## On the coexistence of the dielectric and superconducting states in quasi-one-dimensional systems

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The behavior of the Peierls instability as a function of the location of the electron Fermi level  $\epsilon_{kF}$  is investigated. It is shown that, when the level to which the one-dimensional band is filled deviates from the middle of the band by  $\mu$ , the wave vector, Q, of the charge density wave (CDW) is not equal to  $2k_F$ , and the dielectric gap,  $\Delta_p$ , is shifted with respect to the Fermi level. Although a state with a CDW is an ordered state of the dielectric type, it has, starting from  $\mu > \Delta_p$ , even at T = 0, free carriers above the gap  $\Delta_p$  (to the extent of the noncoincidence of Q and  $2k_F$ ). If bare attraction exists in the Cooper channel, then a state with a CDW still turns out to be unstable against superconducting ordering, and the coexistence of superconductivity and CDW becomes energetically advantageous at  $\mu > \Delta_p$ .

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The low-temperature state of quasi-one-dimensional systems that exhibit metallic behavior at high temperatures continues to be intensively investigated in connection with its expected, not-quite-usual properties.<sup>[1-3]</sup> It has been established, for example, that, depending on the relation between the constants characterizing the bare electron interaction in the one-dimensional system, the ground state of the system may turn out to be an ordered state of the superconducting or dielectric type, or may remain metallic.<sup>[4,5]</sup>

The purpose of the present paper is to ascertain the conditions for the coexistence of the superconducting and dielectric states in a quasi-one-dimensional system in the framework of the conventional self-consistent scheme. We are aware of the limitedness of such an approach, which does not take into account the role of the long-wave fluctuations, which preclude the description of a change in the state of strictly one-dimensional systems in terms of the theory of phase transitions.

We hope, however, that the results of the mean-field approximation will prove to be useful in the discussion of the properties of quasi-one-dimensional systems, since, according to Ref. 6, they do not qualitatively change after allowing for the fluctuation effects in the Ginzburg-Landau scheme for systems with two order parameters:  $\Delta_{\rho}$  and  $\Delta_{s}$ . Furthermore, these results form a basis for comparison with the results obtained by means of other methods, including more rigorous methods.<sup>[5,7]</sup>

Here we pay particular attention to the behavior of the Peierls instability as a function of the level of deviation,  $\mu$ , of the filling of the one-dimensional band from the middle. Let us recall that, according to Ref. 8, if the band is exactly half-filled, i.e., if  $\mu = 0$ , then there develop in the one-dimensional chain a displacement wave  $\varphi_Q$  and an associated charge-density wave (CDW),  $\rho_Q$ , with wave vector  $Q = 2k_F = \pi/d$ . Below we shall show that, without allowance for the umklapp processes, the condition  $Q = 2k_F$  is, as in the jelly model, <sup>[9]</sup> fulfilled regardless of the level to which the band is filled. Allowance for the unklapp processes (the periodicity of the lattice is, in fact, manifested in these processes) leads,

in accordance with Ref. 10, to a situation in which the CDW vector Q that is established at the Peierls transition point does not coincide with  $2k_F$ , i.e.,  $Q \neq 2k_F$ , if there is a finite deviation,  $\mu$ , from the middle of the band (when  $k_F \neq \pi/2d$ ). To wit, at small  $\mu$  the one-dimensional system prefers to maintain a doubled period, i.e.,  $Q = \pi/d$ .<sup>[111]</sup> It is only upon the attainment of a limiting deviation level,  $\mu_{crr}$  that the CDW vector begins to change in the direction of the doubled limiting momentum, but it remains, as before,  $Q \neq 2k_F$ .

It is appropriate in this connection to discuss the origin of the deviation of the level to which the band is filled from the middle of the band. First of all, it can come about because of the overlap of the band under consideration with some other band playing the role of a reservoir and not undergoing a reconstruction in the transition. To a limiting case of a state with a given value of  $\mu$  corresponds an infinitely large density of states of the reservoir. A given value,  $\delta n$ , of the deviation of the electron concentration from the concentration that corresponds to the exactly half-filled band should be regarded as another limiting case. A state with a given  $\delta n$  is characteristic rather of systems with doping if we ignore the possible formation of bound impurity states. <sup>[121]</sup>

If the bare electron interaction in the Cooper channel corresponds to attraction, i.e., if  $\lambda_s < 0$ , then the dielectric and superconducting orderings should be considered simultaneously. From the obtained system of self-consistent equations for the order parameters  $\Delta_p$  and  $\Delta_s$  we can establish precisely the conditions for the coexistence of the dielectric CDW state and superconductivity. Below this is done for the case of a weak superconducting ordering against a background of a dielectric ordering established at a higher temperature, i.e., when the original critical temperatures,  $T_{p0}$  and  $T_{s0}$ , of the pure dielectric and superconducting phases differ so much so that  $T_{p0} \gg T_{s0}$ . In this case we can neglect the inverse effect of the superconductivity on the CDW.

Below we shall show that the conditions for the coexistence of superconductivity and CDW are closely connected with the distinctive features of the excitation spectrum of the dielectric phase, and, in fact, arise only when the Fermi level of the original metallic phase deviates from the middle of the band. Although a state with a CDW is of the dielectric type, its excitation spectrum for  $\mu \neq 0$  has no gap, since the dielectric gap in this case arises not exactly at the Fermi level. This state, which has free carriers above the gap  $\Delta_p$  (to the extent of the noncoincidence of Q and  $2k_F$ ), turns out to be itself unstable against superconducting ordering, and the coexistence of superconductivity and CDW becomes energetically advantageous when  $\mu > \Delta_{p*}$ 

1. In the model Hamiltonian of a one-dimensional metal

$$\mathcal{H} = \sum_{p\sigma} (e_{p} - \mu) a_{p\sigma}^{+} a_{p\sigma}^{+} g \sum_{p\sigma} a_{p+q,\sigma}^{+} a_{p\sigma} (b_{q} + b_{-q}^{+})$$

$$+ V_{D} \sum_{p\sigma} \sum_{p'\sigma'} a_{p+q,\sigma}^{+} a_{p\sigma} a_{p\sigma}^{+} a_{p'-q,\sigma'}^{+} a_{p'\sigma'}^{+} + V_{s} \sum_{p} \sum_{p'} a_{p\sigma}^{+} a_{-p-\sigma}^{+} a_{-p'-\sigma'}^{-} a_{p'\sigma'}^{-}$$
(1)

we retain out of the interaction of the electrons with other and with the lattice only the terms that are responsible for the instabilities in the Peierls (the second and third) and superconducting (fourth) channels. Here  $a_{p\sigma}$  and  $b_Q$  are the annihilation operators for an electron and a photon in states respectively with quasimomenta p and Q ( $\sigma$  is the spin index). We shall assume that the matrix elements  $V_D$  and  $V_s$  include all the possible types of interelectron interaction (Coulomb, exchange of phonons, etc.).

The quasimomentum dependence of the electron energy

$$\varepsilon_p = -W \cos pd \tag{2}$$

(2W is the band width and d is the period of the chain) possesses the obvious property:

$$\varepsilon_p + \varepsilon_{p+Q_0} = 0, \quad Q_0 = \pi/d.$$
 (3)

The shift of the chemical potential  $\mu = \varepsilon_{kF} = -W \cos k_F d$ from its position,  $\mu = 0$  with  $k_F^0 = \pi/2d$ , at the middle of the band takes account in the Hamiltonian (1) of the deviation of the filling of the band from the exactly halffilled situation.

