

# Inhomogeneous current state of an excitonic insulator

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The feasibility of a phase transition into a current state in the region of an incommensurate phase of an excitonic insulator is considered. Correct allowance for the symmetry of the magnetic elements of the Coulomb interaction makes states with homogeneous spontaneous current impossible. The characteristic dimension of the inhomogeneity in the model under consideration is determined by the degree of disparity between the electron and hole Fermi surfaces. The functional of the free energy is constructed and it is shown that the phase of the order parameter is not fixed in the incommensurability region. A model solution is obtained, from which it can be concluded that a current state is realizable in the region of the domain wall of a ferroelectric.

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## 1. INTRODUCTION

Halperin and Rice<sup>1</sup> noted in their review a substantial difference between the states of an excitonic insulator as a function of the order parameter. In the case of the two-band model at a nonzero interband dipole transition element, the situation was particularly interesting (Volkov, Kopaev<sup>2</sup>). Namely, at a real order parameter  $\Delta = |\Delta|e^{i\varphi}$  a transition into a ferroelectric state takes place, and at an imaginary order parameter the transition is into the so-called current state (called also the superdiamagnetic state by Volkov, Ginzburg, and Kopaev<sup>3</sup>). The theory of a phase transition into the current state contains a large number of nontrivial singularities of physical and mathematical character compared with the theory of the transition into the ferroelectric state.<sup>4</sup>

A simple approach, which leads in the case  $\varphi = 0$  and  $\varphi = \pi$  to a homogeneous spontaneous polarization of the system, leads in the case  $\varphi = \pm\pi/2$  to a spatially homogeneous spontaneous current. The latter contradicts the Bloch theorem<sup>3</sup> which states that the ground state of any macroscopic system as a state with zero total momentum (i. e., with zero average current). A correct allowance for the corresponding terms of the Coulomb interband interaction eliminates this contradiction, and the only realizable state with nonzero spontaneous current is an inhomogeneous one in the sense that the average current over the sample is zero.<sup>5</sup> The question of the characteristic dimension of the inhomogeneity was discussed in Ref. 6 only qualitatively.

The present paper is devoted to a clarification of certain possibilities of realization of a current state. The point is that in the simplest scheme of an excitonic insulator<sup>1</sup> a state with an imaginary order parameter is energywise favored (we do not consider the influence of impurity scattering on the phase of the order parameter<sup>7</sup>).

The main results of the paper are the following. In the region of the inhomogeneous state of an excitonic dielectric the most convenient solution can be

$$\Delta(r) = \Delta_{\text{Re}}(r) + i\Delta_{\text{Im}}(r),$$

where  $\Delta_{\text{Re}}(r)$  and  $\Delta_{\text{Im}}(r)$  are the real and imaginary parts

of the order parameter. The spatial changes  $\Delta_{\text{Re}}$  and  $\Delta_{\text{Im}}$  are connected with each other in such a way that  $\Delta_{\text{Im}}(r) \sim \text{grad}\Delta_{\text{Re}}(r)$ . The appearance of  $\Delta_{\text{Im}}$  produces an inhomogeneous current  $j(r)$  that flows around the region of the spontaneous polarization connected with  $\Delta_{\text{Re}}(r)$ .

Under certain conditions there can exist in the region of the inhomogeneous states a solution  $\Delta = i\Delta_{\text{Im}}(r)$  that turns out to be the most convenient. This corresponds to a pure current state.<sup>2</sup> Here and below we are dealing with the ground state, in contrast to the paper of Klyuchnik and Lozovik,<sup>8</sup> who investigated excited states of an excitonic insulator.

The causes of the onset of inhomogeneous states of an excitonic insulator may be non-congruence of individual sections of the electron and hole Fermi surfaces, doping that leads to inequality of the electron and hole densities, the presence of other bands that serve as an electron reservoir and have no energy-spectrum singularities of their own, and others. The characteristic dimension of the spatial inhomogeneity of the order parameter and of the associated physical quantities can be generally speaking, incommensurate with the period of the crystal lattice. We investigate below inhomogeneous states that arise at a specified difference of the electron and hole densities  $N$ . The dimension of the inhomogeneity is proportional in this case to  $(N/v_F)^{-1}$ , where  $v_F$  is the velocity on the Fermi surface.

