

Nonlinear electrical conductivity of a point-contact junction containing a planar defect

Yu. A. Kolesnichenko, M. V. Moskalets, and R. I. Shekhter

Physicotechnical Institute of Low Temperatures, Academy of Sciences of the Ukrainian SSR, Kharkov

(Submitted 25 June 1990)

Zh. Eksp. Teor. Fiz. **98**, 2038–2055 (December 1990)

The influence of the interaction between electrons and phonons localized near a planar defect on the nonlinear electrical conductivity of small-size junctions is studied theoretically. It is shown that the normalized second derivative of the current-voltage characteristic of a point-contact junction (known as the point-contact spectrum) containing a planar defect exhibits singularities due to inelastic relaxation of carriers by interaction with such phonon states. In strong magnetic fields (such that $r_H \ll d$, where r_H is the cyclotron radius of the electron paths and d is the junction size) and also in the case of strong elastic scattering of electrons by a defect, the surface contribution predominates over the contribution of the bulk electron-phonon interaction to the point-contact spectrum. The quantum nature of carrier relaxation interacting with strongly localized phonons governs the contribution made to the point-contact spectrum by the effects of renormalization of the electron mass, giving rise to a specific "quantum background." The results obtained can account for anomalies of the point-contact spectra of tin associated with the electron-phonon interaction at a twin boundary, observed recently by Khotkevich, Yanson, Lazareva *et al.* [Sov. Phys. JETP **71**, 937 (1990)].

INTRODUCTION

The problem of the interaction of conduction electrons with macroscopic defects in metals is currently attracting much attention because of the discovery of enhancement of the superconductivity near twinning planes in tin.^{1,2} The observed effect can be explained in a natural manner by the special properties of the electron and phonon states near a defect. However, direct experimental studies of such an electron-phonon interaction (EPI) localized near a grain boundary are difficult because of the smallness of the effective volume occupied by defects in a metal. In this situation an important role is played by methods for local probing of a metal when the measured effect is due to the contribution of extremely small volumes of a conductor or to a small group of particular electrons.³⁻⁵ One of these methods is known to be determination of the transport phenomena in point-contact junctions whose resistance is governed by the scattering of carriers within a small region ($d \approx 10^2 - 10^3 \text{ \AA}$) in which an electric current is concentrated.^{6,7} Such a region has dimensions comparable with the size of a defect, which provides a unique opportunity for investigating the interaction of carriers with a single scattering object.

This idea was realized in experiments carried out on point-contact junctions with tin and reported in Ref. 8: anomalies were observed in the point-contact spectrum and these were probably associated with the contribution of EPI near a twin boundary.

The method of point-contact spectroscopy of macrodefects required that the contributions of the local EPI at a defect be distinguished from the background of the EPI spectrum of a defect-free metal (representing the bulk contribution to the point-contact spectrum). The local contribution should be very distinctive because of the sensitivity of the effect to the electron transmission coefficient D of a defect and to the ratio of the electron λ_B and localized phonon κ^{-1} wavelengths. An additional opportunity for separating

the bulk defect contributions to the point-contact spectrum is provided by a study of the dependence of the intensity of such a spectrum on an external magnetic field.

We shall develop a theory of point-contact spectroscopy of the EPI localized near a planar defect. We shall use a model (Fig. 1) in which the planar defect intersects the point-contact junction and is oriented at right-angles to its axis, where the phonon states represent surface waves near a defect boundary. Since the depth κ^{-1} at which surface phonons are located is governed by their frequency ω and increases in the limit $\omega \rightarrow 0$, the value of ω controlled by the voltage applied to the point-contact junction determines whether the electron-phonon scattering at the defect is quantum-mechanical ($\kappa^{-1} \lesssim \lambda_B$) or classical ($\kappa^{-1} \gg \lambda_B$). In the quantum case the electron transport resembles the inelastic tunneling of carriers across a carrier, whereas in the classical case it resembles the classical electron-phonon relaxation in point-contact junctions. A smooth transition be-