We shall follow the stability of the phonon subsystem on the example of its interaction, involving momentum transfers  $Q \sim 2k_F$ , with the electrons. The stability is established according to the behavior of the phonon Green function

$$D(\Omega_n, Q) = D_0(\Omega_n, Q) / [1 - g^2 D_0(\Omega_n, Q) \Pi(\Omega_n, Q)], \qquad (4)$$

where  $D_0(\Omega_n, Q)$  is the free-phonon Green function:

$$D_0(\Omega_n, Q) = -1/[\Omega_n^2 + \omega_0^2(Q)],$$

while  $\Pi(\Omega_n, Q)$  is the polarization operator:

$$\Pi(\Omega_n, Q) = -2T \sum_n \sum_p G_p^{(0)}(\omega_n) G_{p-Q}^{0}(\omega_n - \Omega_n), \qquad (5)$$

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which it is sufficient to compute in terms of the noninteracting-electron Green functions  $G_{b}^{(0)}(\omega_{n})^{[13]}$ :

$$G_p^{(0)}(\omega_n) = 1/(i\omega_n - \varepsilon_p + \mu).$$

In normal (N) processes the initial and final electron states should belong to the first Brillouin zone, i.e., |p|,  $|p-Q| < Q_0$ . In the static limit  $\Omega_n - 0$ , we find from (5) that

$$\Pi_{N} = \int_{q}^{\infty} \frac{dp}{2\pi} \left( th \frac{\varepsilon_{p} - \mu}{2T} + th \frac{\varepsilon_{p-q} + \mu}{2T} \right) \frac{1}{\varepsilon_{p} + \varepsilon_{p-q}}, \quad q = Q - Q_{o}.$$
(6)

The umklapp (U) processes make the remaining part of the first Brillouin zone accessible for scattering of phonons of the  $\omega_0(Q)$  mode:  $|p|, |p-Q+H| < Q_0$ ,

$$\Pi_{\nu} = \int_{-\phi_{\nu}}^{q} \frac{dp}{2\pi} \left( \operatorname{th} \frac{\varepsilon_{p} - \mu}{2T} + \operatorname{th} \frac{\varepsilon_{p-q} + \mu}{2T} \right) \frac{1}{\varepsilon_{p} + \varepsilon_{p-q}}.$$
 (7)

Introducing the new variable  $\varepsilon = \varepsilon_{p-q/2}$ , let us rewrite  $\Pi_N$  and  $\Pi_{U}$ :

$$\Pi_{N} = 2N(0) \int_{0}^{\infty} d\epsilon \,\eta(\epsilon) f(\epsilon, \mu_{-}),$$

$$\Pi_{v} = 2N(0) \left[ \int_{0}^{w} d\epsilon \,\eta(\epsilon) f(\epsilon, \mu_{+}) + \int_{w_{1}}^{w} d\epsilon \,\eta(\epsilon) f(\epsilon, \mu_{-}) \right],$$
(8)

where we have introduced the notation

$$f(\varepsilon,\mu) = \left( \operatorname{th} \frac{\varepsilon_{1}-\mu}{2T} + \operatorname{th} \frac{\varepsilon_{1}+\mu}{2T} \right) \frac{1}{2\varepsilon_{1}}, \quad \varepsilon_{1} = \varepsilon \cos(qd/2),$$
$$\mu_{\pm} = \mu \pm \sin(qd/2) \left( W^{2} - \varepsilon^{2} \right)^{\prime h}, \quad W_{1} = W \cos(qd/2),$$

and  $\eta(\varepsilon) = W/(W^2 - \varepsilon^2)^{1/2}$  is the density of states normalized to its value,  $N(0) = L/\pi dW$ , in the middle of the onedimensional band.

The temperature satisfying the equation for the poles of the phonon Green function (4)

$$1 - \lambda_i \Pi_i = 0, \quad i = N, U, N + U, \tag{9}$$

determines the critical temperature,  $T_{p_i}$  for the development of the CDW of the mode  $\omega_0(Q)$  as a function of the location of the Fermi level  $\mu = -W \cos k_F d$  in the band of width 2W, the CDW period  $2\pi/Q$ , and the effective coupling constants  $\lambda_i = 2g_i^2/\omega_0(Q)$ . Allowance for the interelectron interactions leads to the result that as the  $\lambda_i$  we should set

$$\lambda_{i} = [2g^{2}/\omega_{0}(Q) + V_{D}]_{i}, \qquad (10)$$

where the index i = N, U labels the normal and umklapp processes.

We shall restrict ourselves to the consideration of the case of small deviations of the band filling from the middle, i.e., of the  $\mu \ll W$  case. It will be seen below that in this case the wave vector Q that gets established in the CDW system also differs little from  $Q_0 = \pi/d$ (which corresponds to a simple doubling of the period),

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i.e.,  $q = Q - Q_0 \ll Q_0$ . Under these conditions, it is convenient to transform the "exact" equation (10), appropriately changing<sup>[13]</sup> the order of summation when computing  $\Pi(\Omega_n, Q)$  in (5).

In the case of the normal processes we obtain from (9) that

$$\ln \frac{T_{p^{N}}}{T_{p^{0}}} - \operatorname{Re}\left[\psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + i\frac{\mu - \epsilon_{q/2}}{2\pi T_{p^{N}}}\right)\right] = 0,$$
(11)

where  $\varepsilon_{Q/2} = W \sin(qd/2) \approx v_F q/2$ ,  $\psi(x)$  is the digamma function, and  $T_{\neq 0}^N = (2\gamma/\pi) 4W \exp(-1/\lambda'_N)$  is the Peierls doubling temperature (q=0) for the exactly half-filled band, i.e., for  $\mu = 0$ .

To make a judgment about the actual value of the reconstruction temperature  $T_{pp}^{N}$  it is sufficient to know that, according to (11), the max $\{T_{p}^{N}\}$  is attained at  $\varepsilon_{Q/2}$ =  $\mu$ , i.e., at  $Q = 2k_{F}$ , and is equal to  $(T_{p}^{N})_{max} = T_{p0}^{N}$  irrespective of the location of the Fermi level in the onedimensional band. When allowance is made for only the normal processes, the corresponding dielectric gap always arises at the Fermi level. Let us, for completeness, give the dependence on the wave vector Q of  $T_{p}^{N}$ (Fig. 1), expressed for convenience in terms of  $\varepsilon_{Q/2}$ , for several values of the filling-deviation level  $\mu$ ; the  $T_{p}$  max line has been made distinct.

To demonstrate the role of the umklapp processes in the development of the Peierls instability, we shall restrict ourselves to the consideration of the case  $\lambda_U = \lambda_N$ . The corresponding equation for the determination of  $T_p$ with a simultaneous allowance for the N and U processes has the form<sup>[101</sup>

$$\ln \frac{T_{\mathfrak{p}}}{T_{\mathfrak{p}\mathfrak{o}}} - \operatorname{Re}\left\{\psi\left(\frac{1}{2}\right) - \frac{1}{2}\left[\psi\left(\frac{1}{2} + i\frac{\mu - \varepsilon_{\mathfrak{q}/2}}{2\pi T_{\mathfrak{p}}}\right) + \psi\left(\frac{1}{2} + i\frac{\mu + \varepsilon_{\mathfrak{q}/2}}{2\pi T_{\mathfrak{p}}}\right)\right]\right\} = 0,$$
(12)

where  $T_{\rho 0} = (2\gamma/\pi)\Delta_0$  is the transition temperature for  $\mu = 0$ ,  $\varepsilon_{Q/2} = 0$ , and a doubled (because of the fact that  $\lambda_N = \lambda_U = \lambda_p$ ) coupling constant and

$$\Delta_0 = 4W \exp\left(-\frac{1}{2\lambda_p N(0)}\right). \tag{13}$$

In Fig. 2 we show the dependence  $T_{\rho}(\varepsilon_{Q/2})$  for several values of  $\mu$ ; the  $T_{\rho max}$  curve has been made distinct. All

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the quantities  $(T_p, \mu, \varepsilon_{Q/2})$  are in units of  $\Delta_0$ . The role of the umklapp processes is manifested first and foremost in the effective doubling (for  $\lambda_N = \lambda_U$ ) of the coupling constant: into (13) enters  $2\lambda_p$  as compared to  $\lambda_N$  in (11). The type of function  $T_p(\varepsilon_{Q/2})$  is itself changed drastically.