## 2. MODEL HAMILTONIAN AND MATRIX ELEMENTS OF COULOMB INTERACTION

We consider the two-band model traditionally used for the investigation of the transition into the state of an excitonic insulator. We assume that in the vicinity of the point  $k_0$  of the Brillouin zone there are closely located isotropic bands 1 and 2 with dispersion laws

$$\varepsilon_{1,2}(k) = \pm(k^2 - k_0^2)/2m^*, \quad (1)$$

where the wave vector  $k$  differs from  $k_0$ . Assume that the point  $k_0$  the bands 1 and 2 belong to irreducible representations of different parity, so that the dipole-transition matrix element  $P_{12}$  differs from zero. To investigate the transition into the insulator phase it is necessary first to write down the Hamiltonian of the

system either in the Bloch representation or in the Luttinger-Kohn representation. The latter is more convenient, for while it becomes necessary to work in a nondiagonal basis, the form of the matrix elements of the Coulomb interband interaction is relatively simpler to establish.

Thus, the Hamiltonian of the system in the Luttinger-Kohn representation takes the form

$$H = H_0 + H_{rc},$$

$$H_0 = \sum_{\mathbf{k}, i} \varepsilon_i(\mathbf{k}) a_{i\mathbf{k}}^\dagger a_{i\mathbf{k}} + \sum_{\mathbf{k}} \frac{1}{m} \mathbf{P}_{12} \mathbf{k} a_{1\mathbf{k}}^\dagger a_{2\mathbf{k}} + \text{c.c.}, \quad (2)$$

$$H_{rc} = \sum_{i, j, n, l, \mathbf{k}, \mathbf{k}', \mathbf{q}} V_{ijnl}(\mathbf{q}) a_{i\mathbf{k}}^\dagger a_{j\mathbf{k}'}^\dagger a_{n, \mathbf{k}' - \mathbf{q}} a_{l, \mathbf{k} + \mathbf{q}},$$

where  $\varepsilon_i(\mathbf{k})$  are the electron dispersion laws in bands 1 and 2;  $m$  is the mass of the free electron and must be distinguished from the electron effective mass  $m^*$  calculated without allowance for the hybridization of the bands 1 and 2. The Hamiltonian (2) contains the hybridization term of bands 1 and 2 in explicit form, so that even without allowance for the Coulomb interaction  $H_{rc}$  the anomalous Green's functions  $G_{12}^0(\mathbf{k}) = \langle a_{1\mathbf{k}} + a_{2\mathbf{k}} \rangle_{ee}$  corresponding to the Hamiltonian (2) differ from zero.

However,  $\sum_{\mathbf{k}} G_{12}^0(\mathbf{k}) = 0$  because the hybridization term is odd in  $\mathbf{k}$ , and the presence of anomalous mean values does not lead (if  $H_{rc}$  is not taken into account) to any new physical consequences.

We discuss now the important problem of the form of the Coulomb-interaction matrix elements  $V_{ijnl}(\mathbf{q})$ . In practically all the investigations of the excitonic insulators (and in a number of other problems)  $V_{ijnl}(\mathbf{q})$  is replaced by the constant  $V_{ijnl}$  in the high-density approximation. The arguments advanced in favor of this substitution is usually connected with screening (density-density interaction from different bands), while the argument favoring  $V_{1122} \equiv V_2$  and  $V_{1112} \equiv V_3$  is the short-range character of the interactions connected with the interband transitions of a particle pair ( $V_{1122}$ ) or of one particle ( $V_{1112}$ ). But whereas replacement of the interaction  $V_1(\mathbf{q})$  by a constant independent of the momentum is justified in the high-density approximation, it is already less obvious for  $V_2(\mathbf{q})$ , and raises serious objections in the case of  $V_3(\mathbf{q})$ . The point is that this substitution causes complete loss of the information on the symmetry of the system [this is particularly important for  $V_3(\mathbf{q})$ , since the corresponding term in the Hamiltonian leads to the appearance of a source in the right-hand side of the self-consistency equation for the order parameter].

