Tunneling mechanism for conversion of conduction electrons into a charge density wave at the interface between a metal and a Peierls insulator

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(Submitted 23 April 1987)

Pis'ma Zh. Eksp. Teor. Fiz. **46**, No. 3, 99–102 (10 August 1987)

The excitation of the current of a charge density wave at the interface between a metal and a Peierls insulator by a tunneling mechanism, as conduction electrons of the metal tunnel into the valence band of the insulator, is analyzed. The probability for the excitation of a current by this mechanism is calculated.

At low temperatures the current carriers in a Peierls insulator are not free electrons and holes but collective excitations of the phase (φ) of the order parameter (a charge density wave). In a closed electric circuit a Peierls insulator is always in contact with a metal, so there is the important problem of determining the mechanism by which conduction electrons convert into the current of a charge density wave at an interface between a metal and a Peierls insulator.

A conversion mechanism which has been discussed[1,2] in the literature is based on the suggestion that a phase-slippage center is produced in the Peierls insulator. Since at such a center the modulus (Δ) of the order parameter vanishes, an energy on the order of Δ is required for the formation of this center. On the other hand, we know that the conductivity of a charge density wave arises at voltages $eV \ll \Delta$ (see, for example, the review by Grüner and Zettl[3]). How would the electrons of the metal convert into the current of a charge density wave in this case, in the ideal situation in which there are no existing phase-slippage centers in the Peierls insulator? Are there no free electrons or holes, or no impurity levels in the gap?

An additional level must be created in the valence band of the Peierls insulator if electrons are to go from the metallic bank of the contact into this insulator. If the conversion is to be a continuous process, the level must have the energy $(eV/2)$ of the metal electrons at the time of the transition, and the level can be formed solely as a result of the formation of a soliton of the modulus of the order parameter. Since the energy of such a soliton is on the order of Δ, the conversion will go by a tunneling mechanism at voltages $eV \ll \Delta$.

It is physically clear that only pairs of electrons with opposite spins can be transferred into the valence band (or a vacuum) of the Peierls insulator. The process by which an electron is scattered at the metal-insulator interface therefore resembles Andreev scattering at a metal-superconductor interface.

In the field-theory approach, the Lagrangian of a Peierls insulator with a complex order parameter is written[4,5]

$$\mathcal{L} = \frac{\dot{\Delta}^2 + \Delta^2 \dot{\varphi}^2}{g^2 \omega_0^2} - \frac{\Delta^2}{g^2} + \bar{\psi}_s \{ i\gamma_\mu (\partial_\mu - ieA_\mu) - \Delta e^{i\gamma_5 \varphi} \} \psi_s . \tag{1}$$

Here ψ_s is the electron-hole spinor; s is the spin projection index; γ_μ $(\mu = 0.1)$, $\gamma_5 = \gamma_0 \gamma_1$ is the set of Pauli matrices; A_μ is the electric potential; g is the electron-phonon coupling constant; and ω_0 is the frequency of phonons of momentum $2k_F$.

To find the probability for a tunneling conversion of metal electrons into a charge density wave, we must find a solution of the Eculidean equations of motion for model (1) with boundary conditions which fix the values of the modulus $[\Delta_i = \Delta_f = \Delta_0 \sim \epsilon_F \exp(-\pi v_F/g^2)]$ and phase $[\varphi_i = 0, \varphi_f = \varphi(x)]$ of the order parameter in the initial (i) and final (f) states. In the course of the conversion, Δ must be an inhomogeneous function of the coordinates if an electron level is to form inside the gap.

Since the adiabatic condition $\bar{\omega} = (g/\sqrt{\pi v_F})\omega_0 \ll \Delta_0$ holds in a Peierls insulator, the solutions which we are seeking should be chosen by requiring that an energy functional be at an extremum. The dependence of these solutions on the imaginary time τ thus enters implicitly: The adjustable parameters of the static solutions become functions[4,7] of τ:

$$\begin{aligned} \sigma_s(x) &= \Delta \cos\varphi = \Delta_0 - \frac{k_0^2}{\Delta_0} \left\{ 1 - \tanh\left(\frac{k_0(x - x_0)}{v_F} \right) \right\}, \\ \pi_s(x) &= \Delta \sin\varphi = \frac{\omega_e k_0}{\Delta_0} \left\{ 1 - \tanh\left(\frac{k_0(x - x_0)}{v_F} \right) \right\}, \end{aligned} \tag{2}$$

where ω_e is the energy of an electronic level inside the gap, given by

$$\omega_e = \Delta_0 \cos\theta(\tau), \quad k_0 = \Delta_0 \sin\theta(\tau). \tag{3}$$

