Fluctuation increment to the conductivity in quasi-one-dimensional systems near a structure transition

L. P. Gor'kov and I. E. Dzyaloshinskiĭ

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences
(Submitted May 27, 1974)
ZhETF Pis. Red. **20**, 37–41 (July 5, 1974)

It is shown that the contribution made to the conductivity by fluctuations near a structure transition is determined by the kinetics of the electronic interactions. The derived expression does not differ from the earlier results. "Three-dimensionality" of the phonons annihilates the fluctuation growth in the conductivity.

A noticeable conductivity maximum was observed in TTF-TCNQ crystals[1] near $T_s = 60\,^\circ$K. It was confirmed in[2] that in a number of cases this maximum takes the form of a sharp peak. According to the explanation proposed for this effect in[3], a structure transition takes place at the point of conductivity maximum. In the vicinity of the transition, the fluctuation gap in the energy spectrum of the one-dimensional electrons attunes itself in the presence of the current to the motion of these electrons in such a way as to hinder the dissipative processes. Attempts were made in[4,5] to derive the mechanism of[3] from the microscopic theory. The results of[4] and[5] do not agree. Since the calculations of[4] have not been published,[1)] we present below the results of our calculations. These results do not agree with those of[4,5], although in the limiting case of one-dimensional phonons they lead to the same temperature dependence of the increment on the conductivity, $\Delta\sigma \propto (T - T_s)^{-1/2}$, as obtained in[3–5]. What is more important is that when the "three-dimensionality" of the phonons is taken into account the structure transition leads only to a singularity in the derivative of the conductivity.

In a one-dimensional metal, the structure and Cooper transitions cannot be separated in the principal approximation.[6,7] At the same time a phase transition is impossible in the one-dimensional case. An analysis of the role of effects of the three-dimensional structure, undertaken in[7], has shown that a structure transition is realized if the interaction between electrons on different filaments (without their jumping over from filament to filament) is large enough. If the jumping over of electrons prevails, then the one-dimensional singularities go over into Cooper pairing in this case. In the first case we deal also with a softening of the corresponding phonon mode. The fluctuation region of temperatures corresponds to

$$(T - T_s)/T_s > g^2, \tag{1}$$

where g^2 is a certain effective electron-electron interaction constant. We consider below for simplicity the model of a structure transition that takes place at a temperature T_s above the Debye temperature. In this case, in the region of applicability of the self-consistent-field approximation (1), the phonon D function takes the form

$$D^R(\omega, k) = \frac{\omega_0^2(k)}{\omega^2 - \omega_0^2 g_{ph}^2 [f - i\beta\omega]}, \tag{2}$$

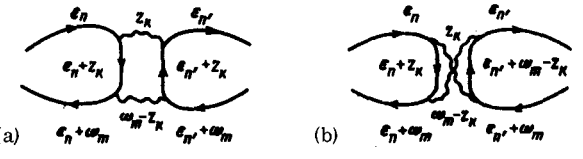
where

$$f = \frac{T - T_s}{T_s} + \frac{7\zeta(3)}{16\pi^2 T_s^2}(v_F k_\parallel)^2 + B g_{ph}^{-2} S^{-1} k_\perp^2; \quad \beta = \pi/8T_s,$$

and g_{ph}^2 is the square of the electron-phonon interaction, S is the cross-section area of the reciprocal lattice, and $B \sim 1$ is a constant that characterizes the dispersion of the phonon frequency. The electron spectrum in the absence of the jumps remains flat ($v_F \equiv v_{zF}$). The fluctuation increments of the conductivity, resulting from the soft mode in (2), are due to the diagrams shown in the figure (see[4,5]), where a wavy line corresponds to the D function of phonons with a transfer $k_\parallel = \pm 2p_F$. For an analytic continuation in ω_m, it is necessary to represent all the sums over the frequencies in the matrix elements of these diagrams in terms of contour integrals. Starting, as in[5], from sums over the phonon frequencies, it is easy to verify that the main contribution to the current matrix element connected with small k and z in (2) is proportional to

$$T^2 \sum_{n,n'=-\infty}^{+\infty} \int \frac{dz}{4\pi i} \operatorname{cth}\frac{z}{2T} D^R_{i\omega_m - z}(D^R_z - D^A_z)$$
$$\times \{ p_z G_{i\epsilon_n} G_{i\epsilon_n + i\omega_m} [G_{z + i\epsilon_n} + G_{i\epsilon_n + i\omega_m - z}]\}$$
$$\times \{ [G_{i\epsilon_{n'} + z} + G_{i\epsilon_{n'} + i\omega_m - z}] G_{i\epsilon_{n'}} G_{i\epsilon_{n'} + i\omega_m} p'_z \}. \tag{3}$$