We consider now the form of the matrix elements  $V_1(\mathbf{q})$  and  $V_{2,3}(\mathbf{q})$  for our model:

$$V_1(\mathbf{q}) = \sum_{\mathbf{G}} B_{11}(\mathbf{G}) B_{22}(-\mathbf{G}) V(\mathbf{q} + \mathbf{G}),$$

$$V_2(\mathbf{q}) = \sum_{\mathbf{G}} B_{12}(\mathbf{G}) B_{21}(-\mathbf{G}) V(\mathbf{q} + \mathbf{G}), \quad (3)$$

$$V_3(\mathbf{q}) = \sum_{\mathbf{G}} B_{11}(\mathbf{G}) B_{12}(-\mathbf{G}) V(\mathbf{q} + \mathbf{G}).$$

Equations (3) are easily obtained from those of Dubovik by making insignificant transformations. We assume

that all the momenta  $\mathbf{k}$ ,  $\mathbf{k}'$ , and  $\mathbf{q}$  in the Hamiltonian lie near  $k_0$ , where, in fact, the effective-mass approximation is valid. In (3) we have

$$B_{ij}(\mathbf{G}) = \int_{V_0} u_{i\mathbf{k}_0}^*(\mathbf{r}) u_{j\mathbf{k}_0}(\mathbf{r}) e^{i\mathbf{G}\mathbf{r}} d\mathbf{r}, \quad (4)$$

where  $u_{i\mathbf{k}_0}(\mathbf{r})$  is the Bloch wave function at the point  $\mathbf{k}_0$ ,  $\mathbf{G}$  is the reciprocal-lattice vector, and  $V_0$  is the volume of the unit cell:

$$V(\mathbf{q} + \mathbf{G}) = V(|\mathbf{q} + \mathbf{G}|^2). \quad (5)$$

In our case the functions  $u_{1\mathbf{k}_0}(\mathbf{r})$  and  $u_{2\mathbf{k}_0}(\mathbf{r})$  have different parities. It is easy to verify, using this circumstance, the following properties of the matrix elements (3):

$$\begin{aligned} V_1(\mathbf{q}) &= V_1(-\mathbf{q}), \quad V_1(0) \neq 0; \\ V_2(\mathbf{q}) &= V_2(-\mathbf{q}), \quad V_2(0) \neq 0, \quad V_2(0) \ll V_1(0); \\ V_3(\mathbf{q}) &= -V_3(-\mathbf{q}), \quad V_3(0) = 0. \end{aligned} \quad (6)$$

It follows thus from (6) that it is wrong to replace  $V_3(\mathbf{q})$  by a constant independent of the momentum. Analysis shows that at small  $\mathbf{q}$  the potentials  $V_2(\mathbf{q})$  and  $V_3(\mathbf{q})$  take the form

$$V_2(\mathbf{q}) = \alpha q^2 + (\mathbf{q}\beta)^2 + V_2(0), \quad (7)$$

$$V_3(\mathbf{q}) = \mathbf{q}\gamma, \quad (8)$$

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are parameters whose explicit form is of no interest to us. All that matters is that  $V_1 \gg V_2$ ,  $V_3$  in the entire range of variation of  $\mathbf{q}$  of interest to us.

As to  $V_1(\mathbf{q})$ , it is easy to obtain from (3) the usual expression,<sup>1</sup> by retaining only the terms with  $\mathbf{G} = 0$ .

### 3. SPONTANEOUS CURRENT IN A SYSTEM WITH IMAGINARY ORDER PARAMETER

According to the classification given in Ref. 2, for a real order parameter  $\Delta$  in a system with bands of the symmetry investigated by us, there arises a spontaneous polarization

$$\vec{\mathcal{P}}(\mathbf{R}) = 2d_{12}\Delta(\mathbf{R}). \quad (9)$$

Here  $\mathcal{P}(\mathbf{R})$  is the polarization averaged over the volume of the old (unreconstructed) unit cell, and  $d_{12}$  is the transition matrix element:

$$d_{12} = \frac{e}{V_0} \int u_{1\mathbf{k}_0}^*(\mathbf{r}) \mathbf{r} u_{2\mathbf{k}_0}(\mathbf{r}) d\mathbf{r}. \quad (10)$$

The order parameter  $\Delta(\mathbf{R})$ , which characterizes the macroscopic change of the polarization, is simply the anomalous Green's function taken at equal arguments  $\mathbf{r} = \mathbf{r}' = \mathbf{R}$ . It is important that the normal Green's functions  $G_{11}$  and  $G_{12}$  do not enter explicitly in the expression (9) for the polarization.

