Character of electron reflection at a normal metal-Peierls semiconductor boundary

S. N. Artemenko and S. V. Remizov

Institute for Radioengineering and Electronics of the Russian Academy of Sciences, 103907 Moscow, Russia

(March 23, 2022)

JETP Letters, Vol. 65, No. 1, 53-58 (10 January 1997)

Abstract

The reflection of electrons incident from a normal metal on the boundary of the metal with a quasi-one-dimensional conductor containing a charge-density wave (CDW) is investigated theoretically. It is shown that the reflection is not of an Andreev character but rather of a Bragg character. This is due to the fact that the CDW is actually an electronic crystal, and its wave vector is a reciprocal lattice vector of the electronic crystal. The ratio of the intensities of the standard and Bragg reflection depends on the phase of the CDW.

It is well known (see, for example, Ref. 1) that an electronic crystal – a charge or spin density wave whose motion under the influence of an electric field is associated with a collective mechanism of conduction – forms in quasi-one-dimensional conductors below the Peierls transition temperature. For definiteness, in what follows we shall study a charge-density wave (CDW), but the results obtained are also applicable to the case of a spin density wave.

There exists a formal analogy between Peierls semiconductors (PSs) and superconductors, since in both cases the condensed state is described by an order parameter \( \Delta = |\Delta| \exp i\varphi \) whose amplitude determines the energy gap in the single-particle excitation spectrum and the derivative of whose phase (in a superconductor with respect to the
coordinate and in a Peierls semiconductor with respect to time) is proportional to the contribution of the condensed electrons to the electric current density. A CDW can be graphically imagined as a condensate consisting of bound pairs of electrons and holes whose momenta differ by the magnitude of the wave vector of the CDW. By analogy to superconductors, where the condensate consists of pairs of electrons with opposite momenta and Andreev reflection is observed at a boundary with normal metal [2], it should be expected that even the reflection of electrons with energy close to the Fermi energy from the normal metal-PS boundary \((N - P)\) has an unusual character. It has been concluded in theoretical works [3,4] that an electron reflected from a PS onto which it was incident from a normal metal moves along the same trajectory along which it was incident on the PS, i.e., the reflection is similar to Andreev reflection, but in contrast to a superconductor the sign of the charge of the incident quasiparticle does not change. The observation of features in the resistance of a contact of a PS with a normal metal which were interpreted as a manifestation of the Andreev-type reflection predicted in Refs. 3 and 4 was recently reported in Ref. 5. In our view, a reflection in which the reflected particle moves along the same trajectory cannot appear at a metal-PS contact, since a quasiparticle in the PS is a superposition of two electrons with momenta differing by the wave vector of the CDW and not with opposite momenta. We shall show that the momentum component parallel to the interface can either be conserved (standard reflection) or change by an amount equal to the CDW wave vector component parallel to the interface (Bragg reflection from an electronic crystal).

We shall be interested in the reflection of electrons with energies of the order of \(k_B T\) or \(\Delta\) near the Fermi energy, since such electrons will determine the conductivity in structures containing a PS.

We consider first the reflection of electrons at the interface between a normal metal and a PS, whose electronic structures differ from one another only by the presence of a CDW in the PS, occupying the space \(x > 0\). This model will enable us to investigate reflection from a CDW in a pure form, since there will be no reflection, associated with the difference in the energy structure of the crystals and having no relation with the CDW, from the interface.
The fact that the CDW was formed in only a part of the crystal could be due to the fact, for example, that the electron-phonon interaction constant vanishes for \( x < 0 \).

To calculate the electronic wave functions in a PS it is often convenient to employ the self-consistent field approximation equations of the Bogolyubov-de Gennes type for superconductors, as was done, for example, in Ref. 3. The envelopes \( u(r) \) and \( v(r) \) – the amplitudes determining the contribution of the states belonging to opposite sheets of the Fermi level, shifted by the wave vector \( Q \) of the CDW, to the total wave functions – serve as the elements of the spinor wave functions. In calculating the wave functions in a nonuniform system by matching at the interface, the total wave functions

\[ \psi = u e^{iQr/2} + ve^{-iQr/2}, \]  

which are solutions of the Schrödinger equation with the potential of the CDW, prescribed for \( x > 0 \) as \( 2|\Delta| \cos (Qr + \varphi) \), must be matched. The matching of the envelopes \( u \) and \( v \) at the interface in the case of a CDW gives, generally speaking, an incorrect result.