It is quite evident that, with the appearance of a deviation,  $\mu$ , from the middle of the band, the max $\{T_p\}$  is first attained at  $\varepsilon_{Q/2} = 0$ . This means that, for small deviation levels  $\mu$ , an instability develops at the point  $T_p$  at double (2d) the period of the initial lattice. The limiting value  $\mu_{\rm cr}$ , right up to which the doubling of the period is still advantageous, is found from the condition Re $\partial^2 \psi(z)/\partial z^2|_{z=(0.5+i\mu_{\rm cr}/2\pi T_p)} = 0$ , and is equal to  $\mu_{\rm cr} = 0.602\Delta_0$ .<sup>[14]</sup>

At higher  $\mu$  levels, the max $\{T_{p}\}$  is now attained at a finite value of  $\varepsilon_{Q/2}$ , but still  $\varepsilon_{Q/2} \neq \mu$ . Thus, the wave vector  $Q = Q_{0} + q$  of the generated displacement wave is not equal to  $2k_{F}$  of the original one-dimensional metal, and, consequently, although the low-temperature phase is of the dielectric type, it has in its conduction band carriers whose concentration is determined not only by thermal excitation across the resulting gap, but also by the extent of the noncoincidence of Q and  $2k_{F}$ . This would correspond at T = 0 to a degenerate semiconductor. The connection between the indicated shift,  $\mu$ , of the chemical potential in the normal phase and the deviation,  $\delta n$ , of the concentration from the concentration corresponding to half filling of the band is established from the formula

$$\delta n = 2N(0) \int_{0}^{\infty} d\epsilon \, \eta(\epsilon) \left[ th(\epsilon + \mu)/2T - th(\epsilon - \mu)/2T \right]$$
(14)

and, under conditions of degeneracy  $(T \ll W)$  of the carriers, has the form

 $\delta n/2N(0) \approx W \arcsin \mu/W \approx \mu$ .

2. Let us turn to the investigation of the reconstruction of the electron spectrum and the lattice as a result of the instability of the phonon subsystem. Let us introduce for consideration the electron temperature function  $G_{p'p}(\tau)^{[131]}$ :





$$G_{p'p}(\tau) = -\langle \hat{T} \, \tilde{a}_{p'}(\tau) a_p^+(0) \rangle,$$

 $\tilde{a}_{p'}(\tau) = \exp(\tau \hat{H}) a_{p'} \exp(-\tau \hat{H}).$ 

The equations of motion for the Fourier components  $G_{\theta',\theta}(\omega_n)$  have the form

$$-\Delta(-Q)G_{p+2q, p} + (i\omega_{n} - \varepsilon_{p+q} + \mu)G_{p+q, p} - \Delta(Q)G_{pp} = 0,$$
  

$$-\Delta(-Q)G_{p+q, p} + (i\omega_{n} - \varepsilon_{p} + \mu)G_{pp} - \Delta(Q)G_{p-q, p} = 1,$$
  

$$-\Delta(-Q)G_{pp} + (i\omega_{n} - \varepsilon_{p-q} + \mu)G_{p-q, p} - \Delta(Q)G_{p-2q, p} = 0,$$
(15)

where the order parameter  $\Delta(Q)$ :

 $\Delta(Q) = g\langle \varphi_Q \rangle + V_D \rho_Q, \tag{16}$ 

is expressible in terms of the amplitude of the  $\omega_0(Q)$ -mode displacement wave,

 $\langle \varphi(z) \rangle = \langle \varphi_{Q} \rangle e^{iQz} + \langle \varphi_{-Q} \rangle e^{-iQz}$ 

and the amplitude,

$$\rho_{Q} = \sum_{p} \langle a_{p-Q}^{+} a_{p} \rangle$$

of the real CDW.

If the wave vector Q is incommensurable with the reciprocal-lattice vector  $2\pi/d$ , then the order of the system (15) formally becomes infinite.

A. In a concrete analysis of the system (15), it is useful to consider the normal processes first, and then allow for the umklapp processes, in the same way as was done above in the study of  $T_{p}$ .

Clearly, for the N processes the states with the quasimomenta p' and p should belong to the first Brillouin zone:  $|p'|, |p| < Q_{0}$ . Then for a CDW with some Q (for definiteness,  $Q - Q_0 = q > 0$ ) there remain out of the complete system (15) only the equations

$$(i\omega_{n}-\varepsilon_{p}+\mu)G_{pp}-\Delta(Q)G_{p-q, p}=1,$$

$$-\Delta(-Q)G_{pp}+(i\omega_{n}-\varepsilon_{p-q}+\mu)G_{p-q, p}=0.$$

$$q 
(17)$$

Similarly, in the equivalent region  $-Q_0 of the first zone only <math>G_{p+Q,p}$  does not vanish (cf. Eq. (6)). Finally, for the electrons with  $|p| < Q - Q_0$  we should set  $G_{p-Q,p} = G_{p+Q,p} \equiv 0$ , since these electrons cannot transfer the momentum Q without leaving the first zone.

Solving (17), we find, for example, in the region q

$$G_{pp} = (i\omega_n + \varepsilon_{p-q} + \mu)/D(p, \omega_n), \ G_{p-q, p} = \Delta(Q)/D(p, \omega_n),$$
$$D(p, \omega_n) = (i\omega_n + \mu - \varepsilon_p) (i\omega_n + \mu + \varepsilon_{p-q}) - |\Delta(Q)|^2.$$

The self-consistency equation for  $\Delta(Q)$  is obtained after eliminating the amplitudes  $\langle \varphi_Q \rangle = \langle b_Q + b_Q^* \rangle / \omega_0^{1/2}(Q)$  from (16) with the aid of the equations of motion for the phonon averages (for greater details, see Ref. 15), and has the form (the index N denotes normal processes):

$$\Delta(Q) = \lambda_N 2T \sum_{n} \sum_{p>q}^{Q} G_{p-q,p}(\omega_n), \quad \lambda_N = [2g^2/\omega_0(Q) + V_D]_N.$$
 (18)

After the summation over n and the substitution

$$\sum_{p}\ldots \rightarrow N(0)\int d\varepsilon \,\eta(\varepsilon)\ldots$$

we obtain the equation of state of the low-symmetry phase with allowance for only the N processes:

$$\frac{1}{\lambda_{N'}} = \int_{0}^{W_{1}} d\epsilon \,\eta(\epsilon) \left( th \,\frac{E-\mu_{-}}{2T} + th \,\frac{E+\mu_{-}}{2T} \right) \Big/ \,2E, \tag{19}$$

where

$$E = (\varepsilon^2 \cos^2 (qd/2) + \Delta^2)^{\nu_h}, \ \mu_- = \mu - (W^2 - \varepsilon^2)^{\nu_h} \sin (qd/2),$$
$$W_1 = W \cos (qd/2), \ \lambda_N' = \lambda_N N(0).$$