The situation is different in the case of an imaginary order parameter  $\Delta$ . Besides the interband component of the spontaneous current, which takes the form

$$j_{12}(\mathbf{R}) = 2 \frac{e}{m} \mathbf{P}_{12} \Delta(\mathbf{R}), \quad (11)$$

$$\mathbf{P}_{12} = \int u_{1\mathbf{k}_0}^*(\mathbf{r}) \frac{\nabla_{\mathbf{r}}}{i} u_{2\mathbf{k}_0}(\mathbf{r}) d\mathbf{r},$$

where

$$\Delta(\mathbf{R}) = i|\Delta(\mathbf{R})|, \quad (12)$$

there is also an intraband current component

$$\mathbf{j}_1 + \mathbf{j}_2 = \frac{e}{2m} \left[ \frac{\nabla_r}{i} - \frac{\nabla_{r'}}{i} \right] [G_{11}(r, r') + G_{22}(r, r')]_{r=r'-R}. \quad (13)$$

An analysis carried out in Ref. 6 has shown that at constant  $\Delta(R)$  the total current in the system is zero [this can be still treated as cancellation of the interband current (11) by the intraband current (13)]. It is impossible to obtain a general expression for the current  $j(R)$  in terms of the order parameter  $\Delta(R)$ , but near the transition temperature and for a slow variation of  $\Delta(R)$  it was shown in Reg. 6 that

$$\mathbf{j}(R) = \delta [\text{rot rot } \mathbf{P}_{12} \Delta(R)], \quad (14)$$

where  $\delta$  is a numerical coefficient.

Thus, only an inhomogeneous current state is produced, in agreement with the Bloch theorem. We note also that  $\text{div} \mathbf{j}(R) = 0$ .

We examine now in greater detail the effective interaction constants for the cases of real and imaginary order parameters. It follows from the results of Sec. 2 that direct diagrams (of the Hartree type), which contain the interband interaction  $V_3(0)$  drop out of consideration. Only the exchange diagrams remain, and their contribution is well known. The interaction constants (disregarding the spin and the phonons) are of the form

$$g_{Re} = \bar{V}_1 + \bar{V}_2 - 4V_3(0), \quad g_{Im} = \bar{V}_1 - \bar{V}_2. \quad (15)$$

The subscripts Re(Im) pertain to real (imaginary) order parameters, while  $\bar{V}_1$  and  $\bar{V}_2$  are the Coulomb interactions taken on the Fermi surface and averaged over the angles. In the Luttinger-Kohn representation the interaction  $V_3(q)$  reduces mainly to a renormalization of the hybridization term in the Hamiltonian (2), and we confine ourselves hereafter to allowance for the interactions  $V_1$  and  $V_2$ . We emphasize, however, that in the Bloch representation  $V_3$  cannot be discarded. The Hamiltonian (2) rewritten in the Bloch representation will not contain a hybridization term. The interaction  $V_3$  has in this case, too, the structure (8), but since  $V_3$  acts as a source in the self-consistency equations, it must be taken into account if a correct expression is to be obtained for  $\Delta(\mathbf{k})$ , with parts even and odd with respect to  $\mathbf{k}$ . It can be shown that allowance for such an odd part of  $\Delta(\mathbf{k})$  is analogous to allowance for the hybridization in the Luttinger-Kohn representation, and ensures mutual cancellation of the interband and intraband currents.

It is clear from the foregoing that it is most convenient to carry out the investigation of the current state in the Luttinger-Kohn representation. The weakly inhomogeneous current state near the phase-transition temperature will be investigated in the next section.

#### 4. TWO-PARAMETER GINZBURG-LUNDAU EXPANSION

We start with the Hamiltonian (2) expressed in the Luttinger-Kohn representation. The complex order parameter  $\Delta$  is defined in the usual manner in terms of the anomalous Green's function of the system  $G_{12}(r, r')$ . It is convenient to separate it into a real and imaginary part,  $\Delta = \Delta_{Re} + i\Delta_{Im}$ . We analyze next

the behavior of the system near the phase-transition temperature. This is easiest to do by constructing the free-energy functional  $F(r)$ . For simplicity we assume that the hybridization parameter  $|P_{12}k_F|/m\varepsilon_F$  is small, so that we confine ourselves to the first nonvanishing terms in the coefficients of the expansion of  $F(r)$  in terms of  $\Delta(r)$ . Assume that the electron and hole densities are not equal and their difference is  $n$ . It is known<sup>10</sup> that in the case of a real order parameter (singlet or triplet), if  $n$  is large enough a transition is possible into an incommensurate state characterized by a superstructure wave vector  $q \sim n/v_F$ . On the  $(n, T)$  phase diagram there is a point of contact of three phases, unreconstructed, reconstructed commensurate, and reconstructed incommensurate- the so-called Lifshitz point. We shall not deal hereafter with the spin structure, and assume that the pairing is singlet both the state  $\Delta_{Re}$  and in the state  $\Delta_{Im}$ . It can be shown that allowance for the possible appearance of triplet pairing introduces no new factors in the analysis that follows.

