{2}/\Delta_{0}^{2})} \left[ 1 - \frac{6\eta}{\Delta_{0}} \left( 1 + \frac{34}{15}\gamma \ln\frac{\omega_{D}^{2}}{\Delta_{0}^{2}} \right)^{-50/41} \right].$$
(40)

Graphs for the polarization operator  $\Pi_1$  do not have external ends and the principal logarithmic contribution will develop when the dashes connect lines with close momenta. In the multiple integrals obtained in this case, the principal logarithmic region is that in which the dashes connect lines with very small momenta. Combining graphs with all possible dashed insertions of the types shown, we obtain a graphic expression of the Sudakov type for  $\delta \Pi_1$ :



$$\Pi_{1} \sim \frac{1}{\gamma} \left\{ \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_{p}^{2}}{\Delta_{0}^{2}} \right)^{\frac{\gamma}{\alpha}} \left[ 1 - \frac{\gamma \eta}{\Delta_{0}} \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_{p}^{2}}{\Delta_{0}^{2}} \right)^{\frac{\omega}{\alpha}} \right] = 1 \right\}.$$
(41)

Calculating the physical quantities, we get, for T = 0,

$$\Delta_{o}^{2} = \sigma(p - p_{c}) \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_{D}^{2}}{\sigma(p - p_{c})} \right)^{-15/10} \times \left[ 1 - \frac{\eta}{[\sigma(p - p_{c})]^{\frac{1}{7}}} \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_{D}^{2}}{\sigma(p - p_{c})} \right)^{-15/102} \right],$$
(42)

$$\chi = \frac{\lambda}{4\pi\sigma(p-p_c)} \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_D^2}{\sigma(p-p_c)} \right)^{\frac{3}{2}} \left( 1 + \frac{\eta}{[\sigma(p-p_c)]^{\frac{1}{2}}} \left( 1 + \frac{34}{15} \gamma \ln \frac{\omega_D^2}{\sigma(p-p_c)} \right)^{-\frac{n}{2}} \right),$$
(43)

$$\mathbf{P}^{2} = \frac{\lambda \sigma (p - p_{c})}{32\pi^{2} \gamma s_{i}^{\nu_{c}}} \left(1 + \frac{34}{15} \gamma \ln \frac{\omega_{p}^{2}}{\sigma (p - p_{c})}\right)^{s_{i}} \left[1 + \frac{5\eta}{[\sigma (p - p_{c})]^{\nu_{h}}} \times \left(1 + \frac{34}{15} \gamma \ln \frac{\omega_{p}^{2}}{\sigma (p - p_{c})}\right)^{-n_{i}}\right].$$
(44)

For finite temperatures, the line of phase transitions is determined by the relation

$$T_{c}^{2} = \frac{9}{20\pi^{2}} \frac{\sigma(p-p_{c})}{\gamma} \left(1 + \frac{34}{15} \gamma \ln \frac{\omega_{D}^{2}}{\sigma(p-p_{c})}\right)^{\pi/s_{1}} \\ \times \left[1 + \frac{5\eta}{[\sigma(p-p_{c})]^{\frac{1}{2}}} \left(1 + \frac{34}{15} \gamma \ln \frac{\omega_{D}^{2}}{\sigma(p-p_{c})}\right)^{-\pi/s_{2}}\right] \\ \chi(T) = \frac{C}{4\pi(T^{2} - T_{c}^{2})} \left(1 + \frac{34}{15} \gamma \ln \frac{\omega_{D}^{2}}{T_{c}^{2}}\right) \\ \times \left[1 + 6\eta \left(\frac{C}{\lambda(T^{2} - T_{c}^{2})}\right)^{\frac{1}{2}} \left(1 + \frac{34}{15} \gamma \ln \frac{\omega_{D}^{2}}{T_{c}^{2}}\right)^{-\pi/s_{1}}\right] \\ P^{2}(T) = \frac{5}{18} \frac{\lambda}{4\pi s^{\frac{3}{2}}} (T_{c}^{2} - T^{2}).$$
(45)

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# 6. CONCLUSION

We know of only a single case of a phase transition at T = 0, namely, the alloy SnTe-GeTe. Using the experimental data of<sup>[10]</sup> for the concentration dependence of  $T_C$  at high temperatures and Eq. (47) from our previous work,<sup>[1]</sup> we can estimate the alloy concentration  $n_C$ for which T = 0 ( $n_C \approx 4-5\%$ ). From these data, we can estimate the amplitude  $\zeta$  ( $\zeta \approx 0.5$ ). Since  $\zeta$  is not very small, the formulas of Sec. 5 must be understood as tentative estimates. Recognizing that the anharmonic constant is very small ( $\gamma \approx 2 \times 10^{-2}$ ), we must expect that the impurity contribution exceeds the logarithmic contribution from the interaction even in the region of applicability of the self-consistent field.

