Tunneling between conductors with a charge-density wave

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The current through a P_1–I–P_2 tunnel junction [$P_{1,2}$ are conductors with a charge-density wave (CDW)] is calculated. It is shown that aside from a term proportional to the product of the densities of states, the current includes a term containing $\cos(\chi_1 - \chi_2)$, where $\chi_{1,2}$ are the phases of the CDW.

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In recent years, considerable progress has been achieved in understanding the properties of quasi-one-dimensional conductors below the Peierls transition point. Thus, for example, the predictions of the theory[1,2] of the structure of the ground state of polyacetylene have been confirmed. Optical[3] and tunneling[4] experiments have shown that levels related to the formation of amplitude solitons are actually formed at the center of the forbidden band of polyacetylene. However, many features of the behavior of Peierls conductors remain unclear. This concerns both the structure of the electronic spectrum and the kinetic characteristics, for example, the mechanism of charge transfer.

Tunneling experiments are one of the most convenient methods for studying the electronic spectrum. On the other hand, the tunnel current between Peierls conductors separated by an insulating layer (a P_1–I–P_2 system) has not been calculated. The example of superconductors, in which the phase transition is similar to the Peierls transition, shows that the tunnel effect in such systems makes it possible to determine the energy structure and a number of new interesting phenomena. Here we shall examine tunneling in systems P_1–I–P_2 and P–I–N, where N is a normal conductor, and we shall show that in addition to the usual current I_1 in the N–I–N system there is an additional current I_2 which is proportional to the energy gap Δ and which depends on the difference between the phases of the charge-density waves. Experimental study of this current will apparently permit determining not only some thermodynamic but also kinetic characteristics.

To calculate the tunnel current in a P_1–I–P_2 junction, we shall use the method of the tunneling Hamiltonian for matrix Green's functions $G_{\alpha\beta}(\mathbf{p}, \mathbf{p}')$.[5] To the Hamiltonian system we shall add the terms

$$\hat{H}_T = \sum_{\alpha,\beta,\mathbf{p},\mathbf{q}} [\, T_{\alpha\beta}(\mathbf{p},\mathbf{q})\, c^{+}_{\alpha\mathbf{p}} a_{\beta\mathbf{q}} + \text{c.c.}] , \tag{1}$$

where $\hat{T} = \hat{T}_0 \hat{1} + T_Q \hat{\sigma}_x$ includes the tunneling matrix elements: T_0 without transfer and T_Q with transfer from one side of the Fermi surface to the other, shifted by the wave vector of the CDW. Below we shall write the equation for the Green's function, introduced by Keldysh, $\hat{G}$ up to terms of order $\hat{T}^2$, respectively. The self-energy part, which corresponds to tunneling, is expressed in terms of the Green's functions of one of the electrodes $\hat{G}_2$ as follows:

$$\hat{\Sigma} = T_0^2 \hat{G}_2 + T_Q^2 \hat{\sigma}_x \hat{G}_2 \hat{\sigma}_x + T_0 T_Q (\hat{\sigma}_x \hat{G}_2 + \hat{G}_2 \hat{\sigma}_x). \tag{2}$$

The equation sought for $\hat{G}_1$, which determines the current I, has the form

$$I \sim i \int d\mathbf{p} \, \mathrm{Sp} \frac{\partial \hat{G}_1(\mathbf{p}, t, t)}{\partial t} = i \int d\mathbf{p} \, \mathrm{Sp} \, [\hat{\Sigma}^R \hat{G}_1 + \hat{\Sigma} \hat{G}_1^A - \hat{G}_1^R \hat{\Sigma} - \hat{G}_1 \hat{\Sigma}^A]. \tag{3}$$

Substituting into (3) the expression for $\hat{\Sigma}$ from (2) and for the functions $\hat{G}^{R(A)}$ and $\hat{G}^5$ in (3) and ignoring, for simplicity, the curvature of the nearly flat opposite sections of the Fermi surface, we obtain

$$I = R_N^{-1} \int_{-\infty}^{+\infty} d\epsilon \, (\mathrm{th}\epsilon_+\beta - \mathrm{th}\epsilon_-\beta) \left[|\epsilon_+ \epsilon_-| + \frac{T_0^2}{T_0^2 + T_Q^2} \Delta_1 \Delta_2 \cos(\chi_1 - \chi_2) \right]$$

$$\times \frac{\theta(|\epsilon_+| - \Delta_1)\theta(|\epsilon_-| - \Delta_2)}{2\sqrt{\epsilon_+^2 - \Delta_1^2}\sqrt{\epsilon_-^2 - \Delta_2^2}} + F(\cos \chi_{1,2}), \tag{4}$$

where $\epsilon_\pm = \epsilon \pm V/2$, V is the voltage across the junction, $\beta = 1/2T$, and $\Delta_{1,2}, \chi_{1,2}$ are the gaps and phases of the CDW at the electrodes. The function $F(\cos\chi_{1,2})$, which is not written out here, depends on the phase of the CDW at each of the electrodes differently. The appearance of F is related to the limited applicability of the tunneling Hamiltonian method in this case of a spatially inhomogeneous structure (presence of CDW at each of the electrodes). It follows by writing (1) in the coordinate representation, with $T_{\alpha\beta}(\mathbf{p}, \mathbf{q})$ independent of $\mathbf{p}$ and $\mathbf{q}$, that $T(\mathbf{x}, \mathbf{x}') \sim T^2 \delta(\mathbf{x})\delta(\mathbf{x}')$, i.e., tunneling occurs at a fixed point in space and for this reason depends on the local density of electrons, i.e., on the CDW phase. A more systematic but more complex method shows that the function F in (4) indeed drops out. This method consists of calculating directly the current in a system consisting of two massive Peierls conductors, which are separated by a delta-function barrier. We also assume that at the interface there is a random inhomogeneous potential, and averaging with respect to this potential is what leads to the disappearance of F.