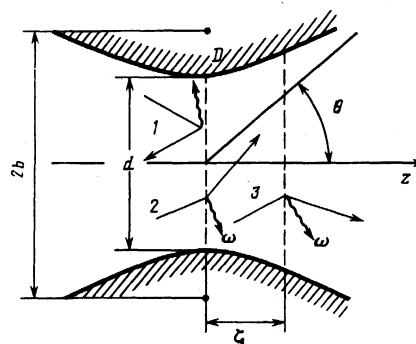


FIG. 1. Model of a point-contact junction in the shape of a single-sheet hyperboloid of revolution with a vertex angle 2θ and an interfacial distance $2b$; d is the smallest diameter. A planar defect of transparency D is located in the central plane $z=0$ or at a distance $\zeta \approx d$ from it. Paths of electrons (1, 2, and 3) interacting with surface phonons of frequency ω are shown schematically.

tween these two qualitatively different cases of the inelastic electrical conductivity can be induced by varying the voltage across the junction.

It is of fundamental importance that the contributions of the local and bulk EPI depend differently on the elastic tunneling coefficient D of electrons crossing the defect. The quantum process of electron-phonon relaxation near a defect, like the inelastic tunneling effect, makes a contribution to the resistivity which is of order D , while bulk relaxation associated with the way in which a tunneling electron is scattered in the bulk and then creates a return tunnel current is proportional to D^2 . We can therefore have a situation in which the contribution to the point-contact spectrum of the EPI localized at a defect is the dominant effect. Identification of this contribution is facilitated by a study of how the intensity in the point-contact spectrum depends on the external magnetic field. The bulk and surface contributions then exhibit different asymptotic behavior in a strong magnetic field (such that $r_H \lesssim d, l_i$; here, r_H is the cyclotron radius of the carrier paths, l_i is the elastic mean free path of electrons, and d is the point-contact junction size), the specific nature of which depends on the transparency D .

Our results will be reported as follows. In Sec. 1 we formulate the model and find the general relationships governing the elastic electrical conductivity and the conditions encountered in point-contact spectroscopy. We analyze the contribution made by the EPI at the defect to the point-contact spectrum (Sec. 2). This contribution is calculated using an effective boundary condition reflecting the quantum nature of the electron-phonon scattering during crossing of the defect boundary. We derive the boundary condition for the electron distribution function (Appendix I). We devote Sec. 3 to an analysis of the bulk relaxation processes in a point-contact junction containing a planar defect. A comparison of both contributions and a discussion of the conditions for the observation of the EPI at a defect is made in the Conclusions.

1. FORMULATION OF THE PROBLEM AND BASIC RELATIONSHIPS

If the size of a planar defect is comparable with the size of a point-contact junction, the defect has a fundamental influence on the electrical conductivity. A typical situation encountered in this case is shown in Fig. 1. The processes of elastic scattering of electrons limit the current across the junction and make an additional contribution to the resistivity. In the absence of the inelastic scattering of carriers by a defect, a system of this kind represents a point-contact tunnel junction whose transparency is governed by the elastic scattering of electrons on the defect plane. It is known^{9,10} that the transport properties of such a junction can be investigated using the semiclassical approach based on formulation of suitable boundary conditions applicable to the electron distribution function and describing elastic scattering as well as quantum passage of carriers across a defect. We assume that, in addition to the processes already mentioned, there are also inelastic channels of quantum transmission due to the interaction of electrons with surface oscillations (phonons or other Bose excitations) located at a distance κ^{-1} from the defect plane. When the localization length κ^{-1} is small compared with the transport lengths of elec-

trons, i.e., when $\kappa^{-1} \ll l_i, l_{ep}, d$ (l_{ep} is the electron-phonon relaxation length), the analysis of the inelastic scattering processes reduces to formulation of semiclassical boundary conditions applicable not only to the elastic but also to the inelastic processes of carrier scattering. In general, such a boundary condition is a relationship linking the distribution function $f_{\mathbf{p}_{\parallel}, -p_{zj}}^{(j)}$ of electrons traveling from the boundary in the j th half-space ($j = 1$ or 2) with the analogous functions $f_{\mathbf{p}_{\parallel}, p_{zk}}^{(k)}$ for carriers arriving from the interior of a metal at the defect (located in the plane σ):

$$f_{\mathbf{p}_{\parallel}, -p_{zj}}^{(j)}(\rho) = (1 - D) f_{\mathbf{p}_{\parallel}, p_{zj}}^{(j)}(\rho) + D f_{\mathbf{p}_{\parallel}, p_{zk}}^{(k)}(\rho) + \bar{W}_j \{f_p^{(1)}(\rho), f_p^{(2)}(\rho)\}, \quad \rho \in \sigma, \quad j \neq k. \quad (1)$$