If pure substances with low  $T_c$  become known, it will be necessary to take into account the anisotropy of the four-phonon interaction and striction, leading to a first-order transition. If the striction and the anisotropy are small, so that they can be neglected at a sufficient distance from the transition point, then it will be necessary in every case to take into account the degeneracy of the critical branch in the direction of polarization. As was shown in Sec. 3, such an account leads to a significant change in the power of the logarithms in comparison with the results of Rechester.

Summing up, we can say that real observation of such low-temperature transitions is extremely difficult because of the exponentially small required temperatures. Even if one succeeds in carrying out the measurements at such a low temperature, many factors (anisotropy, impurity, striction) can distort the picture of the phenomenon so that it will not be described by the logarithmic theory. It would be all the more interesting to observe a transition described by such a theory.

### **APPENDIX**

In the case of a polar cubic crystal, the harmonic Hamiltonian is of the form [11,12]

$$H_{0} = \frac{1}{2} \sum_{\mathbf{k}} \left[ M \dot{\mathbf{u}}_{\mathbf{k}} \dot{\mathbf{u}}_{-\mathbf{k}} + \mathbf{u}_{\mathbf{k}} \hat{A} \mathbf{u}_{-\mathbf{k}} + \dot{\mathbf{x}}_{\mathbf{k}} \dot{\mathbf{x}}_{-\mathbf{k}} + \omega_{0}^{3} \mathbf{x}_{\mathbf{k}} \mathbf{x}_{-\mathbf{k}} \right. \\ \left. + \mathbf{x}_{\mathbf{k}} \hat{S} \mathbf{x}_{-\mathbf{k}} + 2 \mathbf{u}_{\mathbf{k}} \hat{V} \mathbf{x}_{-\mathbf{k}} + \frac{v_{0}}{4\pi} \mathbf{E}_{\mathbf{k}} \mathbf{E}_{-\mathbf{k}} - 2 z \mathbf{x}_{\mathbf{k}} \mathbf{E}_{-\mathbf{k}} \right].$$
(A.1)

Here

$$\hat{A} = Mk^{*}(a_{i}\hat{g}_{i} + a_{t}\hat{g}_{i} + a_{a}\hat{g}_{a}), 
\hat{S} = k^{2}(s_{i}\hat{g}_{i} + s_{i}\hat{g}_{i} + s_{a}\hat{g}_{a}), 
\hat{V} = M^{\prime h}k^{2}(v_{i}\hat{g}_{i} + v_{i}\hat{g}_{i} + v_{a}\hat{g}_{b}); 
g_{i}^{ab} = n_{a}n_{b}, \quad g_{i}^{ab} = \delta_{ab} - n_{a}n_{b}, \quad g_{a}^{ab} = g_{abyb}n_{y}n_{b};$$
(A.2)

the variables u and x denote displacements associated with the acoustic and critical oscillations, respectively, z is the effective change of the ions,  $v_0$  the cell volume, and n = k/|k|.

After the electric field is turned off, a large gap  $\lambda = 4\pi z^2/v_0$  appears in the spectrum of the longitudinal optical oscillations. The quantities u and x are normal oscillations only for small  $k \ll \omega_0 a^{-1/2}$ . For large k, intermingling of the branches takes place. Thus, for k parallel to the principal axes, the frequencies of the transverse vibrations are (see<sup>[11,12]</sup>)

$$\omega_{c,a}^{2}(k) = \frac{1}{2} \{ \omega_{0}^{2} + (s_{t} + a_{t}) k^{2} \pm [(\omega_{0}^{2} + (s_{t} - a_{t}) k^{2})^{2} + 4v_{t}k^{2}]^{\frac{1}{2}} \},$$

and each of the branches is doubly degenerate. For arbitrary directions of k, there are five mutually intermingled branches.

In the case  $\hat{V}^{z} \ll (\hat{A} - \hat{S})^{2}$ , which is realized for example, in BaTiO<sub>3</sub>,<sup>[13]</sup> the intermingled acoustic and

optical branches can be neglected. The frequency of the critical oscillations in this case is of the form

$$\begin{split} & \begin{array}{l} & & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ \phi\left(n\right) = n_{1}^{2}n_{2}^{2} + n_{2}^{2}n_{3}^{2} + n_{3}^{2}n_{1}^{2}, \\ & & \\ \end{array} \left( \begin{array}{l} & & \\ & & \\ & & \\ \end{array} \right) = n_{1}^{2}n_{2}^{2} + n_{2}^{2}n_{3}^{2} + n_{3}^{2}n_{1}^{2}, \\ & & \\ & & \\ & & \\ \end{array} \left( \begin{array}{l} & & \\ & & \\ & & \\ & & \\ \end{array} \right) \end{split} \right)$$

The logarithmic character of the correlation corrections is preserved also in a theory that takes into account the intermingling of the branches and the anisotropy of the spectra. However, the coefficients in the corresponding parquet equations are complicated angular integrals. For simplicity, we limit ourselves to small  $\hat{V}^2 \ll (\hat{A} - \hat{S})^2$ . Here the coefficients of the equations are functions of the ratio  $s_a/s_t$ .