For  $T = T_p$ , when  $\Delta \rightarrow 0$ , Eq. (19) goes over into (10). Let us begin the study of the ground state (T = 0) with the study of a CDW with such Q that at a given value of  $\mu$  the condition

 $\mu - W \sin (qd/2) = \varepsilon_{kF} - \varepsilon_{q/2} < \Delta.$ 

is fulfilled. A direct computation of (19) yields

$$\frac{1}{\lambda_{N'}} = \int_{0}^{n'} d\epsilon \, \frac{\eta(\epsilon)}{E} = \frac{W}{(W_{1}^{2} + \Delta^{2})^{\nu_{1}}} \bigg[ K \left( \frac{W_{1}}{(W_{1}^{2} + \Delta^{2})^{\nu_{1}}} \right) \\ -F \left( \frac{qd}{2}, \frac{W_{1}}{(W_{1}^{2} + \Delta^{2})^{\nu_{1}}} \right) \bigg], \qquad (20)$$

where K is the complete, and F the incomplete, elliptic integral of the first kind. Clearly, for  $q \ll Q_0$ , qd/2 $\ll \pi/2$  and  $W_1/(W_1^2 + \Delta^2)^{1/2} \sim 1$ . Using the asymptotic representations for K and F, we find, neglecting  $\Delta$  in comparison with  $W_1$ ,

$$\frac{1}{\lambda_{N'}} = \frac{1}{\cos\left(qd/2\right)} \ln \frac{4W[1-\sin\left(qd/2\right)]}{\Delta},$$
  
i.e.,

$$\Delta(Q) = 4(W - \varepsilon_{Q/2}) \exp(-1/\lambda_N N(\varepsilon_{Q/2})).$$
(21)

Let us draw attention to the fact that the coupling constant  $\lambda_N$  enters with the enhanced density of states  $N(0)/\cos(qd/2) = N(\varepsilon_{Q/2})$ , but then the energy range in which the interaction is important decreases by a factor of  $[1 - \sin(qd/2)]$  in comparison with the simple doubling of the period at q = 0.

The change,  $\Delta \Omega_D$ , in the electronic part of the free energy,

$$\Delta\Omega_{p} = \int \Delta^{2} \frac{\partial}{\partial \Delta} \left( \frac{1}{\lambda_{N}} \right) d\Delta = -\frac{1}{2} N(\varepsilon_{q/2}) \Delta^{2} , \qquad (22)$$

indicates that the dielectric state is preferred to the initial metallic state, while the variation with respect to Q (or q) clearly determines the self-consistent period,  $2\pi/Q$ , of the CDW that is established at T = 0.

Formally, the equation of state (18) admits of another type of solution,  $\Delta'$ , corresponding to such a wave vector Q in the CDW that  $\mu - \varepsilon_{Q/2} > \Delta'$ :

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where  $\Delta$  is given by the formula (21). The corresponding change  $\Delta \Omega'_D$ , however, turns out to be positive. This proves that the wave vector, Q, of the displacement wave should in any case be such that the condition (19) is <u>fulfilled</u>:  $\varepsilon_{kF} - \varepsilon_{Q/2} < \Delta$ ,

Notice in this connection that there is a difference in the behavior of systems with a given value of the deviation,  $\mu$ , from the middle of the band and with a given value of the carrier-concentration excess,  $\delta n$ , over the concentration that corresponds to the half-filled band. The equation of state (18) in the latter case should be supplemented by the equation

$$\delta n = 2N(0) \int_{0}^{\pi} de \ \eta(e) \ \{ th[(E+\mu_{-})/2T] - th[(E-\mu_{-})/2T] \}, \qquad (23)$$

which expresses the condition for the conservation of charge in the phase transition. For T = 0 and  $\delta n = 0$ , there remains out of all the  $\Delta(Q)$  contained in (18) the solution with  $Q = Q_0$ :

$$\Delta_0^{N} = 4W \exp\left(-1/\lambda_{N'}\right), \qquad (24)$$

which corresponds to exact doubling of the period.

Any given finite value of  $\delta n > 0$  necessarily leads to  $\mu_{-} = \mu - \epsilon_{0/2} > \tilde{\Delta}$ , since we have, on account of (23),

 $n = \delta n/2N(0) \approx (\mu_{-}^{2} - \bar{\Delta}^{2})^{\frac{1}{2}}$ 

Eliminating then from the equation of state  $\mu_{-} = (\bar{\Delta}^2 + n^2)^{1/2}$ , we find the dependence of the order parameter  $\bar{\Delta}$  on *n*:

 $\bar{\Delta} = [\Delta(\Delta - 2n)]^{\nu},$ 

where  $\Delta$  is a quantity which can be computed from the formula (21). The change,  $\Delta \tilde{\Omega}_D$ , in the free energy for  $n < \Delta/2$  is equal to

$$\Delta \widetilde{\Omega}_{p} = -\frac{1}{2} N(\varepsilon_{Q/2}) \left[ \Delta(Q) - 2n \right]^{2}.$$

For  $n > \Delta(Q)/2$  the metallic phase is stable at T = 0.

B. In the case when the umklapp processes are taken into account, the uncoupling of  $G_{\mu \pm nQ, \rho} = 0$  for n > 1 becomes, in contrast to the case of the normal processes, illegitimate, and we are formally obligated to turn to the complete system of equations (15). The presence of the higher harmonics  $G_{\mu\pm nQ, \rho}$  with n > 1 implies that, under the conditions of incommensurability of Q and  $\pi/d$ , instead of the barely unstable displacement of the type  $\langle \varphi \rangle \sim \cos Qz$ , a more complex CDW is established in a self-consistent fashion.

It can, however, be seen from the solution to the system (15) that, compared to the (n-1)-th harmonic  $G_{p\pm(n-1)Q,p}$ ,  $G_{p\pm nQ,p}$  contains a superfluous power of the order parameter  $\Delta$ . The relative order of the corresponding corrections in the self-consistency equations is, in its turn, equal to  $\Delta/W$ . Therefore, in the frame-

work of the Hartree-Fock scheme, we should in the equation for  $\Delta$  retain only the components  $G_{p-Q,p}$  and  $G_{p+Q,p}$ .

To demonstrate the role of the umklapp processes, let us again consider the case of equal constants,  $\lambda_N = \lambda_U = \lambda_p$ , for the normal and umklapp processes.

The self-consistency equation

$$\Delta = \lambda_p 2\pi T \sum_p \sum_n G_{p-Q,p}(\omega_n) = \lambda_p 2\pi T \sum_p \sum_n (\Delta/D_+ + \Delta/D_-),$$

where the summation over p is performed in the first Brillouin zone and

$$D_{\pm}^{2} = \Omega_{\pm}^{2} - \varepsilon^{2} \cos^{2} q d/2 - \Delta^{2}, \ i \Omega_{\pm} = i \omega_{n} + \mu_{\pm},$$

after the summation over  $\omega_n$  and standard transformations, assumes the form

$$\frac{1}{\lambda_{p'}} = \int_{0}^{w} d\epsilon \,\eta(\epsilon) \left[ \operatorname{th} \frac{E-\mu_{-}}{2T} + \operatorname{th} \frac{E+\mu_{-}}{2T} + \operatorname{th} \frac{E-\mu_{+}}{2T} + \operatorname{th} \frac{E+\mu_{+}}{2T} \right] \frac{1}{2E}.$$
(25)

The solution,  $\Delta$ , to Eq. (25) at T = 0 depends essentially on the quantity  $\mu$ .