Here, p_{zj} and \mathbf{p}_{\parallel} are the components (perpendicular and parallel to the defect plane) of the momentum of an electron arriving at the defect from the j th bank of the junction; D is the effective transparency representing the probability of elastic transmission of electrons by a defect; the integral operator \bar{W}_j corresponds to the inelastic scattering channels. Note that the energies of the incident and transmitted electrons satisfy the law of conservation which includes a possible jump of the electric potential ΔV at the junction:

$$\epsilon_{pj} = \epsilon_{pk} + e\Delta V.$$

A rigorous derivation of the boundary condition (1) requires a consistent microscopic analysis. Such an analysis is given in the Appendix I. The presence of the term \bar{W}_j in Eq. (1) determines the specific nature of the problem under consideration and is responsible for the appearance of significant contributions made to a point-contact spectrum by the EPI at a defect boundary.

The electron transport outside a planar defect can be described using an approach which is normally employed in point-contact spectroscopy. We give the principal relationships which will be needed later. The distribution functions $f_p^{(j)}$ are found from the Boltzmann transport equation containing the integrals of the elastic (I_i) and electron-phonon collisions (I_{ep}) in a metal:

$$v \frac{\partial f_p^{(j)}}{\partial \mathbf{r}} + \left(e\mathbf{E} + \frac{e}{c} [\mathbf{vH}] \right) \frac{\partial f_p^{(j)}}{\partial \mathbf{p}} = I_i \{f_p^{(j)}\} + I_{ep} \{f_p^{(j)}\}. \quad (2)$$

Equation (2) together with the boundary condition (1) should be supplemented by conditions representing the elastic scattering of electrons on the surface of a metal¹¹ and by a condition representing the spreading of the current in the interior of a conductor [$f_p^{(j)}(\mathbf{r} \rightarrow \infty) = n_F$, where $n_F(\epsilon_p)$ is the Fermi function]. The electric potential $\varphi(\mathbf{r})$ ($\mathbf{E} = -\nabla\varphi$) is found from the equation of electrical neutrality and satisfies the condition

$$\varphi(\mathbf{r} \rightarrow \infty) = \frac{1}{2} V \text{ sign } z.$$

A static magnetic field is assumed to be oriented along the junction axis [$\mathbf{H} = (0, 0, H)$].

The traditional treatment of point-contact spectroscopy involves an allowance for the inelastic carrier scattering processes on the basis of perturbation theory. The relevant condition applying to the bulk scattering is¹²

$$L \ll \min\{l_{ep}, \lambda_e = (l_i l_{ep})^{1/2}\}, \quad (3)$$

where L is the effective spreading length of an electric current, equal to the junction size d in weak magnetic fields ($r_H > d$) and to dl_i/r_H in strong magnetic fields ($r_H < l_i, d$). A similar condition in the case of spectroscopy of the surface inelastic scattering processes is

$$\kappa^{-1} \ll l_s, \quad (4)$$

where l_s is the characteristic mean free part of electrons in the case of inelastic scattering by surface oscillations near a defect. In this case the term \hat{W}_j in the boundary condition (1) can be allowed for using perturbation theory.

The elastic electrical conductivity of a point-contact junction is found by solving the transport problem to lowest order in the parameters (3) and (4):

$$f_{p0}^{(j)}(\mathbf{r}) = \alpha_p^{(j)}(\mathbf{r}) n_F^+ + [1 - \alpha_p^{(j)}(\mathbf{r})] n_F^-, \quad (5)$$

$$n_F^\pm = n_F [e_p + e\phi(\mathbf{r}) \mp eV/2].$$

The quantity $\alpha_p^{(j)}(\mathbf{r})$ represents the probability that an electron with a momentum \mathbf{p} reaches a point \mathbf{r} from the right-hand bank of a junction and it satisfies Eq. (2) subject to the condition (1) for $I_{ep} = \hat{W}_j = 0$. At the banks of a junction, we have

$$\alpha_p^{(j)}(\mathbf{r} \rightarrow \infty) = \theta(z).$$

If

$$d \gg \min\{l_i, r_H\}, \quad (6)$$

the analysis of the "elastic" electrical conductivity can be reduced to the analysis of the process of carrier diffusion:¹²