The case  $s_a \ll s_t$  was considered above. We now discuss the case  $s_a \gg s_t$ . First, integration can be carried out over the frequency  $\omega$  and the modulus  $|\mathbf{k}|$ , which gives the corresponding logarithm. The coefficient of the logarithm is proportional to  $s^{-3/2}(n)$ . For arbitrary direction of n,  $s(n) \sim s_a$  and for n lying in the planes  $n_i = 0$ , one of the branches has  $s_1(n) \sim s_a$ and the other  $s_2(n) \sim s_t \ll s_a$ . Therefore, in carrying out integration over the angles, the principal contributions are made by the range of directions of n close to such planes, and the component in the Green's function corresponding to  $s_2(n)$ . The polarization of the corresponding oscillations is perpendicular to the given planes. Thus in the range of directions of n close to the plane  $n_i = 0$ ,

$$G_{\alpha\beta}(\mathbf{k},\omega) = \frac{\delta_{\alphai}\,\delta_{\beta\mu}}{\omega^2 + \Delta^2 + k^2(s_i + \frac{3}{2}s_an_i^2)}.$$
 (A.4)

The angular integrals that are developed are of the form

$$\int \frac{d\Omega}{(s_t + \frac{3}{2} s_s n_t^2)^{\frac{3}{2}}} = \sqrt{\frac{2}{3}} \frac{4\pi}{s_t s_a^{\frac{1}{2}}}.$$
 (A.5)

With account of what has been shown, the parquet equations take the form

$$\Gamma_{\alpha\beta\gamma\delta}(x) = \gamma_{\alpha\beta\gamma\delta}^{\dagger} - \int_{0}^{t} dy \sum_{i=1}^{3} \left[ \Gamma_{\alpha\betaii}(y) \Gamma_{ii\gamma\delta}(y) + \Gamma_{ii\gamma\delta}(y) + \Gamma_{ii\gamma\delta}(y) \right]$$
(A.6)

 $+ \Gamma_{\alpha i \gamma i}(y) \Gamma_{i \beta i \delta}(y) + \Gamma_{\alpha \delta i i}(y) \Gamma_{i i \gamma \beta}(y) ].$ 

Using Eq. (4) for the tensor structure of  $\Gamma$  and differentiating (A.6) with respect to the upper limit, we obtain

$$\Gamma_{i}'(x) = -\frac{i}{3} [7\Gamma_{i}^{2}(x) + 2\Gamma_{i}(x)\Gamma_{2}(x)],$$
  

$$\Gamma_{2}'(x) = -\frac{i}{3} [9\Gamma_{2}^{2}(x) + 12\Gamma_{i}(x)\Gamma_{2}(x) + 4\Gamma_{i}^{2}(x)]$$
(A.7)

with the boundary conditions

$$\Gamma_{1}(0) = \gamma_{1}^{*} = \frac{1}{4}\gamma_{1}(6s_{1}/s_{a})^{\frac{1}{2}}, \qquad \Gamma_{2}(0) = \gamma_{2}^{*} = \frac{1}{4}\gamma_{2}(6s_{1}/s_{a})^{\frac{1}{2}}.$$
 (A.8)

In the solution of the set (A.7), we shall use the method outlined in Sec. 2. As a result, we get

$$\varphi' = f(\varphi) = -\frac{\gamma_{1}^{*}}{3} \frac{(7\varphi^{2} + 5\varphi + 4)^{s_{1}}}{(7\lambda^{2} + 5\lambda + 4)^{s_{1}}} C(\varphi, \lambda),$$
  

$$\Gamma_{1} = \gamma_{1}^{*} \left(\frac{7\varphi^{2} + 5\varphi + 4}{7\lambda^{2} + 5\lambda + 4}\right)^{s_{1}} C(\varphi, \lambda);$$
(A.9)

$$\varphi = \Gamma_2/\Gamma_1, \quad C(\varphi, \lambda) = \exp\left\{\frac{88}{7\sqrt{759}} \left[ \arctan\frac{14\varphi + 5}{\sqrt{759}} - \arctan\frac{14\lambda + 5}{\sqrt{759}} \right].$$
  
For  $\gamma_1^* > 0$ , the function  $\varphi \to -\infty$  for

$$x \to x_0 = \int_{\lambda}^{-\infty} \left( \frac{d\varphi}{f(\varphi)} \right),$$

but the stability condition  $\varphi \ge -1$  is violated even earlier. As  $\gamma_1^* \rightarrow 0$  the parameter  $x_0 \sim \gamma_1^{-9/7}$  and there. is a broad range of applicability of the zero-charge solution

$$\Gamma_2(x) = \frac{\gamma_2}{1+3\gamma_2 \cdot x}.$$
 (A.10)

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Similar results are obtained in the case  $\gamma_1^* < 0$ . As is seen from Eqs. (A.7),  $\Gamma_2(x) \neq 0$  even if  $\gamma_2^* = 0$ , i.e., the anisotropy of the spectrum generates the anisotropy of the interaction.

