

# Possible phase transitions in systems of interacting metallic filaments (quasiunidimensional metals)

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The effects of interactions between filaments on the properties of quasiunidimensional metals are discussed. It is shown that, together with the state considered previously,<sup>[9,10]</sup> in which dielectric and superconductive pairing coexist on a single filament, the interaction makes possible either a purely dielectric state of the Peierls type or a mixed state in which the superconducting and dielectric gaps  $\Delta^k$  are essential functions of the filament numbers  $i$  and  $k$ . The influence of transverse motion on the transition temperature and the possibility of superconducting states are taken into account.

## 1. INTRODUCTION AND CHOICE OF MODEL

Experimental studies in recent years have reawakened interest in the properties of one-dimensional systems. The most relevant of these are experiments with complexes based on TCNQ and variable-valency complexes based on Pt and Ir (see, for instance, the review paper by Shchegolev<sup>[1]</sup>). It has been found that for the set of filamentary-structure substances Qn-TCNQ<sup>[1]</sup>, NMP-TCNQ<sup>[2]</sup>, and TTF-TCNQ<sup>[3]</sup> the temperature dependence of the conductivity is metallic in character. At room temperature the conductivity reaches a value of about  $10^2-10^3 \text{ ohm}^{-1} \cdot \text{cm}^{-1}$  with a very high anisotropy ( $\sim 10^2-10^3$ ). In addition, these substances display an unusual "one-dimensional" metal-dielectric transition, accompanied by anomalous damping of the phonon mode<sup>[4]</sup>.

The existence of dynamic instabilities in a one-dimensional metal has been discussed many times. Instability with respect to ion shifts and damping of the phonon mode was discussed by Peierls<sup>[5]</sup> and Froehlich<sup>[6]</sup> (see also Afanas'ev and Kagan<sup>[7]</sup>), and antiferromagnetic instability (giant spin waves) by Overhauser<sup>[8]</sup>. It was shown by Bychkov and the present authors<sup>[9]</sup> that the Peierls instability is always accompanied by an instability of the BCS type, with the formation of Cooper pairs. It was explained in<sup>[9]</sup> that the formulas of Froehlich and Overhauser are incorrect by themselves. They correspond to the Hartree-Fock approximation (or, what is the same thing, the "ladder" approximation), which is inapplicable in the one-dimensional case and leads to a transition with the incorrect sign of the interaction. From<sup>[9]</sup> (the so-called "parquet" approximation) there follows the simultaneous appearance of dielectric (Peierls) and superconducting instabilities. It was later shown by Larkin and one of the present authors<sup>[10]</sup> that the antiferromagnetic instability can appear only in the case of a single electron in the unit cell, when Umklapp processes are significant in the one-dimensional case.

However, the even more rigorous parquet approximation<sup>[9,10]</sup> has extremely limited accuracy in the one-dimensional case. As a phenomenological theory of phase transitions, it corresponds to the molecular field approximation. When fluctuations are included in the one-dimensional case, the transition becomes badly smeared out. The formulas of<sup>[9,10]</sup> have numerical meaning in the region  $T - T_{c0} \gtrsim T_{c0}$  ( $T_{c0}$  is the temperature "according to molecular field theory").

In the present work we intend to take into account the various three-dimensional effects that, on the one hand,

make the "true" transition temperature finite, and on the other permit us to determine the region  $|T - T_c| \lesssim T_c$  in which theories of the Ginzburg-Landau type are applicable.

We consider a system of parallel metallic filaments packed into a plane lattice with distance  $a$  between filaments. In the first approximation, when in principle it should not lead to an incorrect answer, we may neglect electron hopping from one filament to another<sup>[1]</sup>.

For the Green's function of an electron in the temperature method, and for all the correlation functions in the following, it is convenient to use the mixed representation that indicates the momentum  $p$  along the filament and the number  $i, k, l, \dots$  of the corresponding filament. In this representation

$$\mathcal{G}_{\alpha\beta}^i(p) = \frac{\delta_{\alpha\beta}}{i\epsilon_n - v_F(|p| - p_F)};$$

here  $\alpha$  and  $\beta$  are spin indices, and  $\epsilon_n = 2\pi(n + 1/2)T$ . On each filament the region between  $-p_F$  and  $p_F$  in the one-dimensional reciprocal cell  $(-\pi/c, \pi/c)$  is filled by electrons (Fig. 1), so that the total three-dimensional electron density is  $n = 2p_F/a^2\pi$ . In the case when there is exactly one electron per period along the filament,  $p_F = \pi/2c$ .

If the electron hopping is significant we must transform from the "node" representation  $i, k, l, \dots$  to the transverse quasimomentum  $p$ . Then we can write

$$\mathcal{G}_{\alpha\beta}(p, p_\perp) = \frac{\delta_{\alpha\beta}}{i\epsilon_n - v_F(|p| - p_F) - w(p_\perp, p_\perp)},$$

where  $w$  is the "hopping energy," which is small compared to the Fermi energy:  $\epsilon_F = v_F p_F \gg w$ . In the three-dimensional reciprocal cell the absence of hopping corresponds to a plane Fermi surface, and the inclusion of hopping leads to a weak "corrugation" of the Fermi plane.

Even when the electrons move only along their respective filaments, their interactions can still be significant (cf.<sup>[1]</sup>). These include both the direct Coulomb interaction and the indirect interaction through phonons, since the filaments are densely bound ( $a \sim c$ ) in an elastic matrix and the phonon spectrum remains, in principle, three-dimensional. Non-phonon exchange mechanisms of a different type also lead to interactions between separate filaments<sup>[11,12]</sup>. In our model "phonon interactions" will be those that are cut off at energies higher than the Debye energy  $\omega_D$ . Non-phonon interactions are retained up to an energy  $\bar{\omega}$  on the order of the Fermi energy  $\epsilon_F$ .

## 2. BASIC EQUATIONS (NON-PHONON INTERACTIONS)

From the mathematical point of view, the principal difference between the one-dimensional problem of the electron-spectrum instability and the BCS theory of superconductivity is the existence of two special scattering channels. The first (Cooper) channel (Fig. 2a) corresponds to the coupling of two electrons at opposite ends of the Fermi surface (Fig. 1), and contributes a logarithmic integral of order  $\ln(\bar{\omega}/T)$ . The same logarithm is given by the second (Peierls) channel (Fig. 2b), which corresponds to the pairing of electrons with a hole at the opposite end of the Fermi surface. The anomalous scattering in this channel is characterized by momentum  $2p_F$ , and corresponds to Peierls doubling of the period<sup>[5,6]</sup> and a strong Kohn anomaly in the phonon spectrum<sup>[7]</sup>.

In the model with a weak interaction the summation of terms of the form  $(g \ln(\bar{\omega}/T))^n$  leads, owing to the mutual insertion of diagrams 2a and 2b into one another, to a system of parquet equations. We shall select the bare interactions as shown in Fig. 3. The difference from<sup>[10]</sup> consists in the fact that the constants  $g_1^{ik}$  and  $g_2^{ik}$  are now essential functions of the distance between filaments.

In the case of exactly one electron per (one-dimensional) cell,  $p_F = \pi/2c$ , as in<sup>[10]</sup>, logarithmic terms are given not only by the diagrams of Figs. 2a and 2b, but also by the diagrams related to the Umklapp processes  $p_1 + p_2 = p_3 + p_4 \pm 2\pi/c$ . These processes are described by the additional constant  $g_3^{ik}$ .

When hopping is neglected, we can explicitly separate the dependence of the vertex parts  $\Gamma$  on the spins  $(\alpha\beta\gamma\delta)$  and the filament numbers  $(iklm)$ :

$$\Gamma_{\alpha\beta\gamma\delta}^{iklm} (+---) = \gamma_1^{ik} \delta_{\alpha\gamma} \delta_{\beta\delta} \delta_{lm} - \gamma_2^{ik} \delta_{\alpha\delta} \delta_{\beta\gamma} \delta_{lm} \delta_{kl}, \quad (1)$$

where the  $\pm$  signs correspond to electrons lying at one or another of the "Fermi points"  $\pm p_F$ ; the functions  $\gamma_1^{ik}$  and  $\gamma_2^{ik}$  depend only on the longitudinal momenta and the frequencies. If scattering with Umklapp is possible, then together with the amplitude  $\Gamma$  in (1), which conserves the total momentum, we must also, as in<sup>[10]</sup>, take into account the vertex part

$$\Gamma_{\alpha\beta\gamma\delta}^{iklm} (+-+-) = \gamma_3^{ik} (\delta_{\alpha\gamma} \delta_{\beta\delta} \delta_{lm} - \delta_{\alpha\delta} \delta_{\beta\gamma} \delta_{lm} \delta_{kl}). \quad (2)$$

The fundamental scheme of the parquet equations is well known and has been described many times. In addition to<sup>[9]</sup>, a detailed discussion is given in the first work



FIG. 1

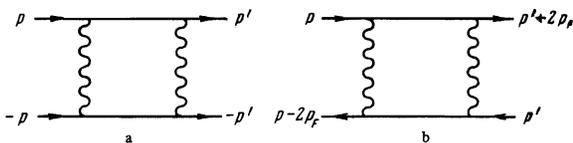


FIG. 2

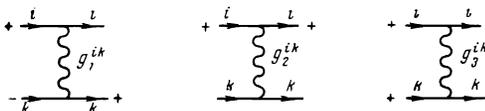


FIG. 3

by Dyatlov et al.<sup>[13]</sup> and in the article by Nozieres et al.<sup>[14]</sup>, where the procedure suggested by Sudakov<sup>[13]</sup> is analyzed in detail.