Let the conducting chains be directed along the \( x \) axis and let the electronic spectrum of the quasi-one-dimensional conductor in the normal state have the form \( E_N = p_x^2/2m + E_\perp(p_\perp) \), where \( |E_\perp| \ll E_F \) and \( E_F = p_{xF}^2/2m \) is the Fermi energy. For definiteness, we shall consider the case when the wave vector of the CDW possesses the components \( Q = (2k_F, Q_y, 0) \). Then in the Peierls state the spectrum has the form \( E_P = \eta \pm \sqrt{\xi^2 + |\Delta|^2} \), where \( \xi = [E(k) - E(k - Q)]/2, \eta = [E(k) + E(k - Q)]/2, \) and the relation between \( u \) and \( v \) in Eq. (1) is determined by \( u = -\Delta v/(\xi + \sqrt{\xi^2 + |\Delta|^2}) \). If the energy is measured from the Fermi energy \( |\epsilon| = |E - E_F| \) is less than \( |\Delta| \), then in the state with the CDW \( |u| = |v| \) to within corrections of order \( \Delta/E_F \). It follows from the form of Eq. (1) that as a result of matching the solutions at \( x = 0 \) it will turn out that, to the same accuracy, the amplitudes \( u \) and \( v \), which in the normal metal correspond to the amplitudes of the incident and reflected waves, are of the same absolute magnitude. Therefore if the wave vector of the CDW possesses a component \( Q_y \) parallel to the interface, then the corresponding component of the electron momentum will change by \( Q_y \) on reflection.
We shall now calculate, by matching the wave functions, the reflection coefficient, neglecting the coordinate dependence of the energy gap near the interface as a result of the proximity effect. Let us assume, for simplicity, that on formation of a CDW the period is doubled in a direction perpendicular to the conducting chains, i.e., $2Q_y$ corresponds to a reciprocal-lattice vector. For $x < 0$ we seek the wave function in the form

$$\psi = \left[e^{ik_xx} + Ae^{-ik_xx} + Be^{-ik_xx+iQ_yy}\right]e^{i(k_yy+k_zz)},$$

where the first term describes the incident wave, the second term describes the standard reflection, and the third term describes Bragg reflection. For $x > 0$ the wave function must be a linear combination of functions of the form

$$\psi = \left[e^{ik_xx} + Ae^{-ik_xx} + Be^{-ik_xx+iQ_yy}\right]e^{i(k_yy+k_zz)},$$

which describe states possessing along the $y$ axis momentum components $k_y$ and $k_y + Q_y$ and the same energy as the state (2). Strictly speaking, the wave functions in the form of plane wave combinations considered above can be equated only if the electronic structure in the N and P regions is the same and the Bloch periodic factors are identical for $x > 0$ and $x < 0$. Nonetheless, to understand qualitatively the effect of the difference of the electronic spectra in the $N$ and $P$ regions, we shall also discuss the result of the matching for the case when the electronic spectra on both sides of the interface are different.

The expressions for the reflection coefficient $R$ in the general case are quite complicated. For this reason, we confine our attention to the limiting case of weak threedimensionality of the spectrum in the conductor with the CDW and we neglect terms of the order of $E_\perp/\epsilon$. For the case when the electronic structure is the same to the left and right of the boundary, we obtain for the ratio of the standard and Bragg reflection intensities

$$|A/B|^2 = (|\Delta| \sin \varphi/ E_F)^2,$$

Therefore, in accordance with what we have said above, $|A| \ll |B|$ and Bragg reflection, where the parallel component of the momentum changes by $Q_y$, dominates. We also note that the relation (3) depends on the phase of the CDW. $|\epsilon| < |\Delta|$ the reflection coefficient $R = 1$, and for $|\epsilon| > |\Delta|$ we obtain $R = |\Delta|^2/(|\epsilon| + \xi)^2$, where $\xi = \sqrt{\epsilon^2 - |\Delta|^2}$.  

4
We now consider the case when the effective masses along the $x$ axis are different in the materials to the left and right of the interface. Then

$$|A/B|^2 = \frac{(m_1 - m_2)^2}{4m_1 m_2} \begin{cases} \sin^2(\varphi + \varphi_0) & |\epsilon| < |\Delta|, \\ (\epsilon/|\Delta|)^2 \cos^2 \varphi & |\epsilon| > |\Delta|, \end{cases}$$