1) For small  $\mu < \Delta$ , CDW with such Q that the condition  $\mu_- < \mu_+ < \Delta$  is fulfilled are admissible. Then for T = 0 we find from (25) the equation

$$\frac{1}{\lambda_{p'}} = 2 \frac{W}{(W_i^2 + \Delta^2)^{\frac{1}{1}}} \operatorname{K}\left(\frac{W_i}{(W_i^2 + \Delta^2)^{\frac{1}{1}}}\right).$$

Using the asymptotic form of the complete elliptic integral K for  $W_1/(W_1^2 + \Delta^2)^{1/2} \sim 1$ , let us solve it for  $\Delta$ :

$$\Delta = \Delta_1 = 4 \left( W^2 - \varepsilon_{Q/2}^2 \right)^{\frac{N}{2}} \exp\left[ -\frac{1}{2\lambda_p} N(\varepsilon_{Q/2}) \right].$$
<sup>(26)</sup>

Notice that allowance for the umklapps leads to an increase in the effective interaction (to its doubling when  $\lambda_N = \lambda_U$ ).

The change in the free energy can be computed as before from the formula (22), and is now equal to

$$\Delta\Omega_1 = -\frac{1}{2}N(\varepsilon_{Q/2})\Delta_1^2, \qquad (27)$$

the max $\{-\Delta \Omega_1\}$  is attained at  $Q = Q_0$ , i.e.,

$$(\Delta_{i})_{opt} = 4W \exp\left(-\frac{1}{2\lambda_{P}N(0)}\right) = \Delta_{0}.$$
(28)

It follows from this that the ground state is insensitive to doping,  $\mu$ , until this quantity exceeds the maximum possible dielectric gap,  $\Delta_0$ , in the system. The CDW that is established corresponds in this case to a simple doubling of the period with  $Q = Q_0$ .

For  $\mu > \Delta$  (when  $\mu_+ > \Delta$  as well), the properties of the ground state are determined by the relation between  $\mu_-$  and  $\Delta_-$ 

2) For example, for the solutions  $\Delta_2$  that are such that  $\mu_- < \Delta_2 < \mu_+$ , the region  $\varepsilon \cos(qd/2) < (\mu_+^2 - \Delta^2)^{1/2}$  drops out from the integration at T = 0, and Eq. (25) assumes the form

$$\frac{1}{\lambda_{p'}} = 2 \frac{W}{(W_{i}^{2} + \Delta_{2}^{2})^{\frac{1}{h}}} \left\{ K\left(\frac{W_{i}}{(W_{i}^{2} + \Delta_{2}^{2})^{\frac{1}{h}}}\right) - \frac{1}{2} F\left(\arcsin\frac{(\mu_{+}^{2} - \Delta_{2}^{2})^{\frac{1}{h}}}{\mu_{+}}, \frac{W_{i}}{(W_{+}^{2} + \Delta_{2}^{2})^{\frac{1}{h}}}\right) \right\}$$

whence, using the asymptotic forms of K and F in the case when  $W_1/(W_1^2 + \Delta_2^2)^{1/2} \sim 1$ , we find that

$$\{\Delta_{2}[\mu_{+}+(\mu_{+}^{2}-\Delta_{2}^{2})^{\prime h}]\}^{\prime h}=4(W^{2}-\varepsilon_{Q/2}^{2})^{\prime h}\exp[-1/2\lambda_{P}N(\varepsilon_{Q/2})].$$
 (29)

The change,  $\Delta\Omega_2$ , that occurs in the free energy during the changeover to the CDW state with these Q is equal to

$$\Delta\Omega_{2} = -N(\epsilon_{q/2})\Delta_{2}^{2}\{1-\mu_{+}/[(\mu_{+}^{2}-\Delta_{2}^{2})^{\nu_{+}}+\mu_{+}]\},$$
(30)

where  $\Delta_2$  is found from Eq. (29).

3) If, on the other hand,  $\Delta < \mu_{-} < \mu_{+}$ , then the order parameter  $\Delta_{3}$  in this case satisfies the equation

$$\{[\mu_{+}+(\mu_{+}^{2}-\Delta_{s}^{2})^{\nu_{1}}][\mu_{-}+(\mu_{-}^{2}-\Delta_{s}^{2})^{\nu_{2}}]\}^{\nu_{1}}=4(W^{2}-e^{2}_{e/2})^{\nu_{1}}\exp[-1/2\lambda_{p}N(e_{e/2})].$$
(31)

but a CDW with such Q turns out to be energetically disadvantageous (since the corresponding calculation yields  $\Delta\Omega_3 > 0$ ), and is not realized at any given  $\mu$ .

From a comparison of the cases 1) and 2) we conclude that in a regime of given  $\mu$  we can have either a dielectric state with a doubled period (when  $\mu < \Delta$ ), or a conducting state of the semiconducting type with the order parameter  $\Delta_2$ , (29), but without a gap in the excitation spectrum (when  $\mu > \Delta$ ). In fact, the value of Q that gets established in the CDW in the  $\mu > \Delta$  case is found from the corresponding variation  $\Delta\Omega_2$ , (30), with respect to Q (or q).

A different behavior is exhibited by the one-dimensional system during the reconstruction in the case when the number,  $\delta n$ , of carriers above the halfway filling mark of the band is given. As before, for the normal processes, the equation of state (25) should be supplemented by the electrical-neutrality equation

$$\frac{\delta n}{2N(0)} = n = \int_{0}^{\pi} d\varepsilon \,\eta(\varepsilon) \left[ \operatorname{th} \frac{E+\mu_{-}}{2T} - \operatorname{th} \frac{E-\mu_{-}}{2T} + \operatorname{th} \frac{E+\mu_{+}}{2T} - \operatorname{th} \frac{E-\mu_{+}}{2T} \right]. \tag{32}$$

If it is given that n=0 at T=0, then, clearly,  $\mu_- < \mu_+ < \Delta$ . In this case the order parameter  $\Delta = \Delta_0$  and the change  $\Delta\Omega$  are determined by the preceding formulas (28) and (27), and  $Q_{opt} = Q_0$ . A fixed value of  $n \neq 0$  can be maintained by the low-symmetry phase at T=0 in two ways:

a)  $\mu_{-} < \Delta < \mu_{+}$ . Equation (32) then gives  $n = (\mu_{+}^{2} - \Delta_{a}^{2})^{1/2}/2$ . Eliminating then  $\mu_{+} = (4n^{2} + \Delta_{a}^{2})^{1/2}$  from Eq. (29), we obtain an equation for the determination of the order parameter  $\Delta_{a}$  in this case:

 $\Delta_{a}^{4}+4n\Delta_{a}\Delta_{1}^{2}-\Delta_{1}^{4}=0,$ 

where the quantity  $\Delta_1$  is given by the formula (26). The change in the free energy is then equal to

$$\Delta\Omega_{a} = -N(\epsilon_{q/2}) \left[ \Delta_{a}^{2} + 4n^{2} - 2n(\Delta_{a}^{2} + 4n^{2})^{\frac{1}{2}} \right].$$
(33)

b)  $\Delta < \mu_{-} < \mu_{+}$ . In this case Eq. (32) reduces at T = 0 to

$$2n = (\mu_{+}^{2} - \Delta_{6}^{2})^{\frac{1}{2}} + (\mu_{-}^{2} - \Delta_{6}^{2})^{\frac{1}{2}}.$$