Since we have $\varphi(x) = \arctan(\pi_s/\sigma_s)$, the phase shift at the time τ is $\Delta\varphi(\tau) = \varphi(x = \infty, \tau) - \varphi(x = -\infty, \tau) = 2\theta(\tau)$. The initial value of the chiral angle is zero, while the final value is found from the conservation of energy during tunneling. The potential energy corresponding to solutions (2) is

$$W(\theta)=eV\Theta_H[\theta_v-\theta]+\Delta_0\ \{2\Theta_H[\theta-\theta_v]\cos\theta+\frac{2}{\pi}\ (\sin\theta-\theta\cos\theta)\}\ , \tag{4}$$

$$\theta_v=\arc\cos\frac{eV}{2\Delta_0}\cong\frac{\pi}{2}-\frac{eV}{2\Delta_0}\ ,\quad eV<<\Delta_0\ , \tag{5}$$

where Θ_H [...] is the unit step function, and we have allowed for the energy of a pair of electrons of the metal. Under the condition $\theta<\theta_v$ (curve AV in Fig. 1a), a tunneling fluctuation (2), (3) that arises causes a doubly degenerate level to split off from the empty conduction band, and it causes this level to descend to the energy of a metal electron at the contact ($eV/2$; the dashed line in Fig. 1b). At point V, the level which is formed is occupied by two electrons with opposite spins. At this instant the energy of the electrons begins to decrease continuously (Fig. 1b). The maximum of the potential energy, $W(\theta=\pi/2)=(2/\pi)\Delta_0$, corresponds to the well-known Brazovskiĭ-Shei soliton solution.[4,7] When an electronic level is doubly filled, this solution becomes absolutely unstable (a sphaleron). The tunneling terminates at $\theta_f\cong\pi-(eV/2\Delta_0)$. The subsequent evolution of the charge density wave toward a phase difference $\Delta\varphi=2\pi(\theta=\pi)$ occurs in a classical manner.

At voltages $eV\ll\Delta_0$ the electrons go into the Peierls insulator, to a level localized at an instanton with a length scale $l\sim k_0^{-1}(\theta=\pi/2)v_F=v_F/\Delta_0$. If the probability for the filling of a level by metal electrons is not to be exponentially suppressed, the center of instanton (2), $x_0(\tau)$, must lie near the contact, in a region of size $k_0^{-1}v_F$. The same restriction follows from an analysis of kinetic energy (1). It is easy to verify that the term $\Delta_0^2\int_{-\infty}^{\infty}dx\dot{\varphi}_s^2$, which appears in the "kinetic" energy of instanton ansatz (2), (3), diverges linearly at the lower limit. This is a physical divergence, caused by the obvious fact that the probability for a vacuum-vacuum transition, $|0\rangle\rightarrow|\pm2\pi$, is zero in an infinite volume. To calculate the "kinetic" energy of the instantons near the contact, we ignore the coordinate dependence of the extremals of (2), and we cut off the integral at a characteristic dimension $l\sim k_0^{-1}(\theta)v_F$. We then find

$$(g\,\omega_0^{-2})\int dx\,(\dot{\Delta}^2+\Delta^2\dot{\varphi}^2)=\frac{M_i(\theta)\ \theta^2}{2}\ ,\quad M_i(\theta)\cong\frac{\Delta_0}{\overline{\omega}^2}\sin^{-1}\theta\ , \tag{6}$$

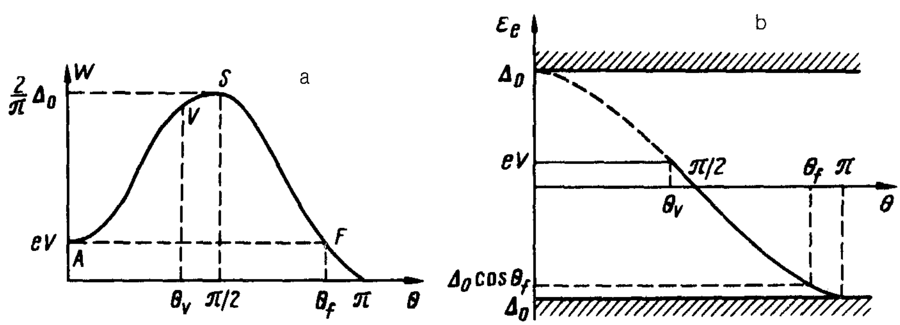

FIG. 1.

and the tunneling action is

$$S = \int_0^{\pi - eV/2\Delta_0} d\theta \, (2M_i(\theta) W(\theta))^{1/2} \sim \frac{\Delta_0}{\overline{\omega}} A, \; A \sim 1. \quad (7)$$

Using (7), we can write the time scale for the tunneling conversion of metal electrons into the Peierls insulator as follows, for typical parameter values of the charge density wave:

$$t \sim \overline{\omega}^{-1} \exp(S) \sim 10^{-8--10} \text{ s}. \quad (8)$$

Our estimates refer to the tunneling conversion of an incommensurate charge density wave at the interface between the metal and the Peierls insulator. In the commensurate case, the current carriers in the Peierls insulator are phase solitons which have an energy $E_\varphi \ll \Delta_0$ and a fractional charge $\pm 2e/M$ (M is the commensurability index[6,8]). By virtue of energy and charge conservation, this conversion mechanism now leads to the formation of a complex of M solitons and is cut off at voltages $eV < ME_\varphi$. It is also clear that at high voltages, $eV \gtrsim (2/\pi)\Delta_0$, the probability for the formation of a charge density wave near a contact will not be of a tunneling nature.

We wish to thank S. N. Artemenko, A. F. Volkov, and I. O. Kulik for useful discussions.

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Translated by Dave Parsons