(4)

where $\varphi_0 = \arctan \xi/\epsilon$. For $m_1 = m_2$ when the answer in Eq. (4) vanishes, the terms of order 1 in the ratio $|A/B|^2$ cancel and therefore the small terms of the order of $(|\Delta|/E_F)^2$, which result in the formula (3), must be taken into account. Therefore, when the electronic spectrum of the crystals on different sides of the interface is different, the standard reflection, where the angle of incidence equals the angle of reflection, is added to the Bragg scattering, and the intensities of both types of scattering are of the same order of magnitude and their ratio depends on the phase of the CDW. If it is assumed that an isotropic metal fills the space $x < 0$, then one obtains an expression differing from expression (4) by the fact that the effective mass $m_1$ in the $N$ region is replaced by $m_1/\cos \theta$, where $\theta$ is the angle of incidence of the electron. Of course, this result is not quantitative, since in matching the wave functions we neglected the periodic Bloch factors in them. Taking account of the real crystal structure would have resulted in the appearance of terms in the expansion of the wave function in a Fourier series in the coordinate which correspond to a change in the momentum by an arbitrary reciprocal lattice vector of both the main and electronic crystals, as a result of which reflection would have also appeared in other directions corresponding to Bragg scattering.

Since the phase of the CDW can change when an electric field directed along the conducting chains is applied to the PS, the dependence of the character of the reflection on the phase of the CDW can be used for experimental investigation of $N - P$ contacts.

We note one other interesting feature of reflection from an $N - P$ contact. This feature is reminiscent of the properties of a normal metal-superconductor contact. As is well known, in a thin layer of normal metal of thickness $d$ bordering a superconductor, bound states with an energy splitting of the order of $\varepsilon_0 = \pi \hbar v_F/d$ (here $v_F = p_x F/m$) appear at energies
\[ |\epsilon| < |\Delta| \] as a result of the Andreev reflection from the superconductor. A similar quantization also appears in a normal metal in contact with a PS if the thickness \( d \) of the normal metal is less than the mean-free path length. The simplest method for investigating such quantization is to calculate the density of states with the aid of the quasiclassical equations for the momentum-integrated Green’s functions, which were employed for investigating the transport properties of PS \[ \text{[3,7]} \]. For our purposes it is sufficient to solve an equation for the retarded Green’s function neglecting the collision integral, in which case this equation has the very simple form

\[ i\hbar v \frac{d\hat{g}}{dx} + (\tilde{\epsilon}\sigma_z + \hat{\Delta})\hat{g} - \hat{g}(\tilde{\epsilon}\sigma_z + \hat{\Delta}) = 0, \tag{5} \]

where the Green’s function \( \hat{g} \) is a \( 2 \times 2 \) matrix with respect to the index corresponding to opposite sheets of the Fermi surface which are displaced by the wave vector \( \mathbf{Q} \) of the CDW, \( \tilde{\epsilon} = \epsilon - \eta (\mathbf{p}_\perp) \), \( \hat{\Delta} = i|\Delta|(\sigma_y \cos \varphi + \sigma_z \sin \varphi) \), and \( \sigma_\alpha \) are the Pauli matrices. Assuming once again that \( |\Delta| \) vanishes abruptly for \( x < 0 \) and that the normal metal occupies the region \(-d < x < 0\), we solve Eq. (5) with the boundary condition \( \text{Tr} \sigma_x g(0) = 0 \) at the boundary of the normal metal with the vacuum. From Eq. (5) we obtain for the function \( g = \text{Tr}(\sigma_z \hat{g}) \), whose real part determines the density of states, in the normal region

\[ g = (\xi + i\tilde{\epsilon}t)/(|\epsilon| + i\xi), \tag{6} \]

where \( t = \tan (2\tilde{\epsilon}d/\hbar v_F + \varphi) \) and it must be assumed that \( \xi \) is an analytic function of \( \epsilon \) in the upper half-plane. The off-diagonal components of \( \hat{g} \) do not vanish even in the normal region, where they oscillate as \( \exp (2\tilde{\epsilon}d/\hbar v_F) \), since the decay length for them equals the mean-free path length and is greater than the thickness of the normal region. In an accurate calculation, we would have to take account of the lowering of the energy gap, which changes the shape of the potential well, in the PS at distances of the order of \( \hbar v_F/|\Delta| \), which happens as a result of the proximity effect. This lowering is due to perturbations of the off-diagonal components of \( \hat{g} \) in the region of the PS near the contact, but the change in the shape of the potential well does not affect the qualitative conclusions and we shall neglect it.
One can see from Eq. (6) that the density of states in the normal metal is an oscillating function of the phase of the CDW as well as of the energy and thickness of the normal region. For energies $|\epsilon| < |\Delta|$ at which bound states appear the density of states has the form

$$N(\epsilon) = \pi \langle (|\xi| + \tilde{\epsilon}t) \delta (\tilde{\epsilon}t - |\xi|) \rangle.$$ \hspace{1cm} (7)

Here $\langle ... \rangle$ indicates averaging over $\mathbf{p}_\perp$. At energies much less than $|\Delta|$ formula (7) reduces to

$$N(\epsilon) = \varepsilon_0 \langle \delta (\tilde{\epsilon} - (2n + 1)\varepsilon_0) \rangle,$$

where $n$ is a positive integer.