(We have left out terms in which the D function contains electron frequencies of the order of either T or $1/\tau$. Here $1/\tau$ is the electron-phonon collision frequency.) The succeeding calculations reduce to a determination of the vertices in (3), consisting of products of three electronic Green's functions. Since the D function (2) has a singularity at a longitudinal-momentum transfer $\pm 2p_F$, the two parts of the diagrams in the figure are not independent. If, say, the integration with respect to the electron momentum takes place in the left electronic loop of diagram (a) near $+p_F$, then the point $+p_F$ makes also a contribution in its right-hand loop. The opposite ends of the Fermi surface contribute to the diagram (b). A special case is $4p_F = 2\pi/a$, where a is



the period along the filament axis. This gives rise to new possibilities connected with Umklapp processes. It is easy to verify that in this case the matrix element should be multiplied by a factor $[1-g_{ph}^{*2}/g_{ph}^2]^2$, where g_{ph}^* corresponds to electron-phonon interaction with Umklapp. Generally speaking, there is no reason why this factor should be considered equal to zero, as was done in[4].

For an analytic continuation of (3) it is necessary to calculate the corresponding sums over the electron frequencies. Changing over to the integrals

$$(T\sum_n \ldots \to \frac{1}{4\pi i}\int \mathrm{th}(z/2T)\,dz\ldots),$$

we call attention to terms of the type

$$\frac{\omega}{2T}\int_{-\infty}^{+\infty} \mathrm{ch}^{-2}\frac{\epsilon}{2T}\,G_\epsilon^R G_{\epsilon+\omega}^A G_{z+\epsilon}^R d\epsilon,$$

which have a kinetic nature and therefore depend significantly on the relation between ω and $1/\tau$. These terms were omitted in[5], since the product of the electron loops (designated A^2 in[5]) was expanded in terms of the *Matsubara* frequencies (it appears that the same procedure was used in[4]). In fact the expression of[5] for $A^2(z) \propto z^2 + 2\omega z$ is replaced at $\omega\tau \ll 1$ by

$$z^2 + \frac{2\pi^3}{7\zeta(3)}(\tau T_s)\omega z.$$

We finally obtain

$$\frac{\Delta\sigma}{\sigma_0} = \frac{v_F 7\zeta(3)}{\pi T_s S(2\pi)^3}\int d^3k\left\{\frac{T-T_s}{T_s} + \frac{7\zeta(3)(v_F k_\parallel)^2}{16\pi^2 T_s^2} + B\frac{k_\perp^2}{g_{ph}^2 S}\right\}^{-1}. \qquad (4)$$

In the one-dimensional case this expression does not contain interaction constants, i.e., it does not depend on the range (cf.[4,5]). The main contribution to the integral (4) is made by large k, where the D function does not take the form (2), and the contribution from the fluctuations constitutes a small increment to the main conductivity. Thus, taking into account the three-dimensional character of the phonons, a square-root singularity exists only for the derivative

$$(1/\sigma_0)\frac{d\sigma}{dT} - \frac{1}{\sqrt{T-T_c}}.$$

The one-dimensional case corresponds formally to $B=0$, but in this case there is no phase transition, and (2) and (4) cease to be valid in the strong-interaction region[6] where, in principle, $\Delta\sigma/\sigma_0$ can become of the order of unity. Smallness of B would mean the absence of dispersion of the corresponding optical frequencies, for which no special reasons can be seen. It seems to us that the result is not limited to the considered phonon model of the structure transition, and has a more general character. Returning therefore to the experiments,[3] we point out that the weak maxima of $\sigma(T_s)/\sigma(300) \sim 10-20$ can be understood in principle in accordance with the remark made by the authors of[9], that the relaxation times increase as a result of the electron-electron processes like $T^{-1}f(\ln T)$. It is impossible to explain in this manner an increase of the conductivity by two orders of magnitude.

[1)] All that is made is a qualitative statement that the fluctuations are important only if the number of electrons per period is not equal to unity.

[1] L. B. Coleman, M. J. Cohen, D. J. Sandman, F. G. Yamagishi, A. F. Garito, and A. J. Heeger, Sol. St. Comm. **12**, 1125 (1973).
[2] M. J. Cohen, L. B. Coleman, A. F. Garito, and A. J. Heeger, "The Electrical Conductivity of TTF-TCNQ," Preprint.
[3] J. W. Bray, J. Bardeen, and D. Allender, Phys. Rev. **9B**, 119 (1974).
[4] B. R. Patton and L. J. Sham, Phys. Rev. Lett. **31**, 631 (1973); Phys. Lett. **47A**, 133 (1974).
[5] S. Strassler and G. A. Toombs, Phys. Lett. **46A**, 321 (1974).
[6] Yu. A Bychkov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. **50**, 738 (1966) [Sov. Phys.-JETP **23**, 489 (1966)].
[7] I. E. Dzyaloshinskiĭ and A. I. Larkin, *ibid.* **61**, 791 (1971) [**34**, 422 (1972)].
[8] L. P. Gor'kov and I. E. Dzyaloshinskiĭ, *ibid.* **67**, 397 (1974) [**39**, No. 1 (1974)].
[9] L. P. Gor'kov and I. E. Dzyaloshinskiĭ, ZhETF Pis. Red. **18**, 686 (1973) [JETP Lett. **18**, 401 (1973)].