Assuming that all the external momenta (in the sense of their distance  $\Delta p = |p| - p_F$  from the corresponding Fermi point) and the frequencies  $\epsilon_n$  are of the same order of magnitude,  $v_F \Delta p \sim \epsilon_n$ , we can verify that all the diagrams in the logarithmic approximation depend only on the single variable

$$\xi = \ln \frac{\bar{\omega}}{\max(v_F \Delta p, T)}.$$

The total vertex parts  $\gamma_1(\xi)$  and  $\gamma_2(\xi)$  are the sums of the bare amplitudes  $g_{1,2}$  and the amplitudes that describe multiple scattering in the Cooper (C) and Peierls (P) channels:

$$\gamma_{1,2}^{ik} = g_{1,2}^{ik} + C_{1,2}^{ik} + P_{1,2}^{ik}. \quad (3)$$

The Sudakov method (see<sup>[10,13,14]</sup>) gives expressions for C and P in terms of  $\gamma$ :

$$C_{1,2}^{ik}(\xi) = - \int_0^\xi d\zeta \gamma_{1,2}^{ik}(\zeta) \gamma_{1,2}^{ik}(\zeta),$$

$$C_2^{ik}(\xi) = - \frac{1}{2} \int_0^\xi [(\gamma_1^{ik}(\zeta))^2 + (\gamma_2^{ik}(\zeta))^2] d\zeta, \quad (4)$$

$$P_1^{ik}(\xi) = \int_0^\xi d\zeta [\gamma_2^{ii}(\zeta) \gamma_1^{ik}(\zeta) - \sum_l \gamma_1^{il}(\zeta) \gamma_1^{lk}(\zeta)],$$

$$P_2^{ik}(\xi) = \frac{1}{2} \int_0^\xi (\gamma_2^{ik}(\zeta))^2 d\zeta.$$

In the case of a single electron per cell ( $g_3 \neq 0$ ) the equations become even more cumbersome. We therefore write down at once the equations for  $\gamma$ :

$$\begin{aligned} \gamma_1^{ik} = g_1^{ik} - \int_0^\xi d\zeta & \left[ \gamma_1^{ik} \gamma_2^{ik} - \gamma_1^{ik} \gamma_2^{ii} + \sum_l \gamma_1^{il} \gamma_1^{lk} \right. \\ & \left. + (\gamma_3^{ik})^2 - \sum_l \gamma_3^{il} \gamma_3^{lk} \right], \end{aligned} \quad (5)$$

$$\gamma_2^{ik} = g_2^{ik} - \frac{1}{2} \int_0^\xi d\zeta [(\gamma_1^{ik})^2 - (\gamma_3^{ik})^2],$$

$$\gamma_3^{ik} = g_3^{ik} + \int_0^\xi d\zeta \left[ \gamma_2^{ik} \gamma_3^{ik} + \gamma_2^{ii} \gamma_3^{ik} + \gamma_1^{ik} \gamma_3^{ii} - \sum_l (\gamma_1^{il} \gamma_3^{lk} + \gamma_3^{il} \gamma_1^{lk}) \right].$$

The new equations (3), (4), and (5) are very complex and cannot be solved in general form. In the absence of interactions between the filaments ( $g^{ik} = 0$  for  $i \neq k$ ) they transform into the solutions that we have already discussed<sup>[9,10]</sup>. We recall that in the absence of Umklapp ( $g_3 = 0$ ) these solutions are of the form

$$\gamma_1 = \frac{g_1}{1 + g_1 \xi}, \quad \gamma_2 = g_2 - \frac{1}{2} \frac{g_1^2 \xi^2}{1 + g_1 \xi}. \quad (6)$$

In the case of attraction ( $g_1 < 0$ ) both vertices have pole singularities<sup>2)</sup>:  $\gamma_1 \approx 2\gamma_2 \approx 1/(\xi - \xi_0)$  with  $\xi_0 = 1/|g_1|$ , which corresponds to a transition temperature  $T_{c0} = \bar{\omega} \exp(-1/|g_1|)$ .

An analysis of the system (3), (4) shows that the solution (6), which is exact in the absence of interactions between the filaments, becomes unstable even with the inclusion of an arbitrarily weak interaction.

The system of integral equations (3) and (4) is in fact equivalent to the following system of differential equations:

$$\frac{d\gamma_1^{ik}}{d\xi} = -\gamma_1^{ik}\gamma_2^{ik} + \gamma_1^{ik}\gamma_2^{ii} - \sum_l \gamma_1^{il}\gamma_1^{lk}, \quad (7)$$

$$\frac{d\gamma_2^{ik}}{d\xi} = -\frac{1}{2}(\gamma_1^{ik})^2$$

with the "initial" conditions

$$\gamma_1^{ik}(0) = g_1^{ik}, \quad \gamma_2^{ik}(0) = g_2^{ik}. \quad (8)$$

Since the right side of the system (7) does not depend explicitly on  $\xi$  and is a homogeneous quadratic function of  $\gamma$ , it can, in principle, have stationary singular solutions of the form

$$\gamma_1^{ik} = \frac{A_{ik}}{\xi - \xi_0}, \quad \gamma_2^{ik} = \frac{B_{ik}}{\xi - \xi_0}, \quad (9)$$

with arbitrary  $\xi_0$ , among which is Eq. (6) with

$$A_{ik} = 2B_{ik} = \delta_{ik}. \quad (10)$$

The purely one-dimensional<sup>[9]</sup> solution (6) corresponds to the special initial conditions  $g_1^{ik} = g_1 \delta^{ik}$  and  $g_2^{ik} = g_2 \delta^{ik}$ .

Let  $g^{ik} \neq 0$  and  $|g^{ik}| \ll |g^{ii}|$ . In the approximation linear in  $\gamma^{ik}$  ( $i \neq k$ ) the equations for  $\gamma^{ii}$  on a single filament do not change form:

$$\frac{d\gamma_1^{ii}}{d\xi} = -(\gamma_1^{ii})^2, \quad \frac{d\gamma_2^{ii}}{d\xi} = -\frac{1}{2}(\gamma_1^{ii})^2,$$

so that near (10) we again have

$$\gamma_1^{ii} = 2\gamma_2^{ii} = \frac{1}{\xi - \xi_0} = \gamma$$

with a shifted pole  $\xi_0 \rightarrow \bar{\xi}_0$ . For small values of  $\gamma^{ik}$  ( $i \neq k$ ) we have

$$\frac{d\gamma_1^{ik}}{d\gamma} = \frac{3}{2} \frac{\gamma_1^{ik}}{\gamma}, \quad \gamma_2^{ik} = 0.$$

Accordingly, the equation of a typical trajectory is  $\gamma_1^{ik} = \text{const} \cdot \gamma^{3/2}$ . A plot of the trajectories using the variables  $\gamma_1^{ik}/\gamma$  and  $\gamma^{-1}$  is given in Fig. 4. The one-dimensional system corresponds to the abscissa axis in Fig. 4. It is apparent that the system can reach the "one-dimensional" singular point (9), (10) only from this axis. Physically this means that the singularities in the vertex part on separate filaments are not independent.

It is not hard to show that the "one-dimensional" solutions of the system (5) are also unstable in the presence of Umklapp<sup>[10]</sup>.