Leaving out the elaborate calculations, we present the general form of the functional  $F(r)$ :

$$\begin{aligned} \frac{F(r)}{2N(0)} = & \tau_{Re} \Delta_{Re}^2 + \tau_{Im} \Delta_{Im}^2 + a_{Re} (\text{grad } \Delta_{Re})^2 + a_{Im} (\text{grad } \Delta_{Im})^2 \\ & + a_{Re}^{(1)} (\mathbf{n} \text{ grad } \Delta_{Re})^2 + a_{Im}^{(1)} (\mathbf{n} \text{ grad } \Delta_{Im})^2 + a_{Re}^{(2)} (\text{div grad } \Delta_{Re})^2 \\ & + a_{Im}^{(2)} (\text{div grad } \Delta_{Im})^2 + A_{Re} \Delta_{Re}^2 + A_{Im} \Delta_{Im}^2 + C (\Delta_{Re}^2 + \Delta_{Im}^2)^2. \end{aligned} \quad (16)$$

Here

$$\begin{aligned} \tau_{Re(Im)} = & \tau_{Re(Im)}^0 - \frac{4n^2}{(\pi T)^2} \varphi_1 (\tau_{Re(Im)}^0 - \nu_{Re(Im)}^0), \\ \tau_{Re(Im)}^0 = & \frac{T - T_{Re(Im)}}{T_{Re(Im)}}, \quad \nu_{Re(Im)}^0 = \frac{n - n_{Re(Im)}}{n_{Re(Im)}}; \end{aligned} \quad (17)$$

$T_{Re(Im)}$  and  $n_{Re(Im)}$  are the coordinates of the Lifshitz point<sup>10</sup> at coupling constants  $g_{Re}$  ( $g_{Im}$ );

$$\begin{aligned} a_{Re} \approx a_{Im} \approx & \frac{1}{6} \frac{v_F^2}{(\pi T)^2} \varphi_2 - \frac{1}{20} \lambda \frac{v_F^2}{(\pi T)^2} \varphi_3 = a, \\ a_{Re}^{(1)} \approx a_{Im}^{(1)} \approx & -\frac{1}{10} \lambda \frac{v_F^2}{(\pi T)^2} \varphi_3 = a^{(1)}, \\ a_{Re}^{(2)} \approx a_{Im}^{(2)} \approx & -\frac{1}{40} \frac{v_F^4}{(\pi T)^4} \varphi_3 = a^{(2)}, \end{aligned} \quad (18)$$

$\mathbf{n}$  is a unit vector in the  $\mathbf{P}_{12}$  direction;

$$\begin{aligned} A_{Re} = & -^3/20 \lambda^2 \varphi_3 + ^1/3 \lambda \varphi_2, \quad A_{Im} = -^3/\lambda^2 \varphi_3 + \lambda \varphi_2, \\ C = & \frac{1}{2} \left[ \frac{1}{(\pi T)^2} \varphi_2 + \frac{8}{(\pi T)^2} \varphi_1 \right], \quad \lambda = \left( \frac{m^*}{m} \right)^2 \frac{|P_{12}^2 v_F^2|}{(\pi T)^2}, \end{aligned} \quad (19)$$

where

$$\begin{aligned} \varphi_1 = & \sum_{k \geq 0} \frac{1}{(2k+1)^3 [1 + (n/\omega_k)^2]^2}, \\ \varphi_2 = & \sum_{k \geq 0} \frac{1 - 3(n/\omega_k)^2}{(2k+1)^3 [1 + (n/\omega_k)^2]^3}, \\ \varphi_3 = & \sum_{k \geq 0} \frac{1 - 10(n/\omega_k)^2 + 5(n/\omega_k)^4}{(2k+1)^3 [1 + n^2/\omega_k^2]^5}, \\ \varphi_4 = & \left[ \sum_{k \geq 0} \frac{(n/\omega_k)}{(2k+1)^2 [1 + (n/\omega_k)^2]^2} \right]^2. \end{aligned}$$