$$\alpha_p^{(j)}(\mathbf{r}) = \alpha^{(j)}(\mathbf{r}) - v_z \tau_i \frac{\partial \alpha^{(j)}}{\partial z} + \frac{\tau_i}{1 + (\Omega \tau_i)^2} \left[(-v_x + \Omega \tau_i v_y) \frac{\partial \alpha^{(j)}}{\partial x} - (v_y + \Omega \tau_i v_x) \frac{\partial \alpha^{(j)}}{\partial y} \right] + \dots, \quad (7)$$

$$\left[\frac{\partial^2}{\partial z^2} + \frac{1}{1 + (\Omega \tau_i)^2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right] \alpha^{(j)}(\mathbf{r}) = 0, \quad (8)$$

where $\tau_i = l_i/v_F$, v_F is the Fermi velocity, and Ω is the Larmor frequency of electrons in a field \mathbf{H} . After substitution in Eq. (1) with $\hat{W}_j = 0$ of the expansion (7), we find that the effective boundary conditions for a planar defect become^{9,13}

$$\frac{dl_i}{l_D} \frac{\partial \alpha^{(j)}}{\partial z} = \alpha^{(1)}(\mathbf{r}) - \alpha^{(2)}(\mathbf{r}) \Big|_{r \in \sigma}, \quad (9)$$

where

$$l_D = \frac{3}{4} d \frac{\langle D | n_z | \rangle}{1 - s/2 \langle D n_z^2 \rangle}$$

is the barrier scattering length, $n_z = v_z/v_F$, and the angular brackets $\langle \dots \rangle$ denote averaging over the Fermi surface.

For $D = 1$, the boundary-value problem described by Eqs. (8) and (9) is identical with the contact problem considered in Ref. 12 using a model of an aperture in an impermeable screen. This model is of general interest because, as shown below, the description of an extended junction in the limit of strong magnetic fields reduces to this model.

We consider a point-contact junction in the form of a single-sheet hyperboloid of revolution characterized by a vertex angle θ (Fig. 1), which governs the effective length of

the junction $b(0) = d/2 \sin \theta$. Equation (8) can be solved directly by compressing the coordinate system along the z axis so that

$$z' = z [1 + (\Omega \tau_i)^2]^{-1/2}, \quad (10)$$

which converts Eq. (8) to the Laplace equation. Then, in the new coordinate system this junction surface is again a hyperboloid but with an effective length

$$b(H) = d/2 \sin \theta', \quad \text{tg } \theta' = \text{tg } \theta [1 + (\Omega \tau_i)^2]^{1/2}. \quad (11)$$

We can see that in the limit $H \rightarrow \infty$ the effective vertex angle θ' of the hyperboloid tends to $\pi/2$ and the solution becomes identical with that obtained using the aperture model. In general, for $D = 1$, we obtain

$$\alpha^{(j)}(\mathbf{r}) = \theta(z) - \text{sign } z \Phi \left(x, y, \frac{z}{[1 + (\Omega \tau_i)^2]^{1/2}} \right), \quad (12)$$

$$\Phi(\mathbf{r}) = \text{arctg} \left\{ \left[\frac{r^2}{2b^2} - \frac{1}{2} + \left(\left(\frac{r^2}{2b^2} - \frac{1}{2} \right)^2 + \frac{z^2}{b^2} \right)^{1/2} \right]^{-1/2} \right\}. \quad (13)$$

The dependence of the junction resistance on the magnetic field is

$$R(H) = \frac{\rho}{d} [1 + (\Omega \tau_i)^2]^{1/2} \text{ctg} \left\{ \frac{1}{2} \text{arctg} [\text{tg } \theta [1 + (\Omega \tau_i)^2]^{1/2}] \right\} \quad (14)$$

(ρ is the resistivity of the junction material). For $H \rightarrow \infty$, the asymptotic behavior of the dependence $R(H)$ is identical with that found in Ref. 12 using the aperture model. This behavior seems natural because in a strong field the lines of flow of the current concentrate along the z axis (Fig. 1) and the spreading pattern becomes very insensitive to the size of the junction, but is governed solely by the shape of its smallest cross section.