In addition to special solutions of the type (9) with a pole  $\xi_0$  which does not depend on the coordinates  $i$  and  $k$  of the filaments (in the following we shall call such poles "stationary"), the system (7) has solutions of a different form. These are the so-called "moving" poles discussed earlier by one of the present authors with Katz and Brazovskii<sup>[15]</sup>. In seeking them it is more convenient to rewrite the system (7) in the two-dimensional momentum

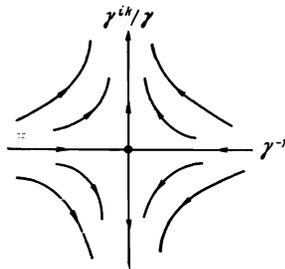


FIG. 4

representation  $q$  with respect to the differences  $\rho_{ik}$  of the two-dimensional coordinates of the filaments:

$$\gamma(q) = \sum_k \gamma^{ik} \exp(iq\rho_{ik}), \quad \gamma^{ik} = \int_S \gamma(q) \exp(-iq\rho_{ik}) \frac{d^2q}{S},$$

where  $S$  is the area of the reciprocal cell (for a square,  $S = 4\pi^2/a^2$ ). We have

$$\frac{d\gamma_1(q)}{d\xi} = -\gamma_1^2(q) + \gamma_1(q) \int \gamma_2(q_1) \frac{d^2q_1}{S} - \int \gamma_1(q-q_1) \gamma_2(q_1) \frac{d^2q_1}{S}, \quad (11)$$

$$\frac{d\gamma_2(q)}{d\xi} = -\frac{1}{2} \int \gamma_1(q-q_1) \gamma_1(q_1) \frac{d^2q_1}{S}.$$

System (11) has a special solution with a polar singularity

$$\gamma_1(q) \approx \frac{1}{\xi - \xi_0(q)}, \quad \gamma_2 \approx 0, \quad (12)$$

where  $\xi_0(q)$  is an essential function of the momentum and is determined by matching with the initial conditions<sup>3)</sup> (8). The transition occurs at the point  $\xi = \ln(\omega/T_{c0}) = \xi_0(q_0)$ ,  $\xi_0(q_0) = \min \xi_0(q)$ . Assuming that near  $\xi_0(q_0)$  the "trajectory" of the pole  $\xi_0(q)$  is of the form

$$\xi_0(q) = \xi_0(q_0) + b(q - q_0)^2, \quad b > 0$$

(see footnote 3), we can verify that the increments of  $\gamma_1$  and  $\gamma_2$  from Eq. (12) near  $\xi = \xi_0(q_0)$  have weaker, non-pole singularities (for additional details see<sup>[15]</sup>).

The character of the transition determined by the moving pole can be assessed from the fact that Eq. (12) corresponds to a simple pole (with residue 1!) in the Peierls channel  $P_1$  in Eq. (4) and to weaker singularities in the channel  $P_2$  and in both Cooper channels. In accordance with<sup>[9,10]</sup>, this means that the transition has the purely dielectric character of a Peierls instability. In this case the phonon frequency  $\omega$  also vanishes ( $q_{\parallel} = 2p_F$ ,  $q_{\perp} = q_0$ ) (see<sup>[9,10]</sup> and Sec. 4). However, this does not mean that the result could have been obtained by a simple summation of ladder diagrams; although the pole is only in the  $P$  channel and its residue is 1, its formation and the trajectory of  $\xi_0(q)$ , and in particular the transition temperature  $T_{c0}$ , are determined by all the parquet diagrams<sup>4)</sup>.

Let us now turn to the special solutions of the "standing pole" type (9). We write the equations for the residues  $A_{ik}$  and  $B_{ik}$ :

$$A_{ik} = A_{ik}B_{ik} - A_{ik}B_{ii} + \sum_l A_{il}A_{lk}, \quad B_{ik} = \frac{1}{2}A_{ik}^2 \quad (13)$$

or

$$A_{ik} = \frac{1}{2}A_{ik}^3 - \frac{1}{2}A_{ik}A_{ii}^2 + \sum_l A_{il}A_{lk}.$$

System (13) does not have any arbitrary parameters of the problem. However, it can be shown<sup>5)</sup> that it has a two-parameter family of solutions. For this purpose we change in Eq. (13) to the momentum representation:

$$A(q) = A^2(q) - \frac{1}{2}A(q) \left[ \int A(q_1) \frac{d^2q_1}{S} \right]^2 + \frac{1}{2} \iint A(q_1)A(q_2)A(q-q_1-q_2) \frac{d^2q_1}{S} \frac{d^2q_2}{S} \quad (14)$$

and as the zeroth approximation we use the solutions of the equation

$$A_0(q) = A_0^2(q). \quad (15)$$

Besides the two obvious solutions  $A_0(q) \equiv 1$  (corresponding to a one-dimensional standing pole) and  $A_0(q) \equiv 0$ , Eq. (14) also has a wide class of "step-function" solu-

tions in which  $A_0(q)$  equals 1 in some portions of the reciprocal cell and zero in the remainder. The "elementary" solution of this type is the "unit function"

$$A_0(q) = \theta_\lambda(q), \quad \theta_\lambda(q) = \theta_{\lambda x}(q_x)\theta_{\lambda y}(q_y);$$

$$\theta_\lambda(q) = \begin{cases} 1, & |q| < \lambda/2 \\ 0, & |q| > \lambda/2 \end{cases} \quad (16)$$

It is easy to see that if the width  $\lambda$  is small compared to the cell dimension  $2\pi/a$ , then, as in the case of a moving pole, the neglected terms in Eq. (14) will only provide a small correction of order  $(\lambda a)^4$  to solution (16). The situation remains the same for any superposition of the elementary solutions:

$$\theta_{\lambda_1}(q) + \theta_{\lambda_2}(q \pm q_{01}) + \theta_{\lambda_3}(q \pm q_{02}) + \dots, \quad (16')$$

when the condition  $\lambda_i \ll |q_{0i} - q_{0k}| \lesssim 2\pi/a$  is satisfied, i.e., when the function (17) consists of a few rather narrow spikes<sup>6)</sup>; see Fig. 5.

The "elementary" solution (16) corresponds to the establishment of long-range correlations, accompanied by slow oscillations of period  $\sim 1/\lambda$ . The corresponding special solution is of the form

$$\gamma_{ik} = \frac{1}{\xi - \xi_0} \frac{4 \sin(\frac{1}{2}\lambda x x_{ik}) \sin(\frac{1}{2}\lambda y y_{ik})}{S x_{ik} y_{ik}}. \quad (17)$$

Although solution (16) is of interest primarily as a proof of the existence of solutions to the general system (13), it is also interesting to consider the nature of the transition to which it corresponds. According to Eq. (4), at small distances there exists a pole  $\sim \lambda^4/(\xi - \xi_0)$  in the Cooper channel, and at large distances, where  $|x_{ik}|, |y_{ik}| \gtrsim 1/\lambda$ , a pole with residue 1 exists in the P channel. Thus, in this extremely peculiar state there exists, against the background of a large dielectric gap (Peierls instability), a superconducting correlation that is small in magnitude but drops off slowly according to a power law.

In addition to these solutions which are "close" to the moving dielectric pole, there exists also a two-parameter set of solutions close to the "one-dimensional standing pole" (10). By making the change of variable  $A(q) = 1 - \frac{1}{2}C(q)$  in Eq. (15) we can show that the "elementary" solution is of the form

$$A_0(q) = 1 - \frac{1}{2}\theta_\lambda(q). \quad (18)$$

The difference now is that the small increments to the solution are of another order of magnitude,  $\sim \lambda^2 a^2$ . The solutions of type (16') are constructed similarly. The elementary solution (18) corresponds to pairing in both the Cooper and dielectric channels, when all four particles lie on a single filament. In addition, according to (18), (17), and (16), long-range Cooper and Peierls correlations of type (17) can be superimposed on these "one-dimensional" pairings.

As we would naturally expect, states such as (18) are unstable in the same sense as the purely one-dimensional states (10) (see Appendix I). However, since the number of such solutions is "continuous," there exist in principle "continuous" regions of the initial data (8) from which these special points can be attained<sup>7)</sup>.

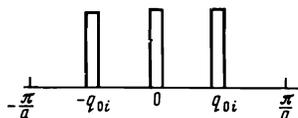


FIG. 5

Investigating the stability of solutions (16) and (16') is a more complex problem. For a two-dimensional system of filaments such an investigation can only be carried out numerically. We shall therefore consider only the case of a one-dimensional filament system, for which analytical methods are completely sufficient (see Appendix I). Only the elementary solution  $\theta_\lambda(q)$  in Eq. (16) is found to be stable; all the combined solutions of type (16') are unstable, although, as in the case of the nearly one-dimensional solutions (18), they can be reached from a "continuum" of initial conditions (see, however, [7]). The structure of the problem concerning the stability of solutions (16) and (16') leaves practically no doubt that the elementary solution (16) also remains stable in the case of a real two-dimensional system of filaments.