We have specially separated in the functional (16) the terms  $A_{Re}$  and  $A_{Im}$ , which contain the first-order corrections in the hybridizations. At the Lifshitz point we have  $\varphi_1 \approx 0$  and it was therefore necessary to retain in  $A_{Re}$  and  $A_{Im}$  the terms of fourth order in  $P_{12}$ . The coef-

ficients  $a^{(1)}$  and  $a^{(2)}$ , and  $a$ ,  $C$  are set equal for  $\Delta_{Re}$  and  $\Delta_{Im}$ , since they differ little near the Lifshitz point, and this difference does not affect the results. The coupling constants  $g_{Re}$  and  $g_{Im}$ , which enter in the definitions of  $\tau_{Re}$  and  $\tau_{Im}$ , are such that in the commensurate phase the temperature  $T_{Re}$  of the transition into the ferroelectric phase exceeds the temperature  $T_{Im}$  of the transition into the superdiamagnetic phase.<sup>2</sup> We shall assume that the constants  $g_{Re}$  and  $g_{Im}$  (and consequently also  $T_{Re}$  and  $T_{Im}$ ) are close, and consider the behavior of the lines of the phase transition into a state with noncommensurate (inhomogeneous)  $\Delta_{Re}$  and  $\Delta_{Im}$ . In this case  $\varphi_2 < 0$ ,  $\varphi_3 < 0$ . Assume that  $\Delta_{Re}$  and  $\Delta_{Im}$  do not coexist in the system. Then, assuming first  $\Delta_{Im} = 0$ ,  $\Delta_{Re} \neq 0$ , we obtain an expression for the transition temperature:

$$\tau_{Re} + A_{Re} + aq_{Re}^2 + a^{(2)}q_{Re}^4 + a^{(1)}(nq_{Re})^2 = 0. \quad (20)$$

We determine  $q_{Re}^2$  by minimizing the functional with respect to this parameter (we seek the solution in the form  $\Delta_{Re}(r) = \Delta_{Re} \cos q_{Re} r$ ; as indicated by Volkov and Dugushev,<sup>11</sup> the representation of the solution in this form near the Lifshitz point is valid accurate in terms cubic in  $\Delta_{Re}$ ):

$$q_{Re}^2 = -\frac{a}{2a^{(2)}}, \quad q_{Re} \perp P_{12}; \quad q_{Re}^2 = -\frac{a+a^{(1)}}{2a^{(2)}}, \quad q_{Re} \parallel P_{12}. \quad (21)$$

Substituting next (21) in (20), we easily note that the highest temperature of the transition into the inhomogeneous (incommensurate state) state corresponds to the transition  $q_{Re} \perp P_{12}$ . The transition line  $T_{Re}(n)$  in the vicinity of the Lifshitz point  $\Theta$  is shown in the figure (curve 1). The Lifshitz point is defined in the case of the transition into the ferroelectric phase as the intersection of the line (20) with the line  $a = 0$ .

We now obtain the line  $T_{Im}(n)$  that characterizes the phase transition into the current state, under the condition that no transition takes place into the ferroelectric state. In the commensurate state this would correspond to the condition  $g_{Re} < g_{Im}$ , which is apparently impossible, so that the transition into the ferroelectric state takes place earlier, and  $T_{Re}(n) > T_{Im}(n)$ . In the inhomogeneous (incommensurate) phase, as we shall now show, the situation may be different. We seek the imaginary order parameter  $\Delta_{Im}(r)$  in the form  $\Delta_{Im}(r) = \Delta_{Im} \cos q_{Im}(r)$ , putting  $\Delta_{Re} = 0$ . We obtain for the transition temperature in this case:

$$\tau_{Im} + A_{Im} + aq_{Im}^2 + a^{(2)}q_{Im}^4 + a^{(1)}(nq_{Im})^2 = 0, \quad (22)$$

and for the parameter  $q_{Im}$  we have

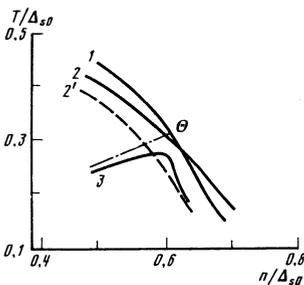


FIG. 1.

