Conductivity peak in the neighborhood of the Peierls transition

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It is shown that the temperature dependence of the perpendicular conductivity has a maximum near the Peierls transition. If the filaments have gaps, then a corresponding maximum may also appear in the parallel conductivity.

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An increase of conductivity above the Peierls transition in TTF-TCNQ salts is one of the well-known effects in the physics of quasi-one-dimensional compounds.[1] There is a school of thought that this increase is associated with the collective excitations. Below we examine a model in which the collective excitations lead to such increase. Investigation of the intrinsic transverse conductivity in real quasi-one-dimensional systems may prove to be very important because the conducting filaments may be broken in some places. Thus, the effective longitudinal conductivity is possible only if the electrons can flow from one filament to another.

We shall examine a system of conducting filaments with such breaks. Let us assume that the average distance between the breaks is equal to l. Let us also assume that this distance is much larger than all the microscopic dimensions of the system and, in particular, much larger than the amplitude of the jumps T_{ij} of the electrons from one filament to another. Thus, the circumfluence of the gaps in the filaments can be described by the classical equations. Assuming that the conductivity at the gap is low and that the intrinsic parallel conductivity in the region between the gaps $\sigma_{\parallel}$ is much larger than the transverse conductivity $\sigma_{\perp}$, we obtain after a basic examination the following expression for the effective parallel conductivity

$$\sigma_{\text{eff}} \sim l^2/d^2\, \sigma_{\perp}, \tag{1}$$

where d is the distance between the filaments.

Equation (1) shows that the longitudinal conductivity σ_{eff} measured experimentally may depend greatly on the intrinsic transverse conductivity. An analogous equation for the impurities with a Gaussian distribution was obtained in Ref. 2.

We shall calculate $\sigma_{\perp}$ in the following model. Let us assume that the attraction of electrons on one filament is stronger than the interaction of the different filaments. Thus, a gap begins to form at a certain temperature T_{c0}. Let us assume that the adiabatic condition is not fulfilled, so that the system has a tendency of undergoing both a Peierls transition and a superconducting transition. The low-lying excitations in the system are described by the phase Hamiltonian.[3,4] Taking into account the interaction of the different chains, we can write this Hamiltonian in the form

$$\hat{H} = \frac{1}{2}\sum_i \int \left[\hat{\rho}_i^2 K^{-1} + Kv^2\left(\frac{\partial \hat{\phi}_i}{\partial x}\right)^2 - \sum_j{}' \left(J_1 \cos\left(2\hat{\phi}_i(x) - 2\hat{\phi}_j(x)\right) \right.\right. \tag{2}$$

$$\left.\left. + J_2 \cos \pi \int_{x_0}^{x} \left(\hat{\rho}_i(x') - \hat{\rho}_j(x')\right) dx' \right) \right].$$

In expression (2) $\hat{\rho}_i$ and $\hat{\phi}_i$ are the density and the phase operators of the ith filament, respectively. The commutator of these variables is

$$[\hat{\rho}_i(x), \hat{\phi}_j(x')] = i\delta_{ij}\delta(x - x').$$

The quantity K represents compressibility and v denotes the speed of sound. The third and the fourth terms describe the interaction of the superconducting and dielectric fluctuations of the different filaments, respectively. The summation is taken over the nearest neighbors. A three-dimensional transition both to the dielectric and to the superconducting state can occur, depending on the relation between the constants J_1 and J_2. Examining the interaction between the chains in the approximation of the self-consistent field, we obtain the equations for the temperatures of the super-conducting T_{c1} and the dielectric T_{c2} transitions[4]:

$$1 = \frac{zJ_1}{2}\int_0^{1/T_{c1}} \int_{-\infty}^{\infty} G_0(x, \tau)\, d\tau\, dx,$$

$$1 = \frac{zJ_2}{2}\int_0^{1/T_{c2}} \int_{-\infty}^{\infty} \Pi_0(x, \tau)\, d\tau\, dx, \tag{3}$$

where z is the number of nearest neighbors

$$G_0(x, \tau) = \langle \exp(2i\phi(x, \tau) - 2i\phi(0, 0)) \rangle_0,$$

$$\Pi_0(x, \tau) = \exp\left[i\pi\left(\int_{x}^{x} \rho(x', \tau)\, dx' - \int_{x_0}^{0} \rho(x', 0)\, dx' \right)\right]. \tag{3a}$$

Equation (3a) is averaged over the states of the free Hamiltonian without allowance for the interaction of the chains. In explicit form the correlator $G_0(x,\tau)$ is[3,4]

$$G_0(x, \tau) = (T/T_{c0})^{\alpha}[\sinh \pi(x/v + i\tau)\sinh \pi(x/v - i\tau)]^{-\alpha/2}, \tag{4}$$

where $\alpha = 2(\pi K v)^{-1}$

The difference between the $\Pi(x,\tau)$ correlator and the $G(x,\tau)$ correlator is that α^{-1} is substituted for α in the former.