Eliminating from this relation and Eq. (31) the quantity  $\mu$ , we obtain an equation for the order parameter  $\Delta_b$ :

$$\Delta_{b} = [\Delta_{1} (\Delta_{1} - 2|n^{2} - \varepsilon_{q/2}^{2}|^{N})]^{N}, \qquad (34)$$

where  $\Delta_1$  is computed as before from the formula (26). The change in the free energy is equal to

$$\Delta \Omega_{b} = -N(\varepsilon_{q/2}) \left[ \Delta_{1} - 2 |n^{2} - \varepsilon_{q/2}^{2}|^{\frac{1}{2}} \right]^{2}.$$
(35)

The condition  $\mu_{-} = \Delta$  determines in the  $n - \varepsilon_{Q/2}$  plane the equation of some curve,

$$(n+\varepsilon_{Q/2})^2|n^2-\varepsilon_{Q/2}^2|=\varepsilon_{Q/2}^2\Delta_1^2,$$

that delimits states of the type a) and b) with one and the same carrier concentration n in the conduction zone of the reconstructed phase. We infer from the expressions for the corrections,  $\Delta\Omega_a$  and  $\Delta\Omega_b$ , to the thermodynamic potentials on this curve,

$$\Delta\Omega_{a} = -\frac{1}{2}N(\varepsilon_{q/2})\left[\Delta_{1}^{2} + 2(n+\varepsilon_{q/2})^{2}\right]\left(\frac{n-\varepsilon_{q/2}}{n+\varepsilon_{q/2}}\right)^{2},$$
  
$$\Delta\Omega_{b} = -\frac{1}{2}N(\varepsilon_{q/2})\Delta_{1}^{2}\left(\frac{n-\varepsilon_{q/2}}{n+\varepsilon_{q/2}}\right)^{2},$$

that for a given *n* the states with those *Q* for which  $\mu_- < \Delta < \mu_+$ , i.e., states of the type a), are more advantageous. Thus, the period  $2\pi/Q$  that gets established at T = 0 in the one-dimensional system should be found from  $\Delta\Omega_a$ , (33).

3. For the simultaneous consideration of the instabilities of the one-dimensional metal in the superconducting and Peierl's channels, let us introduce, besides the functions  $G_{pp}$  and  $G_{p-Q,p}$ , the nondiagonal anomalous function

$$F(x, x') = -\langle \widehat{T} \psi_{\sigma}(x) \psi_{-\sigma}(x') \rangle.$$

As before, let us restrict ourselves to the case of equal constants,  $\lambda_U = \lambda_N = \lambda_p$ , for the normal and umklapp scattering processes in the Peierls channel. After Fouriertransforming the equation of motion for the components, the electron Green functions assume the form

$$\begin{pmatrix} i\omega_{n}-\varepsilon_{p}+\mu & -\Delta_{p} & \Delta_{s} & 0\\ -\Delta_{p} \cdot & i\omega_{n}-\varepsilon_{p-q}+\mu & 0 & \Delta_{s}\\ \Delta_{s} \cdot & 0 & i\omega_{n}+\varepsilon_{p}-\mu & \Delta_{p}\\ 0 & \Delta_{s} \cdot & \Delta_{p} \cdot & i\omega_{n}+\varepsilon_{p-q}-\mu \end{pmatrix}$$

$$\begin{pmatrix} G_{p,p} \\ G_{p-q,p} \\ F_{p,-p} \\ F_{p,-p} \\ F_{p,-p} \end{pmatrix} = \begin{pmatrix} 1\\ 0\\ 0\\ 0 \\ 0 \end{pmatrix}$$
(36)

where

$$\Delta_{s} = -\lambda_{s} 2\pi T \sum_{p} \sum_{n} F_{p,-p}(\omega_{n}), \quad \Delta_{p} = -\lambda_{p} 2\pi T \sum_{p} \sum_{n} G_{p-q,p}(\omega_{n}). \quad (37)$$

Notice that into the equations of motion is inevitably drawn, along with  $F^*_{p,p}$ , the component  $F^*_{p-Q,p}$  of the

anomalous function, although it has itself no logarithmic singularity. For this reason, the corresponding component of the superconducting-order parameter is not retained in (36). Assuming that the superconducting interaction includes all the possible superconductivity mechanisms (e.g., the excitonic, <sup>[1,6]</sup> etc.), we can assume the constants  $\lambda_s$  and  $\lambda_p$  to be independent phenomenological parameters of the theory.

The solution to a system of the type (36) in the simple  $Q = Q_0$  case of the conventional doubling was investigated in detail in Refs. 15 and 16. The classification of the solutions to the system (36) according to the relation between the phases of the order parameters  $\Delta_p$  and  $\Delta_s$ remains entirely valid under the conditions of incommensurability of Q and  $\pi/d$ . Below we consider the socalled symmetric solution, when  $\Delta_s$  and  $\Delta_p$  are both real and of the same sign, which solution, according to Ref. 16, has the broader existence domain.

The solution to the system (36) has the form

$$DG_{pp} = (i\omega - \varepsilon_{p} + \mu) [(i\omega + \varepsilon_{p} - \mu) (i\omega + \varepsilon_{p-q} - \mu) - \Delta_{p}^{2}] - (i\omega + \varepsilon_{p} - \mu) \Delta_{s}^{2},$$

$$DG_{p-q, p} = \Delta_{p} [(i\omega + \varepsilon_{p-q} - \mu) (i\omega + \varepsilon_{p} - \mu) - \Delta_{p}^{2} - \Delta_{s}^{2}],$$

$$DF_{p,-p}^{+} = \Delta_{s} [\omega^{2} + (\varepsilon_{p-q} - \mu)^{2} + \Delta_{p}^{2} + \Delta_{s}^{2}],$$

$$DF_{p-q,p}^{+} = -\Delta_{s} \Delta_{p} (\varepsilon_{p} + \varepsilon_{p-q} - 2\mu),$$
(38)

where D is the determinant of the system (36). The functions  $G_{p-Q,p}$  and  $F_{p,-p}^{*}$  from (38) when substituted into (37) determine the self-consistency equations for  $\Delta_{p}$  and  $\Delta_{s}$ .

At T = 0 these equations can be written in the form

$$1/\lambda_{p'} = [J_{1}(W, \mu_{+}) + J_{1}(W, \mu_{-})]/2, \qquad (39)$$

$$\frac{1}{\lambda_{*}} = [J_{1}(\tilde{\omega}, \mu_{+}) + J_{1}(\tilde{\omega}, \mu_{-}) + \mu_{+}J_{2}(\tilde{\omega}, \mu_{+}) + \mu_{-}J_{2}(\tilde{\omega}, \mu_{-})]/2, \quad (40)$$

where

$$J_{1}(A,\mu) = \frac{1}{2} \int_{0}^{A} de \frac{1}{E} \left( \frac{E+\mu}{\omega_{+}} + \frac{E-\mu}{\omega_{-}} \right),$$
  
$$J_{2}(A,\mu) = \frac{1}{2} \int_{0}^{A} de \frac{1}{E} \left( \frac{1}{\omega_{-}} - \frac{1}{\omega_{+}} \right),$$
 (41)

 $E = (\varepsilon^2 + \Delta_p^2)^{\frac{1}{2}}, \ \omega_{\pm} = [(E \pm \mu)^2 + \Delta_s^2]^{\frac{1}{2}}, \ \lambda' = \lambda N(0),$ 

 $\tilde{\omega}$  is the cutoff energy for the effective interaction in the superconducting channel ( $\tilde{\omega} \sim \omega_D$ ), while the density of states has been replaced by the constant N(0).