In the low-transparency limit of the tunnel barrier for

$$Dd \ll \min(l_i, r_H), \quad (15)$$

we find that the boundary condition (9) becomes¹³

$$\frac{\partial \alpha^{(j)}}{\partial z} = - \frac{l_D}{dl_i} \Big|_{r \in \sigma} \quad (16)$$

and the solution of the boundary-value problem for a junction in the form of an aperture ($\theta = \pi/2$) can be written down similarly to Eq. (12), whereas the function $\Phi(\mathbf{r})$ is given by

$$\Phi(\mathbf{r}) = \frac{l_D}{\pi dl_i} \int_{\rho \in \sigma} \frac{d^2 \rho}{|\mathbf{r} - \rho|}. \quad (17)$$

The resistance of the contact is then given by

$$R(H) = R_T + \frac{32}{3\pi^2} \frac{\rho}{d} [1 + (\Omega \tau_i)^2]^{1/2}, \quad (18)$$

where $R_T = 2\rho l_i / \pi dl_D$ is the tunnel resistance of the barrier. An increase in the magnetic field allows us to go from the case of low transparency of the tunnel barrier [$l_D \ll \min(l_i, r_H)$], when its resistance predominates, to the case of a junction with direct conduction ($r_H \ll l_D, l_i$) when the main contribution comes from the region through which the current spreads in the banks of the junction with longitudinal size $L = dl_i/r_H$ and transverse size d (Ref. 13). In this

case the presence of the tunnel barrier has practically no effect on the electrical conductivity of the point-contact junction.

The above solution of the elastic boundary-value problem governs the inelastic corrections to the point-contact junction current. We shall analyze these corrections in the next sections.

2. POINT-CONTACT SPECTRUM OF INELASTIC ELECTRON SCATTERING BY A PLANAR DEFECT

The allowance for the interaction between electrons and surface oscillations localized near the defect is related to retention of the term \hat{W}_j in the boundary condition (1). The distribution functions $f_p^{(j)}$ occurring in the "collision integral" \hat{W}_j are the functions of Eq. (5) representing the zeroth approximation. The term $\hat{W}_j \{f_{p_0}^{(1)}, f_{p_0}^{(2)}\} \equiv \hat{W}_j(\mathbf{p}, \mathbf{p})$ in the boundary condition then corresponds to a source concentrated in the defect plane $\mathbf{p} \in \sigma$. The corrections to the distribution function $f_{p_0}^{(j)}$ can be calculated using the Green's function of the transport problem in the elastic limit. In accordance with the transformations given in Appendix II, the correction to the point-contact junction current associated with the contribution of the surface oscillations at a planar defect can be represented in the form

$$I_s = \frac{2e}{(2\pi)^3} \int_{\rho \in \sigma} d^2\rho \int d^3p v_z \sum_{j=1}^2 \alpha_{-p}^{(j)}(\rho, -\mathbf{H}) \hat{W}_j(\rho, \mathbf{p}). \quad (19)$$

Here and later we use a system of units in which $\hbar = 1$. Since the size κ^{-1} of the zone where surface phonons are generated is generally comparable with the de Broglie wavelength of electrons (inelastic relaxation under quantum transmission conditions), the transport current is governed not only by the processes of emission or absorption of real phonons, but also by the appropriate renormalization of the electron spectrum. We can therefore distinguish two contributions to the "phonon correction" to the current: the contribution $I_s^{(1)}$ corresponding to real scattering processes, and the contribution $I_s^{(2)}$ related to the processes of virtual transitions of electrons under the action of a "phonon" perturbation. The term $I_s^{(1)}$ governs the point-contact spectrum of the EPI at a defect, whereas $I_s^{(2)}$ corresponds to the presence of a "quantum background" in the relevant point-contact spectrum in the frequency range $\omega > \omega_D$ (ω_D is the maximum frequency of surface phonons). We shall now estimate these contributions separately.