### 3. EFFECTS OF HOPPING. THE MOVING COOPER POLE

We now discuss the role of electron hopping. Neglecting the overlap integrals between the filaments, whose characteristic value we denote by  $V_{12}$ , the three-dimensional electron spectrum is flat. The inclusion of hopping distorts the Fermi surface of the electrons, leading to a finite effective mass in the transverse direction. The amount of this distortion, in energy units, is of order  $w \approx V_{12}^2/\epsilon_F$ . At low temperatures the deviation of the Fermi surface from a plane affects the values of the logarithmic integrals in the Peierls channel in Fig. 2b. Actually, the logarithmic cutoff at the lower limit in the Cooper channel at  $\mathbf{k} = \mathbf{p}_1 + \mathbf{p}_2 = 0$  always occurs at  $v_F \Delta p = T$  because of the invariance of the spectrum under time inversion,  $\epsilon(-\mathbf{p}) = \epsilon(\mathbf{p})$ . In the Peierls channel the appearance of logarithmic integrals is due to the degenerate form of the electron dispersion law. Thus at small  $w$  the overlap between filaments enters into the parquet equations only as the cutoff limit of the Peierls cross sections; it becomes significant when  $w$  is comparable (on the logarithmic scale) with the transition temperature specified by the pole in Eq. (6), (9), or (12). We may therefore assume that  $w$  is exponentially small, so that, as before, we will neglect electron transitions from one filament to another in the initial inter-electronic interactions. The transitions enter the problem only because the electron Green's function  $\mathcal{G}^{ik}(p)$  is nondiagonal in  $i$  and  $k$ .

Consider, for example, the diagram of Fig. 6 for the vertex part with longitudinal momentum transfer  $2p_F$ . In principle, here  $l \neq i$  and  $m \neq s$ . However, if we take the Fourier components with respect to the transverse momenta  $t$ , the internal part of the diagram is proportional to

$$\int U(t_1 - t') U(t' - t_2) \frac{d^2 t'}{v_F} \ln \frac{\bar{\omega}}{w(t')},$$

where  $U$  corresponds to the interaction between the filaments, the integration is carried out over the three-dimensional Fermi surface (which effectively coincides with a plane), and  $v_F \approx v_{Fz}$ . Neglecting, with logarithmic accuracy, the dependence of  $w(t')$  on the point  $t'$ , we see that the vertex in Fig. 6 is nonzero only when  $l = i$  and

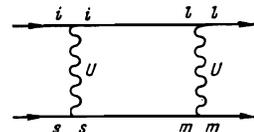


FIG. 6

$m = s$ . In other words, in this approximation we still retain the picture of separate filaments that was used to derive the system (3)–(5). The only difference is that the cutoff in the Peierls channel is limited by the value of  $w$ . If  $\nu = \ln(\bar{\omega}/w) > \xi_0$ , where  $\xi_0 = \ln(\bar{\omega}/T_0)$  is the pole of Eq. (6), (9), or (12), the jumps affect only the fluctuation region below  $T_0$ . Now let  $\nu < \xi_0$ . In this case the Peierls channel has no pole and there is no dielectric transition.

We introduce the Cooper vertex part  $\gamma^{ik}(\nu, \xi)$ , where the momenta  $p_1, p_2, p_3$ , and  $p_4$ , measured from the Fermi surface, are of order  $w/v_F$ , but  $p_1 + p_2 \sim T/v_F \ll w/v_F$ . Employing the usual procedure for separating the cross section in which the variable of integration is smallest, we obtain the equations

$$\gamma_+^{ik}(\nu, \xi) = \gamma_+^{ik}(\nu) - \int_{\nu}^{\xi} \gamma_+^{ik}(\nu, \zeta) \gamma_+^{ik}(\nu, \zeta) d\zeta, \quad (19)$$

$$\gamma_+^{ik}(\nu, \xi) = \gamma_+^{ik}(\nu) - \frac{1}{2} \int_{\nu}^{\xi} [(\gamma_+^{ik}(\nu, \zeta))^2 + (\gamma_+^{ik}(\nu, \zeta))^2] d\zeta.$$

By solving these we find

$$\gamma_{\pm}^{ik}(\nu, \xi) = [\pm 1/2(\xi - \nu) + 1/\gamma_{\pm}^{ik}(\nu)]^{-1}, \quad (20)$$

where  $\gamma_{\pm} = \gamma_1 \pm \gamma_2$ . When  $\xi < \nu$ ,  $\gamma^{ik} \equiv \gamma^{ik}(\xi)$ . The pole  $\tilde{\xi}_0$  in Eq. (20) specifies the Cooper singularity if  $\tilde{\xi}_0 > \nu$ , i.e., if  $\tilde{T}_0 < w$ . In the opposite case the pole in Eq. (20) has no meaning.

There are two possible cases with respect to the transition temperature  $T_0$  obtained by neglecting the overlap integral between filaments:  $\tilde{T}_0 > T_0$  and  $\tilde{T}_0 < T_0$ . Thus, if  $\nu$  is close to  $\xi_0$  (on the logarithmic scale), we obtain formally from Eq. (15)

$$\tilde{\xi}_{0\pm}^{ik} = \nu \pm 2(\xi_0 - \nu) / (A_{ik} \pm 1/2 A_{ik}^2). \quad (21)$$

For example, in the solution for a single filament (with the interaction between the filaments small compared to  $w$ )  $A_{ik} = \delta_{ik}$ :

$$\tilde{\xi}_{0\pm} = \nu + 1/3(\xi_0 - \nu), \quad T_{c\pm} \sim T_{c0}(T_{c0}/w)^{1/3}.$$

The second pole in Eq. (21), which would correspond to a solution with  $T_{c-} > w$ , does not exist. For the general form of  $A_{ik}$ , obviously, both cases are possible. The poles  $\tilde{\xi}_{0+}^{ik}$  and  $\tilde{\xi}_{0-}^{ik}$  correspond to singlet and triplet pairing, respectively, where  $i \neq k$  implies the combining of electrons on different filaments. The transition is specified by the largest of the temperatures in Eq. (21).

To establish a definite correspondence with the three-dimensional formulation of the BCS theory, we write in place of Eq. (20) the three-dimensional equations in the momentum representation in the following schematic form, corresponding to the ladder approximation ( $p_1 = -p_2$ ):

$$\Gamma(p_1, p_3) = \Gamma^0(p_1, p_3) + \int_{\nu}^{\xi} \overline{\Gamma(p_1, l) \Gamma(l, p_3)} d\zeta, \quad (22)$$

where the momenta  $p$  and  $l$  lie on the three-dimensional (nearly planar) Fermi surface, the logarithmic integration is taken along the normals to the Fermi surface, and the bar denotes the integral over this surface.  $\Gamma^0$  has the same meaning as in Eq. (20). The pole part in the vertex part  $\Gamma(p_1, p_3)$  has the usual form

$$\frac{\Delta(p_1) \Delta(p_3)}{\xi - \xi_0}$$

where  $\Delta(p)$  determines (when  $\xi > \nu$ ) the dependence of

the resultant energy gap on the point of the Fermi surface. By establishing the correspondence, in our approximation, between Eq. (22) and the representation that uses the filament numbers, we easily find that the pole in Eq. (20) at a given  $|\rho_{ik}| = \rho(i - k)$  corresponds to the following form of  $\Delta(p)$ :

$$\Delta(q) \propto \sum_{i=-i} \exp(iq\rho_{ik}),$$

where the sum is taken over all neighbors in the two-dimensional lattice. In particular, the pole with  $i = k$  corresponds to a gap that does not depend on the vector  $q$ . Thus the standing pole of Eqs. (6) and (9), with hopping between the filaments taken into account, becomes at  $w > T_{c0}$  the Cooper pole of the three-dimensional problem. If  $p_1 + p_2 = q \neq 0$  in the vertex part, then with the inclusion of the nonlogarithmic terms the pole in the Cooper channel becomes a moving pole:

$$\tilde{\xi}_0(q) = \tilde{\xi}_0 + (v_F/T_c)^2 (\alpha q_{\parallel}^2 + \beta w^2 q_{\perp}^2 / \epsilon_F),$$

where  $\alpha$  and  $\beta$  are numerical coefficients. The usual estimates indicate that at  $w \gg T_c$  the region of the essential singularity around the transition point extends over a temperature interval  $\Delta T/T_c \sim (T_c/w)^4$ .

#### 4. PHONONS

The problem of the interaction with phonons requires separate consideration, because their energies are limited by frequencies on the order of the Debye frequency  $\omega_D \ll \epsilon_F$ . Thus for  $T > \omega_D$  the interaction via phonons provides no contribution to the principal logarithmic terms in the vertex part, since in all the logarithmic integrals in the diagrams of Fig. 7 (where the broken line denotes the phonon D-function) the phonon line enters at energies above the Debye energy. Accordingly, at high temperatures the vertex part is given by the old equations (3), (4), and (5) with the bare interaction  $g$  specified by the non-phonon mechanism. However, as one of the present authors has shown<sup>[16]</sup>, an electronic phase transition with  $T_c > \omega_D$  cannot occur at temperatures corresponding to the pole in  $\Gamma$ . In this case (a pole in  $\Gamma$  at  $T_{c0} > \omega_D$ ) it is always preceded by a purely structural dielectric transition in the ion system.