$$q_{Im}^2 = -\frac{a}{2a^{(2)}}, \quad q_{Im} \perp P_{12}; \quad q_{Im}^2 = -\frac{a+a^{(1)}}{2a^{(2)}}, \quad q_{Im} \parallel P_{12}. \quad (23)$$

Exactly as in (21), the highest transition temperature  $T_{Im}(n)$  is reached at  $q_{Im} \perp P_{12}$ . From (21) and (23) it follows that in this case  $q_{Im} = q_{Re}$ . Inasmuch as  $\varphi_2 < 0$  in the incommensurate phase, it follows from (20) and (22) that even at  $g_{Re} > g_{Im}$ , owing to the difference between the coefficients  $[-\varphi_2$  and  $-(\frac{1}{3})\varphi_2]$  of the term linear in  $\lambda$ , the temperature  $T_{Re}(n)$  may turn out to be lower than  $T_{Im}(n)$ , i. e., the hybridization suppresses the inhomogeneous ferroelectric state more strongly than the inhomogeneous current state. The figure shows a plot of  $T_{Im}(n)$  (curve 2). By selecting the system parameters (by making  $g_{Re}$  and  $G_{Im}$  close enough) we can obtain on the  $(T, n)$  diagram a transition into the inhomogeneous current state in a definite concentration region  $n > n_{Im}^*$  [where  $n_{Im}^*$  is determined by the intersection of the curves  $T_{Re}(n)$  and  $T_{Im}(n)$ ] when the temperature is lowered. The question of the upper limit of the concentration  $n$ , at which a transition into the current state is possible, remains open, however. It is quite probable that this limit coincides with the largest concentration  $n_{cr} = 0.755\Delta_{s0}$  at which a phase transition is possible at all.<sup>10</sup>

The most probable is a ratio of the constants  $g_{Re}$  and  $g_{Im}$  such that  $T_{Re}(n) > T_{Im}(n)$  on the entire phase diagram. It is natural to consider the question of the coexistence of the singlet and triplet order parameters near the Lifshitz point.<sup>11</sup> Simplifying the analysis, we shall assume that the difference between  $g_{Re}$  and  $g_{Im}$  is large enough so that  $A_{Re}$  and  $A_{Im}$  make rather small contributions to the relation between  $T_{Re}(n)$  and  $T_{Im}(n)$  and can be left out (a more rigorous analysis confirms the validity of this approach). We assume that at the temperature  $T_{Re}(n)$  a solution of  $\Delta_{Re}(r)$  was generated in the form  $\Delta_{Re} \cos q \times r$ , with  $q \perp P_{12}$ . The quantity  $q$  itself and its change with decreasing temperature is of no interest to us. The coefficient of  $\Delta_{Im}^2(r)$  in the functional (16) depends substantially on the choice of the solution  $\Delta_{Im}(r)$ .

We discuss now the situation when  $\Delta_{Im}(r) = \Delta_{Im} \sin q \times r$ , i. e., it is shifted by  $\pi/2$  in phase relative to  $\Delta_{Re}(r)$ . In this case it is easy to verify, by integrating over the volume, that the effective coefficient  $\alpha_{Im}$  of the term quadratic in  $\Delta_{Im}$  in the expansion of the free energy is equal to

$$\alpha_{Im} = \tau_{Im} + aq^2 + a^{(2)}q^4 + \frac{1}{2}C\Delta_{Re}^2. \quad (24)$$

At the same time it can be easily shown that

$$\Delta_{Re}^2 = -\frac{2}{3}C_1^{-1}[\tau_{Re} + aq^2 + a^{(2)}q^4]. \quad (25)$$

From (14) and (25) we see that at

$$\alpha_{Im} = \tau_{Im} - \frac{1}{3}\tau_{Re} + \frac{2}{3}(aq^2 + a^{(2)}q^4) = 0$$

the term quadratic in  $\Delta_{Im}$  in the functional (16) reverses sign, and generation of  $\Delta_{Im}(r)$  against the background of  $\Delta_{Re}(r)$  is possible. Recognizing that  $\tau_{Im} = \tau_{Re} + \ln\delta$ , where

$$\delta = \frac{\Delta_{Re}^0}{\Delta_{Im}^0}, \quad \Delta_{Re(Im)}^0 = \delta \exp\left[-\frac{1}{g_{Re(Im)}N(0)}\right], \quad (26)$$

we obtain the condition for the coexistence of  $\Delta_{Re}$  and  $\Delta_{Im}$ :

$${}^2/s\tau_{Re} + \ln \delta + {}^2/s(aq^2 + a^{(2)}q^4) = 0. \quad (27)$$

The line  $T_c(n)$  corresponding to Eq. (27) was approximately plotted in the figure (curve 3).