The equation for the three-prong graph  $\mathcal{T}_1$  is of the form

$$\mathcal{T}_{i}(x)\delta_{\alpha\beta} = \delta_{\alpha\beta} - \int_{0}^{x} dy \sum_{i=1}^{3} \mathcal{T}_{i}(y) \Gamma_{ii\alpha\beta}(y)$$

Using the tensor structure of  $\Gamma$  and differentiating the equation with respect to x, we get

$$\mathscr{T}_{i}'(x) = -\mathscr{T}_{i}({}^{\mathfrak{s}}/{}_{\mathfrak{s}}\Gamma_{\mathfrak{s}} + \Gamma_{\mathfrak{s}}), \quad \mathscr{T}_{i}(0) = \mathfrak{1}.$$
 (A.11)

In the extreme anisotropic case  $\gamma_1^* = 0$ ,  $\Gamma_1(x) = 0$ ,

$$\mathcal{T}_{1}(x) = (1 + 3\gamma_{2} x)^{-\gamma_{2}}.$$
 (A.12)

The polarization vector  $\Pi_1(x)$  is

$$[I_{1}(x) \sim \int_{0}^{1} dy \mathcal{T}_{1}^{2}(y) \sim [(1 + 3\gamma_{2} \cdot x)^{\gamma_{1}} - 1].$$
 (A.13)

- <sup>1)</sup>The case of a large anisotropy of the spectrum  $s_a \ge s_t$  is considered in the Appendix.
- <sup>1</sup>D. E. Khmel'nitskiĭ and V. L. Shneerson, Fiz. Tverd. Tela 13, 832, 2158 (1971) [Soviet Phys.-Solid State 13, 687 (1971)].
- <sup>2</sup>A. B. Rechester, Zh. Eksp. Teor. Fiz. **60**, 782 (1971) [Soviet Phys.-JETP **33**, 423 (1971)]; Dissertation, Institute of Theoretical Physics, USSR Academy of Sciences, 1972.

- <sup>3</sup>A. I. Larkin and D. E. Khmel'nitskiĭ, Zh. Eksp. Teor. Fiz. 56, 2087 (1969) [Soviet Phys.-JETP 29, 1123 (1969)].
- <sup>4</sup>V. V. Sudakov, Dokl. Akad. Nauk SSSR 111, 338 (1956) [Soviet Phys.-Doklady 1, 662 (1957)].
- <sup>5</sup>D. E. Khmel'nitskii, Zh. Eksp. Teor. Fiz. **61**, 2110 (1971) [Soviet Phys.-JETP **34**, 1125 (1972)].
- <sup>6</sup>A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoi teorii polya v statisticheskoi fizike (Methods of Quantum Field Theory in Statistical Physics) Fizmatgiz, 1962 [Pergamon, 1965].
- <sup>7</sup>I. T. Dyatlov, V. V. Sudakov and K. A. Ter-Martirosyan, Zh. Eksp. Teor. Fiz. **32**, 767 (1957) [Soviet Phys.-JETP **5**, 631 (1957)].
- <sup>8</sup> L. D. Landau and E. M. Lifshitz, Staticheskaya fizika (Statistical Physics) Nauka, 1964 [Pergamon, 1969].
  <sup>9</sup> Yu. Kagan and Ya. A. Iosilevskii, Zh. Eksp. Teor. Fiz.
- 46, 2166 (1964) [Soviet Phys.-JETP 19, 1462 (1964)].
- <sup>10</sup> J. N. Bierly, L. Muldawer, and O. Beckman, Acta Metall. 11, 447 (1963).
- <sup>11</sup> V. G. Vaks, Zh. Eksp. Teor. Fiz. 54, 910 (1968) [Soviet Phys.-JETP 27, 486 (1968)].
- <sup>12</sup>B. Ya. Balagurov, V. G. Vaks, and B. I. Shklovskii, Fiz. Tverd. Tela 12, 89 (1970) [Soviet Phys.-Solid State 12, 70 (1970)].
- <sup>13</sup>G. Schirane, B. C. Frazer, V. J. Minkiewiez, J. A. Leake, and A. Linz, Phys. Rev. Lett. 19, 234 (1967).

Translated by R. T. Beyer 34