Actually, when  $T > \omega_D$  it is more convenient to write the usual equation for the D-function in terms of the polarization operator (with  $q_{\parallel} \approx 2p_F$ ,  $\omega_D = 0$ ):

$$D^{-1}(0, q) = -\omega_0^2(q) - \Pi, \quad (23)$$

$$\Pi = \text{diagram 1} + \text{diagram 2}$$

The vertex part of the polarization operator in Eq. (23) depends only on the nonphonon mechanisms. Accordingly, the logarithmic integral in the loop in Eq. (23) is also cut off at the nonphonon energy  $\bar{\omega} \sim \epsilon_F$ . The bare phonon frequency  $\omega_0(q)$  is, as we have already indicated, an essential three-dimensional function of the momentum  $q$ .

We cite here the expressions for  $\Pi$  in several special cases.

1. Nonphonon interactions absent. Here  $\Pi$  is given by the simple loop in Eq. (23):

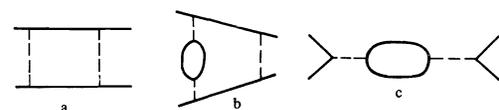


FIG. 7

$$\Pi(\mathbf{q}) = -\frac{1}{2} \omega_0^2(\mathbf{q}) g_{ph}^2(\mathbf{q}) \ln \frac{\bar{\omega}}{T}, \quad (24)$$

where  $g_{ph}$  is the electron-phonon constant. The transition occurs at the temperature where  $D^{-1} = 0$ , i.e.,

$$1 - \frac{1}{2} g_{ph}^2 \ln(\bar{\omega}/T_c) = 0, \quad (25)$$

if the value of  $T_{c0}$  given by this equation is actually larger than the Debye energy  $\omega_D$ .

**2. Nonphonon mechanism.** In this case the dielectric transition is "amplified." For instance, in the case of a "one-dimensional" pole (6) with  $g_1 < 0$ , the polarization operator itself becomes infinite at  $\xi = \xi_0 = 1/|g_1|$ . Let  $T_0 = \bar{\omega} \exp(-\xi_0) > \omega_D$ . Near  $T_0$  a singular term  $^{[10]}$  appears in Eq. (25):

$$1 - \frac{1}{2} g_{ph}^2 \frac{1}{(\xi_0 - \xi)^{1/2}} \frac{\exp^{(1/2 - g_2/g_1)}}{|g_1|^{1/2}} = 0 \quad (26)$$

and the dielectric transition must occur before the "one-dimensional" transition, for any value (even a low value) of the constant  $g_{ph}$ .

Since it is effectively impossible to determine the non-unidimensional solutions to the parquet equations (3), (4), and (5) in analytic form, we shall cite here only the expression for the singular part  $\Pi$  near the "moving" pole (12). In accordance with its meaning as a pole in the P channel, we also find for  $\Pi$  the following simple pole<sup>9)</sup>:

$$\Pi(q_{\parallel} \approx 2p_{\parallel}, q_{\perp}) \sim -\frac{g_{ph}^2(\mathbf{q}_{\perp})}{\xi_0(\mathbf{q}_{\perp}) - \xi}, \quad (27)$$

where  $\xi_0(\mathbf{q}_{\perp})$  is the trajectory of the "moving" pole.

Thus, at  $T > \omega_D$  there is no purely electronic transition due to nonphonon mechanisms. It is forestalled, in quasi-unidimensional metals, by a structural Peierls transition<sup>[5,6]</sup>.

One further point should be made with respect to Eqs. (24)–(27). In the phonon D-function there appears the "bare" phonon spectrum  $\omega_0(\mathbf{q})$ , which has no particular meaning. The real spectrum is specified by the poles of the exact phonon Green's function. Therefore, in the expressions for the polarization operator it is the temperature dependence of the phonon frequencies that has physical meaning. The remaining terms represent renormalizations, which can be included, for instance, in the determination of the phonon spectra near the melting temperature.

When  $T < \omega_D$  the phonon mechanism does not differ essentially from the nonphonon mechanism. Here the diagrams of Fig. 7 also contribute to  $\Gamma$ . Their inclusion leads only to the "renormalization" of the interaction constants and the limits of the integration in Eqs. (3)–(5):

$$\xi = \ln(\bar{\omega}/T) \rightarrow \xi = \ln(\omega_D/T), \quad (28)$$

$$g_1 \rightarrow \gamma_1(\xi_D) - g_{ph}^2, \quad g_2 \rightarrow \gamma_2(\xi_D), \quad g_3 \rightarrow \gamma_3(\xi_D),$$

where  $\gamma_1(\xi_D)$ ,  $\gamma_2(\xi_D)$ , and  $\gamma_3(\xi_D)$  are solutions of the system (3)–(5) at the point  $\xi_D = \ln(\bar{\omega}/\omega_D)$ . In particular, for the one-dimensional solution (6)<sup>[9]</sup> we have

$$g_1 \rightarrow \frac{g_1}{1 + g_1 \xi_D} - g_{ph}^2, \quad g_2 \rightarrow g_2 - \frac{1}{2} \frac{g_1^2 \xi_D}{1 + g_1 \xi_D}.$$

The Peierls ion shift now occurs only simultaneously with the transition in the electron system<sup>[9]</sup>, and Eq. (23) for D is replaced by

$$D = \text{---} + \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} \text{---} \quad (29)$$

where the broken line is the free-phonon function  $D_0$

$= -1/\omega_0^2(\mathbf{q})$ , and the vertex in the third term of Eq. (29) includes diagrams such as that in Fig. 7c. At the transition point D approaches infinity in the same manner as  $\Pi$  in Eqs. (27) and (26) (cf. <sup>[9,10]</sup>). If there are several phonon branches that interact with the electrons, D becomes infinite in Eq. (29) when one of the phonon frequencies becomes zero at the transition point.

## 5. APPLICABILITY OF OUR RESULTS

The basic equations (4), (5) or (11) were obtained with the logarithmic accuracy  $g \ln(\bar{\omega}/T) \sim 1$ . Thus, for instance, in solution (6) for a single filament<sup>[9]</sup> the polar singularity point  $T_0$  was determined only apart from a factor. By making use of the expression obtained for the gap at zero temperature in the exact solution for one of the one-dimensional models<sup>[18]</sup>,

$$\Delta \sim g^{1/2} \bar{\omega} e^{-1/|g|}$$

and assuming that  $\Delta \sim T_0$ , we find that additional terms appear in the denominators of Eq. (6):

$$1 + g \left( \ln \frac{\bar{\omega}}{T} + \frac{1}{2} \ln g + \text{const} \right). \quad (30)$$

Therefore, in the preceding analysis we have essentially assumed that the higher-order corrections with respect to the logarithmic approximation in Eq. (30)

$$1 + g \ln \frac{\bar{\omega}}{T} + \Sigma \left( g, \frac{\omega}{T} \right) \quad (31)$$

have a structure which allows us (near  $1 + g \ln(\bar{\omega}/T) \ll 1$ ) to write Eq. (31) in the form

$$g(\xi - \xi_0). \quad (32)$$

In the one-dimensional case there is no phase transition and, strictly speaking, the vertex part can become infinite only at  $T = 0$ . However, since the terms  $g \ln(\bar{\omega}/T)$  in Eq. (31) represent the basic approximation, expression (32) for the vertex should certainly be valid over some range of temperatures. To estimate this range, i.e., the region of applicability of Eq. (32) within the region where the vertex part is large, becomes an extremely difficult problem in the purely one-dimensional case<sup>[9]</sup>. In particular, we cannot exclude the possibility that the inclusion of non-parquet diagrams will separate the singularities (6) in the Cooper and Peierls channels. This uncertainty also relates to the special standing-pole solution (9).

Although we have no way to resolve this question exactly, we can still make the following comments. In solution (9) dielectric pairing of electrons and holes is possible, of course, because the filament system is essentially three-dimensional. The familiar proof by Hohenberg<sup>[19]</sup> that superconducting averages  $\Delta = \langle a_p a_{-p} \rangle$  are impossible in the one-dimensional case is based on the continuity equation

$$\frac{\partial \rho}{\partial t} + \text{div } \mathbf{j} = 0,$$

which, in the absence of hopping from one filament to another, holds true also in our model. We have not extended the proof of<sup>[19]</sup> to the case  $\Delta_{ik} \neq 0$  at  $i \neq k$ , but if  $A_{ii} \neq 0$  in Eq. (9), then the temperature of a real transition with the formation of a superconducting gap in the spectrum contains an additional order of smallness due to the hopping energy  $w$ .