Thus, inside from the usual term in the current, which is proportional to the product of the densities of states $|\epsilon_\pm|/|\sqrt{\epsilon_\pm^2 - \Delta_{1,2}^2}$ and the difference of the quasiparticle distribution functions, there is a term proportional to $\Delta_1 \Delta_2 \cos(\chi_1 - \chi_2)$. We note that the first term I_1 corresponds to a quasiparticle current in the Josephson junction, while the second term I_2 corresponds to the imaginary part of the Josephson current $\mathrm{Im} I_c(V)$.[6] The current I_2 differs from 0 for $V \neq 0$ and at low temperatures $T \ll \Delta$ it is not small for $V > \Delta_1 + \Delta_2$. At low temperatures, in the case $\Delta_1 = \Delta_2 = \Delta$, we obtain

$$I = I_1 + I_2, \qquad I_1 = R_N^{-1} \left[(2\Delta + V) \mathbf{E}(\alpha) - \frac{4\Delta(\Delta + V)}{2\Delta + V} \mathbf{K}(\alpha) \right] \theta(\alpha),$$

$$I_2 = R_N^{-1} \frac{T_0^2}{T_0^2 + T_Q^2} \frac{4\Delta^2 \theta(\alpha)}{V + 2\Delta} \mathbf{K}(\alpha) \cos(\chi_1 - \chi_2), \qquad \alpha = \frac{V - 2\Delta}{V + 2\Delta}. \tag{5}$$

The presence of amplitude solitons[1,2] leads to the appearance of levels at the center of the forbidden band. In this case, for low soliton concentration, the local density of states near the soliton is given by

$$\nu(\epsilon) = \theta(|\epsilon| - \Delta)\frac{|\epsilon|}{\sqrt{\epsilon^2 - \Delta^2}}\left(1 - \frac{\Delta^2}{2\epsilon^2 \operatorname{ch}^2(x/\xi_0)}\right) + \frac{\pi\Delta\delta(\epsilon)}{2\operatorname{ch}^2(x/\xi_0)},$$

where ξ_0 is the correlation length. Then the *I–V* curve of the *P–I–N* system at low temperature has the form

$$I(V) = R_N^{-1}\left\{\theta(V - \Delta)\left[\sqrt{V^2 - \Delta^2} - 2n\xi_0\Delta \operatorname{arctg}\frac{\sqrt{V^2 - \Delta^2}}{\Delta}\right] + \pi n\xi_0\Delta \operatorname{th}\frac{V}{2T}\right\},$$

where n is the soliton concentration per chain.

We note that the results obtained concern systems with a doubled period such as (CH_x), where the phase $\chi = k\pi$ and $\cos(\chi_1 - \chi_2) = \pm 1$, as well as incommensurate systems and systems that do not have twofold commensurability, where χ can assume different values. In the last case, if a current $I_\parallel$, parallel to the plane of the junction and giving rise to motion of CDW, is passed through one of the electrodes (we assume that the conducting filaments are parallel to the plane of the junction), then the phase χ_1 begins to vary with time and an alternating tunneling current $I_\sim$ is generated in the junction with frequency depending on $I_\parallel$. The characteristics $\chi_1(t)$ and $I_\sim(t)$ are determined by the type of motion of the CDW: Does it move as a whole or, for example, is there a motion of soliton domain walls, which separate the regions with different values of χ_1. In particular, if the CDW moves as a whole, then the frequency of oscillations of $I_\sim$ will increase with increasing $I_\parallel$ (ignoring pinning $\chi_1 \sim I_\parallel t$) and when an external alternating signal acts on the junction, a resonance will be observed in the dependence $I(I_\parallel)$ for fixed V if the frequencies of the external and characteristic oscillations coincide.

In principle, the coordinate dependence of χ, which is caused by the presence of soliton domain walls or fluctuations χ due to interaction of CDW with impurities, can lead to averaging of the term with $\cos(\chi_1 - \chi_2)$ in (5). However, this does not occur in junctions with sufficiently small area.

[1]S. A. Brazovskiĭ, Pis'ma Zh. Eksp. Teor. Fiz. **28**, 656 (1978) [JETP Lett. **28**, 606 (1978)].
[2]W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1978).
[3]N. Suzuki *et al.*, Phys. Rev. Lett. **45**, 1209 (1980).
[4]V. Leo, G. Gusman, and R. Deltour, Phys. Rev. B **26**, 3285 (1982).
[5]S. N. Artemenko and A. F. Volkov, Zh. Eksp. Teor. Fiz. **80**, 2018 (1981) [Sov. Phys. JETP **53**, 1050 (1981)].
[6]K. K. Likharev, Rev. Mod. Phys. **51**, 101 (1979).

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