Henceforth, we shall assume that $T_{c2} > T_{c1}$, so that at T_{c2} a three-dimensional dielectric transition occurs. The applied external field, which is perpendicular to the filaments, can be calculated by substituting $\phi_i - \phi_j \to \phi_i - \phi_j - eAd$. The collective part of the current can be written in the form

$$j = 2eJ_1 < \sin(2\phi_i - 2\phi_{i+1} - 2eAd) >. \tag{5}$$

The current in Ref. 5 is an averaged Josephson current. In addition to this current, there is also a single-particle current at finite temperatures. We shall not examine this current, since the three-dimensional transition has little influence on it. Assuming that the external field A is weak, we obtain in the usual way the expression for the response function $Q(\omega)$:

$$Q(\omega_n) = 4e^2 J_1^2 \int_0^{1/T} \int_{-\infty}^{\infty} G^2(x, \tau)(e^{i\omega_n \tau} - 1)dx d\tau. \tag{6}$$

After the calculations in Eq. (6) an analytic continuation from the Matsubari frequencies $i\omega_n \to \omega + i\delta$ must follow. The $G(x,\tau)$ function differs from the $G_0(x,\tau)$ function in that the averaging is done over the total Hamiltonian (2). However, in the region of high temperatures $T \gg T_{c2}$, the interaction of the chains in Eq. (2) is unimportant. In this case the G function coincides with G_0. The calculation in Eq. (6) with use of Eq. (4) and the subsequent analytic continuation can be easily performed by deforming the contour $(0, 1/T)$ into a sum of the contours $(i\infty, 1/T + i\infty)$ $(0, i\infty)$ and $(i\infty + 1/T, 1/T)$. After the calculations we obtain

$$Q(\omega) = \frac{e^2 v J_1^2}{\pi^2 T^2}\left(\frac{T}{T_{co}}\right)^{2a} \sin^{-1}\pi a \Gamma^{-2}(a)\left[\sin^2\pi\left(\frac{a}{2} + \frac{i\omega}{4T\pi}\right)\left|\Gamma\left(\frac{a}{2} + \frac{i\omega}{4\pi T}\right)\right|^4 - \sin^2\frac{\pi a}{2}\Gamma^4\left(\frac{a}{2}\right)\right]. \tag{7}$$

At low frequencies $Q(\omega)$ depends linearly on the frequency. The perpendicular conductivity $\sigma_\perp(0)$ is

$$\sigma_\perp(0) = \frac{e^2 v J_1^2}{4\pi^2 T^3}\left(\frac{2T}{T_{co}}\right)^{2a} \Gamma^4\left(\frac{a}{2}\right)\Gamma^{-2}(a). \tag{8}$$

Equation (8) shows that the conductivity $\sigma_\perp$ is a power function of the temperature in the high-temperature region. The index α depends on the interaction at one filament. For a weak interaction this index is close to unity.

At temperature $T \ll T_{c2}$ the last term in the Hamiltonian (2) becomes important. In this region Eqs. (8) and (9) cannot be used. At $J_1 \ll J_2$ the third term in Eq. (2), as previously, can be ignored. At $T = 0$ the G function in Eq. (6) depends only on $r^2 = (x/v)^2 + \tau^2$. Going over to the polar coordinates r and θ and integrating over the angle θ, we obtain

$$Q(\omega_n) = 8\pi e^2 J_1^2 \, v \int_0^\infty G^2(r)(J_0(\omega_n r) - 1)\, r\, dr. \tag{9}$$

If $G(r)$ decreases sufficiently fast, then $Q(\omega)$ is analytic for small $|\omega|$. The expansion of this function begins with ω^2.

Expanding the second cosine in Eq. (2) and using the self-consistent field approximation analogous to that in Ref. 5, we obtain the asymptotic form of the $G(r)$ function at large distances $r \gg \kappa$

$$G(r) \sim (\kappa / T_{c0})^{2a} \exp(-\kappa r), \tag{10}$$

where $\kappa = CT_{c2}$ and C is a number of the order of unity.

Substituting Eq. (10) in Eq. (9), we can see that the expansion over small ω begins with ω^2, and the conductivity is equal to zero. Apparently, this result is also valid at $J_1 \sim J_2$.

It was assumed above that the resistance at the gaps is large. In practice, however, the flow across the gaps may be large. Thus, the tunneling across the gap resembles qualitatively the examined tunneling from one filament to another. The corresponding equations can also be obtained by averaging with the Hamiltonian (2). Taking into account the contribution from the current across the gaps, will lead to a more complex expression than Eq. (1) for the effective conductivity. In this case the ratio $\sigma_{\text{eff}}/\sigma_\perp$ is no longer a constant. The defects and the commensurability give rise to the appearance in Eq. (2) of cosines that contain the density integrals. The influence of such terms on the conductivity is analogous to the influence of the last term in Eq. (2), which decreases it. This is in qualitative agreement with the results of Refs. 6 and 7. *The increase of conductivity observed experimentally is described approximately by the* $\sigma \sim T^{-1}$ *law,*[8] *which corresponds to the case* $\alpha \approx 1$. The numerical estimates obtained with the help of Eqs. (3) and (8) for $J_1 \sim J_2$, $T \sim T_{c2}$, and $\alpha \approx 1$ give the value $\sigma_\perp \sim 1$ $\Omega^{-1} \cdot \text{cm}^{-2}$. This value agrees in order of magnitude with the measurements of Marshall *et al.*[6]

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