At the same time it should be noted that the existence of a finite superconducting gap is not necessary in order for a superconducting current to flow. All that is needed

for superconductivity is a change in the density of current states. Unfortunately, the logarithmic approximation does not permit us to determine exactly the structure of the states below the transition point. An approximate qualitative determination is given in Appendix II. It appears, however, that the standing-pole solutions represent many new possibilities.

For the moving pole the situation is much simpler. In this case it is possible to use the molecular-field approximation everywhere except for a small region of true singularity near the phase-transition point. It is easiest to understand this from an example. Consider the dependence of the polarization operator  $\Pi(q_{\parallel}, \mathbf{q}_{\perp})$  on the longitudinal and transverse momenta in Eq. (23) for the D-function. Then in Eq. (24), because of the flat shape of the spectrum, the integration in the electron loop leads to a term that depends only on the longitudinal momentum  $q_{\parallel}$  ( $v_F q_{\parallel} \ll T$ ):

$$\ln \frac{\bar{\omega}}{T} \rightarrow \ln \frac{\bar{\omega}}{T_0} - \alpha \left( \frac{v_F q_{\parallel}}{T_0} \right)^2 - \frac{T - T_0}{T_0}$$

(where  $\alpha$  is a number). Both  $\omega_0(\mathbf{q})$  and  $g_{ph}^2(\mathbf{q})$  depend on the transverse momentum  $\mathbf{q}_{\perp}$ , but this dependence is weak:

$$\omega_0(\mathbf{q}) = \omega_0 \left( 1 + C_1 \left( \frac{q_{\perp}}{q_0} \right)^2 \right), \quad g_{ph}^2(\mathbf{q}) = g_{ph}^2 \left( 1 + C_2 \left( \frac{q_{\perp}}{q_0} \right)^2 \right), \quad (33)$$

where the expansion is about the reciprocal-lattice point at which Eq. (23) becomes zero. The order of magnitude of  $q_0$  is atomic ( $q_0 \sim 2\pi/a$ ). Thus, near the transition point  $T_0$ :

$$1 - 1/2 g_{ph}^2 \ln(\bar{\omega}/T_0) = 0,$$

and we have

$$D(\mathbf{q}, T) = \frac{(g_{ph} \omega_0)^{-2}}{\tau + \alpha (v_F q_{\parallel}/T_0)^2 + g_{ph}^{-2} \beta (q_{\perp}/g_0)^2} \\ \tau = (T - T_0)/T_0.$$

This result also applies directly to the most general case, in which all the interactions involved in the problem show a dependence on the transverse momentum (33). Finally, in the case of a moving pole we have for the vertex part near the transition point

$$\gamma(\tau, \mathbf{q}) = [\tau + \alpha (v_F q_{\parallel}/T_0)^2 + \beta g^{-1} (q_{\perp}/q_0)^2]^{-1}, \quad (34)$$

where  $\alpha$  and  $\beta$  are numerical coefficients, and  $g$  represents the order of smallness of the interaction.

From the viewpoint of the theory of phase transitions, Eq. (34) behaves like the correlation function near the transition point<sup>[20]</sup>. From the familiar formulas for the fluctuations of the order parameter (see, e.g.,<sup>[20]</sup>) we find that outside a narrow neighborhood of the transition temperature

$$\tau \gg g^2, g_{ph}^4 \quad (35)$$

the fluctuations are small. At the end of Sec. 3 we have noted that when the number of jumps is sufficient to cause the formation of a moving Cooper pole, the analogous estimate is of the form

$$\tau \gg (T_c/\omega)^4. \quad (36)$$

Outside the temperature range specified by Eq. (35) or (36), the corresponding structural or superconducting transition can be described by a theory of the Ginzburg-Landau type.

It is not without interest to show that the estimate (35) coincides with the region of applicability of the

parquet equations (within the accuracy of terms including  $g \ln g$  and  $g$ ). In fact, we can estimate the contribution from the first of the non-parquet diagrams (the "envelope") shown in Fig. 8. At high temperatures its contribution is  $g^4 \ln(\omega/T)$  (relative magnitude  $\sim g^2$ ). Near  $\tau \rightarrow 0$  the principal terms in Eq. (34) are those that contain sums over the filaments, since in the solution with the moving pole the  $\gamma^{ik}$  themselves are small.

The order of magnitude of the diagram in Fig. 8 is

$$\frac{1}{T^2} \sum_i \int d q_{\parallel 1} d q_{\parallel 2} (\gamma_1^{i1}(q_{\parallel 1}))^2 (\gamma_1^{i2}(q_{\parallel 2}))^2. \quad (37)$$

For the Fourier component with respect to the difference  $i - k$  with  $\mathbf{q}_{\perp} \neq 0$  we have

$$\frac{1}{T^2} \int \gamma_1(t_1, q_{\parallel 1}) \gamma_1(\mathbf{q}_{\perp} - t_1, q_{\parallel 1}) \gamma_1(t_2, q_{\parallel 2}) \gamma_1(\mathbf{q}_{\perp} - t_2, q_{\parallel 2}) d^2 t_1 d^2 t_2 d q_{\parallel 1} d q_{\parallel 2}.$$

By substituting Eq. (34) in this expression we obtain the estimate  $g^2/\tau$ . The condition for the smallness of this quantity coincides with Eq. (35).

## 6. CONCLUSION

As we have seen, the fact of three-dimensionality has significant effects on the given model of quasi-unidimensional filaments. The purely one-dimensional solution for a single filament<sup>[9,10]</sup> is, in general, unstable, and can exist only if the interaction between the filaments is so small that the actual transition is due solely to hopping effects. We have shown, however, that although the interaction between filaments can lead to a dielectric structural transition, there is also the possibility that it will lead, as before, to a transition with simultaneous dielectric and superconducting pairing. In the latter case the actual transition point clearly is dependent on the hopping processes from one filament to another. In the opposite case, when the probability of an electron transition from one filament to another, while still small, becomes predominant (the quasi-three-dimensional spectrum), the system becomes capable of superconducting pairing alone. Here, however, in contrast to the BCS theory, the system of parquet equations must be used to determine the transition temperature.

Above, for lack of space, we did not dwell in detail upon the case of only one electron in the reciprocal cell ( $2p_F = \pi/c$ ). In this case there is an additional scattering corresponding to Umklapp processes, which in the one-dimensional case creates the possibility of independent antiferromagnetic ordering<sup>[10]</sup>. An analysis of the general equations (5) similar to that given above shows that the moving pole can arise either in  $\gamma_1$  separately or in  $\gamma_1$  and  $\gamma_3$  simultaneously. Similarly, the standing pole is possible either in  $\gamma_1$  and  $\gamma_2$  only, or in all three amplitudes at once. Since the singularity in  $\gamma_3$  is related to the dielectric scattering channel, sufficiently large hopping will suppress both dielectric and antiferromagnetic pairing.

We can now list all the possibilities for the states in the given system at low temperatures.

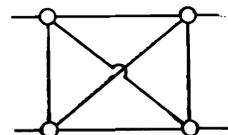


FIG. 8

1. Dielectric state: a structural transition due to the moving pole in  $\gamma_1$ .

2. Dielectric state with antiferromagnetic ordering: a moving pole in  $\gamma_1$  and  $\gamma_2$ .

3. Superconducting state with changed lattice structure: a standing pole in  $\gamma_1$  and  $\gamma_2$ .

4. Superconducting state with antiferromagnetic ordering and changed structure: a standing pole simultaneously in  $\gamma_1$ ,  $\gamma_2$ , and  $\gamma_3$ .

5. Superconducting state: jumps predominant.

6. Normal metallic state.

The details of these states can be explained only outside the framework of the logarithmic approximation, although, as we saw above, there are many possibilities here also.

We have discussed here only the thermodynamic picture of the transitions. Therefore, in speaking of the superconducting transition we have in mind the formation of an energy gap in the spectrum due to Cooper pairing. The current state, the conductivity and the paraconductivity, and similar questions, which are of primary interest in experimental work [1-4], have been left out of consideration. While leaving these problems to a later article, we may nevertheless point out a rather fundamental difficulty, namely, that any defects and impurities, in the Mott sense [21], will lead to the localization of the electron states in the one-dimensional case. Thus, at zero temperature the metallic state in a single filament possesses zero conductivity, as Berezinskiĭ recently confirmed by direct calculations [23].