Therefore, according to Eq. (7), the electron spectrum in the $N$ layer consists of bands of width $E_\perp$ (the width, determined by the function $\eta(\mathbf{p}_\perp)$, of the electron energy band in the perpendicular direction). If the electron spectrum is strongly one-dimensional $E_\perp < \varepsilon_0$, then the allowed energy bands are separated by regions of forbidden energies, otherwise they overlap and the energy dependence of the density of states is of a stepped form. An estimate gives $\varepsilon_0 \approx 70$ K for $v_F = 3 \cdot 10^7$ cm/s and $d = 0.1 \mu$m. At sufficiently low temperatures ($T < \varepsilon_0$, $E_\perp$) energy quantization can be observed in measurements of the conductivity of the normal region in the contact plane or in measurements of the density of states performed with the aid of tunneling or point contacts to the normal region. The application of an electric field in the direction of the chains changes the phase of the CDW, and for this reason, according to Eq. (7), the field should influence the density of states. To observe quantization, the width of the contact should not exceed the phase correlation length, since the phase of the CDW depends on the coordinates as a result of impurity pinning.

It was assumed above in the analysis of quantization that with the exception of the presence of the CDW for $x > 0$ the electronic spectrum is the same on both sides of the contact. The effect of the differences in the electronic spectrum can be estimated by matching the wave functions, as done in the investigation of reflection. It is found that in the case of a contact of two different quasi-one-dimensional metals with $|k^{N}_{xF} - k^{P}_{xF}| \ll |k^{N}_{xF} + k^{P}_{xF}|$,
where $k_{xF}^{N}$ is the Fermi wave vector in the normal region and $k_{xF}^{P}$ is the Fermi wave vector in the PS, the quantization condition is obtained if the argument of the tangent $2\tilde{\epsilon}d/(\bar{h}v_{F})$ in formula (7) is replaced by $\tilde{\epsilon}_{N}d/(\bar{h}v_{F}) + 2(k_{xF}^{N} - k_{xF}^{P})d$, where the dependence of the energy on $p_{\perp}$ in the normal region appears in $\tilde{\epsilon}_{N}$ in the same way as in the similar dependence in $\tilde{\epsilon}$ for a PS. Therefore the thickness of the $N$ region enters the quantization condition not only in the form 60 but also in the form of the product $(k_{xF}^{N} - k_{xF}^{P})d$, which for large differences in $k_{xF}$ should blur the quantization effects even as a result of small variations of the thickness $d$.

Thus we have found that when electrons incident from a normal metal onto the interface with a PS are reflected, the component of their wave vector parallel to the interface is either conserved or changes by an amount equal to the projection of the wave vector of the CDW on the contact plane. The intensity of different types of reflection depends on the phase of the CDW and therefore can change when an electric field is applied. Specifically, the reflection of electrons from the region with a Peierls gap under certain conditions can result in quantization of the energy spectrum of the electrons near the Fermi energy.

We thank V. A. Volkov for a discussion of this work and also I. G. Gorlova and A. A. Sinchenko for a discussion and for familiarizing us with the experimental data prior to publication. This work is supported by Russian Fund for Fundamental Research (Grant 95-02-05392) and MTP "Physics of Solid-State Nanostructures" (Grant 1-018).
REFERENCES

[1] G. Gr"uner, *Density Waves in Solids*, (Addison-Wesley, Reading, Massachusetts, 1994).

[2] A.F. Andreev, Zh. Eksp. Teor. Fiz. 46, 1823 (1964) [Sov. Phys. JETP 19, 1228 (1964)].

[3] A.L. Kasatkin and E.A. Pashitskii, Fiz. Nizk. Temp. 10, 640 (1984).

[4] A.L. Kasatkin and E.A. PashitskiT, Fiz. Tverd. Tela (Leningrad) 27, 2417 (1985) [Sov. Phys. Solid State 27, 1448 (1985)].

[5] A.A. Sinchenko, Yu. I. Latyshev, S. G. Zybtsev et al., JETP Lett. 64, 285 (1996).

[6] S.N. Artemenko and A.F. Volkov, Zh. Eksp. Teor. Fiz. 81, 1872 (1981) [Sov. Phys. JETP 54, 992 (1981)].

[7] S. N. Artemenko and A. F. Volkov, Chapter 9 in *Charge Density Waves in Solids*, edited by L. Gor’kov and G. Gr"uner (Elsevier Science, Amsterdam, 1989).