The question of the coexistence of the dielectric and superconducting phases reduces, in the framework of the above-adopted formulation of the problem, to the question whether there exists a thermodynamically-advantageous nontrivial simultaneous solution to the "equations of state" (39) and (40) with  $\Delta_p \neq 0$  and  $\Delta_s \neq 0$ . The answer to this question can be obtained by investigating the case of a weak (in comparison with the dielectric) superconducting order, i.e., the case when  $\Delta_s \ll \Delta_p$ . Then we can set in Eq. (39)  $\Delta_s = 0$ , which corresponds to the neglect of the inverse effect of the superconducting ordering on the dielectric ordering. We can also set  $\Delta_s = 0$  in the integrals  $J_1(\tilde{\omega}, \mu_{\pm})$  in Eq. (40), since these integrals do not have singularities when considered as functions of  $\Delta_s$ . The quantity  $\Delta_s$  should, however, be

retained in the terms with  $J_2(\tilde{\omega}, \mu_{\pm})$  when a divergence, which indicates the instability of the dielectric phase against Cooper pairing, arises in them at  $\Delta_s = 0$ . After this, the necessary integrations can easily be performed and, depending on the relation between  $\mu_{\pm}$  and  $\Delta_p$ , three essentially different cases should be distinguished (cf. Sec. 2).

a)  $\mu_{-} < \mu_{+} < \Delta_{p}$ . We set everywhere  $\Delta_{s} = 0$ , since in this case  $J_{2}(\tilde{\omega}, \mu_{\pm})$  does not diverge at  $\Delta_{s} = 0$ , and find from (39) and (40) the expression

$$\frac{1}{\lambda_{p}'} = \ln \frac{2W}{\Delta_{p}}, \quad \frac{1}{\lambda_{\star}'} = \ln \frac{2\omega}{\Delta_{p}} + \frac{1}{2} [a(\mu_{+}) + a(\mu_{-})], \quad (42)$$

where

$$a(\mu) = \frac{\mu}{(\Delta_{p}^{2} - \mu^{2})^{\frac{1}{1}}} \operatorname{arctg} \frac{\mu}{(\Delta_{p}^{2} - \mu^{2})^{\frac{1}{1}}}.$$

Since  $1/\lambda'_{p} = \ln(2W/\Delta_{p0})$  and  $1/\lambda'_{s} = \ln(2\tilde{\omega}/\Delta_{s0})$ , where  $\Delta_{p0}$  and  $\Delta_{s0}$  are the order parameters of the pure dielectric and superconducting phases, let us rewrite (42) in the form of a unified relation,

$$\ln \left( \Delta_{p0} / \Delta_{s0} \right) = \frac{1}{2} \left( a(\mu_{+}) + a(\mu_{-}) \right), \tag{43}$$

which expresses the condition for the formation of the superconducting phase against a background of the dielectric phase at a given  $\mu < \Delta_{p0}$ . It can be seen from (43) that the smallness of the Cooper interaction  $\Delta_{s0} < < \Delta_{p0}$  can be compensated by the large magnitude of  $\mu_*/(\Delta_p^2 - \mu_*^2)^{1/2}$ , provided the quantity  $\mu_* \approx \mu + v_F q/2$  comes close to the edge of the forbidden band,  $2\Delta_p$ , of the dielectric phase. On the other hand, the equilibrium value of  $Q_{opt}$  for  $\Delta_s = 0$  is determined exclusively by the properties of the dielectric phase. In the present case  $\mu < \Delta_{p0}$  and, according to (28), we should set  $Q_{opt} = Q_0$ , i.e.,  $\mu_* = \mu_- = \mu$ . Therefore, instead of (43) we have

$$\ln \frac{\Delta_{p0}}{\Delta_{s0}} = \frac{\mu}{(\Delta_{p0}^2 - \mu^2)^{\frac{1}{1}}} \arctan \frac{\mu}{(\Delta_{p0}^2 - \mu^2)^{\frac{1}{1}}},$$
 (44)

from which we can determine the value of  $\mu$  necessary for the onset of the Cooper ordering for a given relation between the bare interactions  $\Delta_{s0}$  and  $\Delta_{p0}$ .

b) For  $\mu_{-} < \Delta_{\rho} < \mu_{+}$ , we retain  $\Delta_{s}$  in  $J_{2}(\tilde{\omega}, \mu_{+})$ . We find by much the same procedure used above that

$$\ln \frac{\Delta_{p_0}}{\Delta_{s_0}} = \frac{1}{2} \left[ \frac{\mu_+}{(\mu_+^2 - \Delta_p^2)^{\nu_1}} \ln \frac{4(\mu_+^2 - \Delta_p^2)}{\Delta_s [\mu_+ + (\mu_+^2 - \Delta_p^2)^{\nu_1}]} + \frac{\mu_-}{(\Delta_p^2 - \mu_-^2)^{\nu_1}} \operatorname{arctg} \frac{\mu_-}{(\Delta_p^2 - \mu_-^2)^{\nu_1}} \right].$$
(45)

The condition (45) is resolved with respect to  $\Delta_s$  by the BCS-type formula

$$\Delta_{s} = \frac{4(\mu_{+}^{2} - \Delta_{p}^{2})}{\mu_{+} + (\mu_{+}^{2} - \Delta_{p}^{2})^{\frac{1}{h}}} \exp\left\{-\frac{2(\mu_{+}^{2} - \Delta_{p}^{2})^{\frac{1}{h}}}{\mu_{+}}\left[\ln\frac{\Delta_{p0}}{\Delta_{s0}} -\frac{1}{2}\frac{\mu_{-}}{(\Delta_{p}^{2} - \mu_{-}^{2})^{\frac{1}{h}}}\operatorname{arctg}\frac{\mu_{-}}{(\Delta_{p}^{2} - \mu_{-}^{2})^{\frac{1}{h}}}\right]\right\},$$
(46)

where as  $\Delta_p$  we should substitute its value computed from (29) for the purely dielectric ordering.

The change that occurs in the free energy during the transition with the two order parameters  $\Delta_{\rho}$  and  $\Delta_{s}$  can be computed from the formula<sup>[16]</sup>

$$\Delta\Omega_{sp} = -\int_{c} \Delta_{p}^{2} \frac{d\lambda_{p}}{\lambda_{p}^{2}} - \int_{c} \Delta_{s}^{2} \frac{d\lambda_{s}}{\lambda_{s}^{2}},$$

where it is convenient to choose the integration path C, which joins the coordinate origin and the point with the given  $\lambda_p$  and  $\lambda_s$ , such that initially  $\lambda_s = 0$ , while  $\lambda_p$  varies from zero to  $\lambda_p$ . Along the remaining path  $\lambda_p = \text{const}$ , while  $\lambda_s$  varies from zero to  $\lambda_s$ . As a result, we obtain

$$\Delta \Omega_{sp}^{(b)} = \Delta \Omega_2 - N(0) \frac{1}{2} - \frac{\mu_+}{(\mu_+^2 - \Delta_p^2)^{\frac{1}{2}}} \frac{\Delta_s^3}{2}, \qquad (47)$$

where  $\Delta\Omega_2$  is the result of the integration over the section with  $\lambda_s = 0$ , a result which coincides, naturally, with the change that occurs in the free energy during the Peierls ordering, (29). It can be seen from (47) that the coexistence of superconductivity and the dielectric ordering is more advantageous than the purely dielectric ordering.