In light of all the above we would like to point out that experiments [3] on TTF-TCNQ have indicated the presence of a dielectric transition in this system. Measurements of the phonon spectrum in Magnus salts [4] also indicate a damping of the phonon mode. The above arguments tend to be confirmed by the observed narrowness of the region of dip in the phonon frequencies  $\Delta q_{\parallel}/q_{\parallel}$ . From Eq. (33), the corresponding value is  $\Delta q_{\parallel}/q_{\parallel} \sim T_0/\epsilon_F$ .

In conclusion the authors wish to thank B. S. Mityagin for his valuable advice, and A. I. Larkin, S. P. Novikov, and Ya. G. Sinai for many useful discussions.

## APPENDIX I

Let us consider the stability of the "standing" poles (9). Writing

$$\gamma_1(q) = \frac{A(q)}{\xi} + \frac{\delta_1(q)}{\xi^{\Lambda}}, \quad \gamma_2(q) = \frac{B(q)}{\xi} + \frac{\delta_2(q)}{\xi^{\Lambda}},$$

where  $A(q)$  and  $B(q)$  are solutions of Eqs. (13) and (14),  $\delta_1$  and  $\delta_2$  are small increments, and  $\Lambda$  are characteristic numbers that determine the stability, we obtain the linearized equations (11) for  $\delta$ :

$$\begin{aligned} \Lambda \delta_1 = & 2A(q)\delta_1 - A(q) \int \delta_2(q_1) \frac{d^2 q_1}{S} - \delta_1(q) \int B(q_1) \frac{d^2 q_1}{S} \\ & + \int B(q-q_1) \delta_1(q_1) \frac{d^2 q_1}{S} + \int A(q-q_1) \delta_2(q_1) \frac{d^2 q_1}{S}, \quad (\text{A.I.1}) \\ \Lambda \delta_2 = & \int A(q-q_1) \delta_1(q_1) \frac{d^2 q_1}{S}. \end{aligned}$$

The system (A.I.1) specifies the eigenfunctions  $\delta_1$  and  $\delta_2$  and the corresponding eigenvalues  $\Lambda$ . If among the latter there are any  $\Lambda > 1$ , the corresponding "standing" pole will be unstable.

Let us now consider the "elementary" solution of the type (16). It is apparent at once that in this case the dangerous eigenvalues (larger than 1) lie near  $\Lambda = 2$  (with accuracy  $\sim \lambda^4$ ). It is also clear that in the earlier approximation the value of the function  $\delta$  in the outer region  $|q| > \lambda/2$  can be expressed, using Eq. (A.I.1), in terms of their values in the internal region. After we eliminate the external regions and express  $\delta_2$  in terms of  $\delta_1$ , we obtain a closed integral equation for  $\delta_1$  in the internal region, into which we must substitute the expressions for  $A$  and  $B$ , including the terms that follow from (16).

In the following calculations we shall use a one-dimensional momentum  $q$ , assuming also, for simplicity, that the distance between filaments is  $a = 1$ . We have:

$$\begin{aligned} A(q) = & \left[ 1 + \frac{1}{8\pi^2} \left( \frac{\lambda^2}{4} + q^2 \right) \right] \theta_{\lambda}(q) + \frac{1}{16\pi^2} \left( \frac{3\lambda}{2} - |q| \right)^2 (\theta_{\lambda}(q) - \theta_{\lambda}(q)), \\ B(q) = & \frac{1}{4\pi^2} (\lambda - |q|) \theta_{\lambda}(q) \end{aligned} \quad (\text{A.I.2})$$

and the equation for  $\delta_1$  in the internal region  $|q| < \lambda/2$ :

$$\begin{aligned} \left[ 2 - \Lambda - \frac{\lambda^2}{16\pi^2} + \frac{q^2}{4\pi^2} \right] \delta_1 - \frac{\lambda}{8\pi^2} \int_{-\lambda/2}^{\lambda/2} \delta_1(q_1) dq_1, \\ + \frac{1}{4\pi^2} \int_{-\lambda/2}^{\lambda/2} \delta_1(q_1) (\lambda - |q - q_1|) dq_1 = 0. \end{aligned} \quad (\text{A.I.3})$$

Equation (A.I.3) is equivalent to a differential equation with boundary conditions that correspond to the two possible solutions of (A.I.3): symmetric ( $\delta_S(q) = \delta_S(-q)$ ) and antisymmetric ( $\delta_A(q) = -\delta_A(-q)$ ). Introducing the notation

$$\delta_{s,a} = \frac{Q_{s,a}}{v+q^2}, \quad v = (2-\Lambda)4\pi^2 - \frac{\lambda^2}{4},$$

we obtain a second-order equation for  $Q_{s,a}$ :

$$\frac{d^2 Q_{s,a}}{dq^2} - \frac{2Q_{s,a}}{v+q^2} = 0$$

with the boundary conditions

$$\frac{dQ_s(0)}{dq} = Q_s \left( \frac{\lambda}{2} \right) = Q_s(0) = \frac{dQ_a(\lambda/2)}{dq} = 0.$$

The equation can be solved by quadratures:

$$Q = C_1(v+q^2) + C_2(v+q^2) \int_0^q \frac{dq_1}{(v+q_1^2)^2}.$$

For the even solutions  $Q_S$  the constant  $C_2 = 0$ :

$$Q_s = C(v+q^2)$$

and the condition  $Q_S(\lambda/2) = 0$  then clearly gives

$$v_s = -\lambda^2/4 \quad \text{or} \quad \Lambda_s = 2.$$

It can be shown that the eigenvalue  $\Lambda_S = 2$  corresponds to a simple shift of the pole position by a constant amount, and does not mean a loss of stability.

An investigation of the antisymmetric case shows that it corresponds to the eigenvalue

$$\Lambda_a = 2 + \frac{\lambda^2}{16\pi^2} (y^2 - 1),$$

where  $y \approx 1.20$  is the root of the equation

$$\ln \frac{y+1}{y-1} = 2y.$$

However, the presence of an antisymmetric perturbation does not imply the instability of solution (16), because when  $\gamma(q)$  is antisymmetric in momentum space the vertices are also asymmetric,  $\gamma^{ik} = -\gamma^{ki}$  (because they are real in coordinate space). But any reasonable interaction  $g^{ik}$  between the filaments will naturally depend symme-

trically on the distance between  $i$  and  $k$ , and this symmetry will be conserved in all solutions of Eqs. (3)–(5) for  $\gamma_{ik}$ . Thus the unstable antisymmetric perturbation is not physical.

The situation changes when we consider the stability of solutions in the more general form of (16). Calculations (which we shall not cite here) show that in this case, together with  $\Lambda = 2$ , there appear perturbations that are nontrivial and unstable, but symmetric on the whole. We can similarly demonstrate the instability of solutions of type (19).

## APPENDIX II

We showed above that a theory of the Ginzburg-Landau type is valid outside the region (35) below the transition point. In all essentially parquet-type problems we are unable to formulate the nonlinear equations for the gap  $\Delta$ , and are forced to consider only their linearized version.

The problem of determining the gap for a pure one-dimensional pole (6) has already been solved by the present authors<sup>[9]</sup>. We shall therefore present only the final results.

It was shown in<sup>[9]</sup> that each gap  $\Delta$  (in<sup>[9]</sup> there were two: the Cooper and dielectric gaps) is an essential function of the two logarithmic variables,  $\Delta(\eta, \xi)$ :

$$\xi = \frac{1}{2} \ln \frac{\bar{\omega}^2}{\Delta_1^2 + \Delta_2^2 + \dots}, \quad (\text{A.II.1})$$

which contains the sum  $\Delta_1^2 + \Delta_2^2 + \dots$  of all the anomalous nonzero pairings, and the variable

$$\eta(p) = \ln \frac{\bar{\omega}}{v_F |p \mp p_F|}, \quad (\text{A.II.2})$$

which determines the dependence of the gap on the distance from the Fermi surface when  $\eta < \xi$ , i.e., when  $v_F^2 (\Delta p)^2 > \Delta_1^2 + \Delta_2^2 + \dots$ . The function  $\Delta(\eta, \xi)$  satisfies the same equations as the vertex parts, but in contrast to  $\gamma$  in Eqs. (3), (4), and (5) it depends on two momenta with different orders of magnitude (the variables  $\xi$  and  $\eta$ ). There are two types of such vertices:  $\gamma_C(\eta, \xi)$  and  $\gamma_P(\eta, \xi)$ . They correspond respectively to the situations of Figs. 2a and 2b with

$$\xi = \ln \frac{\bar{\omega}}{v_F |p \mp p_F|} > \eta = \ln \frac{\bar{\omega}}{v_F |p' \mp p_F|}.$$