From the analysis of the functional (16) it is easily seen that coexistence of  $\Delta_{Re}$  and  $\Delta_{Im}$  is impossible in the homogeneous case. The most suitable from among the inhomogeneous solutions at small  $q$  is a solution of the type

$$\Delta_{Re}(r) = \Delta_{Re} \cos qr, \quad \Delta_{Im}(r) = \Delta_{Im} \sin qr. \quad (28)$$

The question of the advantage of one type of solution over another is answered in the same manner as for the coexistence of singlet and triplet order parameters.<sup>11</sup>

The results allow us to predict the following structure of the band state in the case of ferroelectric ordering. Inside the ferroelectric "domains," where the spontaneous polarization, which is proportional to  $\Delta_{Re}$ , changes very little, coexistence of  $\Delta_{Re}$  and  $\Delta_{Im}$  is impossible, and no spontaneous current is produced in this region. Near the "domain" boundary, in the region where the polarization is drastically inhomogeneous, a spontaneous current is produced and its maximum density takes place in the region of the strongest variation of the polarization. Thus, a "domain wall" of sorts is produced, in which the phase of the order parameter  $\Delta(r)$  changes from  $\varphi = 0$  to  $\varphi = \pi/2$  and then from  $\varphi = \pi/2$  to  $\varphi = \pi$ . The mathematical analysis of this structure should be based on the functional (16) with allowance for the higher harmonic components. The functional  $F(r)$  takes in terms of the new variables (the amplitude  $|\Delta|$  and the phase  $\varphi$ ) the form

$$\frac{F(r)}{2N(0)} = \tau_{Re}|\Delta|^2 + (\tau_{Im} - \tau_{Re})|\Delta|^2 \sin^2 \varphi + a[(|\Delta'|)^2 + |\Delta|^2(\varphi')^2] + a^{(1)}(n|\Delta'|)^2 + a^{(11)}|\Delta|^2(\varphi'n)^2 + a^{(2)}[(|\Delta|'' - |\Delta|\varphi'')^2 + 4(|\Delta'|)^2(\varphi')^2] + A_{Re}|\Delta|^2 + (A_{Im} - A_{Re})|\Delta|^2 \sin^2 \varphi + C|\Delta|^4. \quad (29)$$

A mathematical analysis of the equations of the minimization of the functional (29) is quite complicated and calls for a separate study.

From among the foregoing results, special notice should be taken of the fact that the transverse structure of an inhomogeneous state [whether "current" or "mixed" (28)] is more favored than a longitudinal one near the transition temperature. In fact, at  $q \parallel P_{12}$ , as follows from the definition of the current (14), we would obtain  $j = 0$ , i. e., no longitudinal currents can exist in the investigated system.

This means that in principle states are possible in which the phase of the order parameter is equal to  $\pm\pi/2$  (or varies in space, going through  $\pm\pi/2$ ), but no spontaneous current can be produced in this case. In

our model, such states are not favored near the transition temperature compared with the "true" current states ( $q \perp P_{12}$ ) for the following reason. Since the system is uniaxial (there is only one preferred vector  $P_{12}$ ) the Fermi surfaces of the electrons and holes are anisotropic, but congruent. The conditions of electron-electron pairing are most favorable in directions perpendicular to  $P_{12}$ , inasmuch in these directions the pairing covers the greater part of the phase space.

We have assumed that the cause of the formation of the inhomogeneous state (current or ferroelectric) is that the electron and hole Fermi surfaces do not coincide (e. g., as a result of doping). Another cause may be the noncongruence of the Fermi surfaces or of at least some of their sections. A qualitative analysis based on the model of Kopaev and Mnatsakanov<sup>12</sup> shows that in this case, too, at sufficiently large noncongruence, an inhomogeneous state of the type considered above is produced.

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