c)  $\Delta_p < \mu_- < \mu_+$ . In this case we find, in the same was as we found (46), that

$$\Delta_{s} = b(\mu_{+}) b(\mu_{-}) \exp\left\{-2 \ln \frac{\Delta_{p_{0}}}{\Delta_{s_{0}}} / \left(\frac{\mu_{+}}{(\mu_{+}^{2} - \Delta_{p}^{2})^{\frac{\mu_{+}}{\mu_{-}}}} + \frac{\mu_{-}}{(\mu_{-}^{2} - \Delta_{p}^{2})^{\frac{\mu_{+}}{\mu_{-}}}}\right)\right\},$$
(48)

where

$$\ln b(\mu) = \frac{\mu/(\mu^2 - \Delta_p^2)^{\frac{1}{\mu}}}{\mu_+/(\mu_+^2 - \Delta_p^2)^{\frac{1}{\mu}} + \mu_-/(\mu_-^2 - \Delta_p^2)^{\frac{1}{\mu}}} \ln \frac{4(\mu^2 - \Delta_p^2)}{\mu_+(\mu^2 - \Delta_p^2)^{\frac{1}{\mu}}},$$

while as  $\Delta_{\rho}$  we should substitute the solution to (31) for the dielectric ordering in the  $\Delta < \mu_{-} < \mu_{+}$  case. The corresponding change in the free energy is equal to

$$\Delta\Omega_{sp}^{(c)} = \Delta\Omega_{s} - N(0) \frac{1}{2} \left[ \frac{\mu_{+}}{(\mu_{+}^{2} - \Delta_{p}^{2})^{\frac{1}{2}}} + \frac{\mu_{-}}{(\mu_{-}^{2} - \Delta_{p}^{2})^{\frac{1}{2}}} \right] \frac{\Delta_{s}^{2}}{2}, \quad (49)$$

where  $\Delta\Omega_3$  is the result of the computation on the  $\lambda_s = 0$ segment. Because of the positiveness of  $\Delta\Omega_3$ , we concluded in Sec. 2 that a CDW with such Q that  $\mu \pm \varepsilon_{Q/2}$  $>\Delta_p$  is not realizable at a given  $\mu > \Delta_p$ . In spite of the fact that, when  $\mu_{-}$  is sufficiently close to the edge of the allowed band, the sign of  $\Delta\Omega_{sp}^{(c)}$ , (49), can on the whole change, we cannot say with certainty that a state with a  $\Delta_s$  of the type (48) is realizable.

Thus, the consideration of even the case of very weak superconducting ordering,  $T_{s0} \ll T_{\rho0}$ , to which we restrict ourselves here, shows that, upon the deviation of the Fermi level of a one-dimensional metal from the middle of the band, there arise conditions for the coexistence of a dielectric distortion and superconductivity. The coexistence manifests itself in the fact that the state with CDW that gets established in the one-dimensional system when  $\mu > \Delta_{\rho}$  is unstable against arbitrarily weak Cooper pairing, and lowers its symmetry with the superconducting order parameter  $\Delta_{s0}$ , which satisfies a BCS-type equation. From this standpoint quasi-one-dimensional objects, in which the dielectric order sets in sooner than in most other materials, deserve consideration when potential candidates for one-dimensional super-

conductivity are being selected. By properly controlling the magnitude of the deviation,  $\mu$ , of the Fermi level from the middle of the band, we can secure a transition into a conducting state of the semiconducting type because of the presence of  $\delta n$  free carriers above the dielectric gap  $\Delta_p$ ,  $\delta n$  being determined by the extent of the noncoincidence of Q and  $2k_F$ .

Notice that, according to (46), the superconducting order parameter  $\Delta_s$  can, depending on the location of  $\mu$ , attain values considerably exceeding  $\Delta_{s0}$ , which are accessible in the absence of dielectric ordering. This distinctive feature, which was earlier noted in threedimensional systems with simultaneous dielectric and superconducting order, <sup>[15,16]</sup> is explained by the fact that the superconducting order under consideration is established against a background of an enhanced density of states, which is due to the dielectric order.

Similarly, the corresponding critical temperature  $T_s$  can, depending on  $\mu$ , significantly exceed the critical temperature,  $T_{s0}$ , of the purely superconducting transition. This all the more indicates the need for a careful study of the low-temperature phase of quasi-one-dimensional systems with an electron concentration different from one per unit cell.

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- <sup>1</sup>W. A. Little, Phys. Rev. 134, A1416 (1964).
- <sup>2</sup>L. B. Coleman, M. J. Cohen, D. J. Sandman, F. G. Yamaguchi, A. F. Garito, and A. F. Heeger, Solid State Commun. 12, 1125 (1973).
- <sup>3</sup>I. F. Schegolev, Phys. Status Solidi A12, 9 (1972).
- <sup>4</sup>Yu. A. Bychkov, L. P. Gor'kov, and I. E. Dzyaloshinski, Zh. Eksp. Teor. Fiz. **50**, 738 (1966) [Sov. Phys. JETP **23**, 489 (1966)].
- <sup>5</sup>I. E. Dzyaloshinskii and A. I. Larkin, Zh. Eksp. Teor. Fiz. **61**, 791 (1971) [Sov. Phys. JETP **34**, 422 (1972)].
- <sup>6</sup>K. Levin, D. L. Mills, and S. L. Cunningham, Phys. Rev. B10, 3821 (1974).
- <sup>7</sup>M. Kimura, Prog. Theor. Phys. 53, 955 (1975).
- <sup>8</sup>R. Peierls, Quantum Theory of Solids, Oxford Univ. Press, London, 1955 (Russ. Transl., IIL, 1956).
- <sup>9</sup>H. Frölich, Proc. R. Soc. A233, 296 (1954).
- <sup>10</sup>M. C. Leung, Phys. Rev. B11, 4272 (1975).
- <sup>11</sup>I. E. Dzyaloshinskii, in: Collective Properties of Physical Systems, Nobel 24, 1973, p. 144; J. R. Schrieffer, in: Collective Properties of Physical Systems, Nobel 24, 1973, p. 145; Yu. V. Kopaev, Tr. Fiz. Inst. Akad. Nauk SSSR 86, 34 (1975).
- <sup>12</sup>Yu. V. Kopaev and A. I. Rusinov, Fiz. Tverd. Tela (Leningrad) **11**, 1306 (1969) [Sov. Phys. Solid State **11**, 1059 (1969)].
- <sup>13</sup>A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, Metody kvantovoi teorii polya v statisticheskoi fizike (Methods of Quantum Field Theory in Statistical Physics), Fizmatgiz, 1962 (Eng. Transl., Prentice-Hall, Englewood Cliffs, New Jersey, 1963).
- <sup>14</sup>G. J. Sarma, Phys. Chem. Solids 24, 1029 (1963).
- <sup>15</sup>Yu. V. Kopaev and R. Kh. Timerov, Zh. Eksp. Teor. Fiz. **63**, 290 (1972) [Sov. Phys. JETP **36**, 153 (1973)].
- <sup>16</sup>A. I. Rusinov, Do Chan Kat, and Yu. V. Kopaev, Zh. Eksp. Teor. Fiz. 65, 1984 (1973) [Sov. Phys. JETP 38, 991 (1974)].

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