In our problem all four forms of anomalous pairings are possible:

$$\langle a_{1s} a_{-1t} \rangle_{s,t}, \quad \langle a_{2ps}^+ a_{2pt} \rangle_{s,t},$$

where the indices  $s$  and  $t$  denote singlet ( $s$ ) or triplet ( $t$ ) pairing with respect to the spin variables. We denote the corresponding gaps (or anomalous mass operators<sup>[9]</sup>) by  $\Delta_S, t(\eta, \xi)$  and  $\kappa_{S,t}^k(\eta, \xi)$ ; of course, these are also functions of the filament numbers. In<sup>[9]</sup> we established the following relationships<sup>[10]</sup> between  $\gamma_{C,P}$  and  $\Delta, \kappa$ :

$$\begin{aligned} \Delta_s \sim \gamma_{C+} \sim \gamma_{C1} + \gamma_{C2}, \quad \Delta_t \sim \gamma_{C-} \sim \gamma_{C1} - \gamma_{C2}, \\ \kappa_s \sim \gamma_{P1}, \quad \kappa_t \sim \gamma_{P2}. \end{aligned}$$

The equations for  $\gamma_{P,C}$  have the following form (cf. <sup>[9,14]</sup>):

$$\begin{aligned} \gamma_{C\pm}(\eta, \xi) = \gamma_{\pm}(\eta) \mp \frac{1}{2} \int_{\eta}^{\xi} d\zeta \gamma_{C\pm}(\eta, \zeta) \gamma_{\pm}(\zeta), \\ \gamma_{P1}(\eta, \xi) = \gamma_1(\eta) - \int_{\eta}^{\xi} d\zeta \left[ \sum_t \gamma_{P1}(\eta, \zeta) \gamma_t(\zeta) \right] \end{aligned}$$

$$\begin{aligned} - \frac{1}{2} \gamma_{P1}(\eta, \zeta) \gamma_2(\zeta) - \frac{1}{2} \gamma_{P2}(\eta, \zeta) \gamma_1(\zeta) \Big], \\ \gamma_{P2}(\eta, \xi) = \gamma_2(\eta) + \frac{1}{2} \int_{\eta}^{\xi} d\zeta \gamma_{P2}(\eta, \zeta) \gamma_2(\zeta). \end{aligned} \quad (\text{A.II.3})$$

It was shown in<sup>[9]</sup> that the linear homogeneous equations for the gaps  $\Delta$  and  $\kappa$  have solutions at the same values of  $\xi$  at which the corresponding  $\gamma_{C,P}$  become infinite. The dependence on  $\eta$  of the term in  $\gamma_{C,P}$  that tends to infinity then determines the dependence of the gaps on the momentum (i.e., on  $\eta$ ).

For the moving pole (12), none of the vertices, except  $\gamma_{P1}$ , becomes infinite. According to Eq. (A.II.3) the latter vertex has the same form of pole,

$$\gamma_{P1}(\eta, \xi; \mathbf{q}) = \frac{1}{\xi - \xi_0(\mathbf{q})},$$

so that

$$\kappa_s(\eta, \mathbf{q}) = \text{const}, \quad \kappa_t = \Delta_s = \Delta_t = 0$$

and  $\kappa_S = \bar{\omega} \exp(-\min \xi_0(\mathbf{q}))$ , as in the BCS theory.

For an arbitrary standing pole, the system (A.II.3) does not have a simple form. If we take a standing pole of type (16), then by neglecting terms of smallness  $A_{ik}^2$  where possible we obtain

$$\gamma_{C\pm}(\eta, \xi) = \gamma_{\pm}(\eta) \exp \left\{ \mp \frac{1}{2} \int_{\eta}^{\xi} d\zeta \gamma_{\pm}(\zeta) \right\}$$

$$\gamma_{P1}(\eta, \xi; \mathbf{q}) = \gamma_1(\eta; \mathbf{q}) \exp \left\{ - \int_{\eta}^{\xi} d\zeta \gamma_1(\zeta; \mathbf{q}) \right\}.$$

$$\gamma_{P2}(\eta, \xi) = \gamma_2(\eta) \exp \left\{ \frac{1}{2} \int_{\eta}^{\xi} d\zeta \gamma_2(\zeta) \right\}.$$

Near the poles (9) with  $A_{ijk}$  and  $B_{ijk}$  specified by Eqs. (13), (16), and (17) we have, in the old approximation,

$$\gamma_{P1}(\eta, \xi; \mathbf{q}) = \frac{\theta_s(\mathbf{q})}{\xi - \xi_0},$$

$$\gamma_{P2}(\eta, \xi) = \frac{A_{ik}^2}{2(\eta - \xi_0)} \left( \frac{\xi - \xi_0}{\eta - \xi_0} \right)^{A_{ik}^{2/4}}, \quad (\text{A.II.4})$$

$$\gamma_{C\pm}(\eta, \xi) = \frac{A_{ik}}{\eta - \xi_0} \left( \frac{\eta - \xi_0}{\xi - \xi_0} \right)^{\pm A_{ik}^{1/2}};$$

$$A_{ik} = \frac{4 \sin^{1/2} \lambda x_{ik} \sin^{1/2} \lambda y_{ik}}{S x_{ik} y_{ik}}. \quad (\text{A.II.5})$$

The formulas (A.II.4) show that in such a transition:

1) singlet Peierls pairing depends on the distance between the filaments,

$$\kappa_s(\eta) \sim A_{ik};$$

2) triplet Peierls pairing is absent;

3) singlet Cooper pairs occur only at distances between the filaments such that  $A_{ik} > 0$ , and here

$$\Delta_s(\eta) \sim A_{ik} (\eta - \xi_0)^{-1 + A_{ik}^{1/2}};$$

4) triplet Cooper pairing occurs at distances such that  $A_{ik} < 0$ :

$$\Delta_t(\eta) \sim A_{ik} (\eta - \xi_0)^{-1 - A_{ik}^{1/2}}.$$

For small distances between the filaments,  $\rho_{ik} \lambda \lesssim 1$ , the  $A_{ik}$  are constant and positive ( $A_{ik} \sim \lambda^2/S$ ), so that, as in the case of a one-dimensional pole, dielectric and singlet Cooper pairing will exist at these distances. At large distances  $A_{ik}$  begins to oscillate, which, according to the preceding formulas, leads to alternating singlet  $\Delta_S$  and triplet  $\Delta_t$  Cooper pairs.

- <sup>1</sup>In fact, a need not be too large compared to the period  $c$  along the filaments, since in TCNQ complexes the strong directionality of the electron orbitals tends to suppress the hopping.
- <sup>2</sup>We recall, to avoid misunderstandings, that in our normalization of Eqs. (3)–(5) and choice of the variable  $\xi$  the constants  $g$  and the  $\gamma$  themselves are measured in units of  $\pi v_F$ . To transform to the usual notation of the BCS theory we must make the substitutions  $g \rightarrow g/\pi v_F$  and  $\gamma \rightarrow \gamma/\pi v_F$ .
- <sup>3</sup>In reality, this matching and the determination of  $\xi_0(q)$  can be accomplished only by the numerical integration of Eq. (11). In [<sup>15</sup>] these calculations were carried out for some particular model and it was found that  $\xi_0(q)$  is of the form  $\xi_0(q) = \xi_{\min} + bq^2$ .
- <sup>4</sup>Note also that the moving pole is a "stable" singularity of system (7), since, on the one hand, it contains the arbitrary function  $\xi_0(q)$ , and thus can be joined to the entire region of the initial conditions, and on the other hand the corrections to solution (12) have a weaker singularity.
- <sup>5</sup>The authors are deeply grateful to B. S. Mityagin for having pointed out to them solutions of the type (16) and (18).
- <sup>6</sup>The only condition is that solution (16) must be an even function, since both  $A^{1k}$  and its Fourier transform  $A(q)$  are real.
- <sup>7</sup>There are strong arguments to indicate, however, that these initial conditions themselves must be of the long-range type (17).
- <sup>8</sup>The condition  $T_{C0} > \omega_D$  was the model criterion for the validity of the 1954 theory of Froehlich [<sup>6</sup>] (see also [<sup>7</sup>]). Metal-dielectric transitions in semiconductors under similar conditions ( $T_C > \omega_D$ ) were also discussed by Kopaev and Timerov [<sup>17</sup>].
- <sup>9</sup>For the procedure by which  $\Pi$  is calculated in the parquet approximation, see [<sup>9,10,14</sup>].
- <sup>10</sup>In making comparisons we must keep in mind that the dependence of  $\gamma$  on the spin indices was introduced in [<sup>9</sup>] in a different manner than in Eq. (1). To reconcile Eq. (1) with [<sup>9</sup>] we must make the substitutions  $\gamma_1 \rightarrow \gamma_1$  and  $\gamma_1 \rightarrow \gamma_1 - \gamma_2$ .
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