a) Point-contact spectrum of the surface electron-phonon interaction

Using the actual form of the collision integral \hat{W}_j obtained in the Appendix I, we can represent a point-contact spectrum (which is the normalized second derivative of the current $I_s^{(1)}$ with respect to the voltage) in its standard form

$$\frac{1}{R(0)} \frac{dR}{dV} = \frac{16ed}{3v_F} \int_0^\infty \frac{d\omega}{T} S\left(\frac{\omega - eV}{T}\right) G_s(\omega), \quad (20)$$

where

$$S(x) = \frac{d^2}{dx^2} \left(\frac{x}{e^x - 1} \right),$$

T is the absolute temperature

$$G_s(\omega) = 2\pi \left(\int \frac{dS_p}{v} \right)^{-1} \sum_{\tau} \int \frac{dS_p}{(2\pi)^3 v} \int \frac{dS_{p'}}{v'} |V_{\mathbf{p}_{\parallel} - \mathbf{p}'_{\parallel}, \tau}|^2 \times K_s(\mathbf{p}, \mathbf{p}') \delta(\omega - \omega_{\mathbf{p}_{\parallel} - \mathbf{p}'_{\parallel}, \tau}). \quad (21)$$

The point-contact function of the interaction with surface phonons $G_s(\omega)$ includes an integral with respect to the two-dimensional vector $\mathbf{q} = \mathbf{p}_{\parallel} - \mathbf{p}'_{\parallel}$ of the generated phonons, whereas the value of the momentum Δp_z transferred by electrons is not limited (in contrast to three-dimensional phonons) by the condition $\Delta p_z \lesssim q$. Therefore, the EPI function for surface phonons characterized by $q \ll p_F$ contains in addition to the bulk EPI function, a large factor of order $p_F/q \gg 1$. The transport form factor for the surface inelastic scattering process $[K_s(\mathbf{p}, \mathbf{p}')]$ is governed by the probabilities of the classical motion of electrons and by the processes of quantum scattering near a defect:

$$K_s(\mathbf{p}, \mathbf{p}') = \left[\int_{\rho \in \sigma} d^2\rho \langle v_z \alpha_p^{(j)}(\rho) \rangle \right]^{-1} \frac{3\pi v_F \kappa^{-1}}{32d} \theta(p_z) \theta(p_z') \times \sum_{j,k,l=1}^2 W_{kl}^{(j)} \times \int_{\rho \in \sigma} d^2\rho \alpha_{-\mathbf{p}_{\parallel}, \mathbf{p}_{zj}}^{(j)}(\rho, -\mathbf{H}) [\alpha_{\mathbf{p}_{\parallel}, \mathbf{p}_{zk}}^{(k)}(\rho, \mathbf{H}) - \alpha_{\mathbf{p}_{\parallel}, \mathbf{p}_{zl}}^{(l)}(\rho, \mathbf{H})]. \quad (22)$$

The effective probability for scattering $W_{kl}^{(j)}$ by a barrier is calculated in Appendix I [Eq. (I.14)]. The general expression (22) simplifies in two limiting cases of barriers characterized by high and low transparency. For $D \ll 1$, the model of a δ -function barrier²⁾ yields

$$K_s(\mathbf{n}, \mathbf{n}') = -\frac{8}{3} \frac{\kappa^{-1}}{d} \theta(n_z) \theta(n_z') (n_z n_z')^2 [\bar{\kappa}^2 - (n_z - n_z')^2] \times \Delta^2(n_z - n_z') \Delta^2(n_z + n_z'), \quad (23)$$

where

$$\Delta(n_z) = \frac{\bar{\kappa}}{\bar{\kappa}^2 + n_z^2}, \quad \bar{\kappa} = \frac{\kappa}{p_F}, \quad n = \frac{v}{v_F},$$

and κ^{-1} is the depth of penetration of a surface oscillation with a two-dimensional momentum $\mathbf{q} = \mathbf{p}_{\parallel} - \mathbf{p}'_{\parallel}$.

We note two important circumstances that follow from Eq. (23). Firstly, the intensity in a point-contact spectrum is independent of the tunnel barrier transparency, of the transport electron relaxation lengths, and of the applied magnetic field, but is governed (to lowest order in $D \ll 1$) simply by barrier relaxation of electron states which are in local equilibrium in each of the junction banks ($f_{p_0}^{(j)} = n_F [\epsilon_p + (-1)eV/2]$). Secondly, when the reciprocal of the depth of localization κ of a phonon perturbation is considerably greater than the momentum of the scattered phonons $|p_z - p_z'|$, the relaxation processes occur in the quantum vicinity of a barrier ($\sim \lambda_B$) and the sign of the point-contact spectrum is negative, like the sign of the corresponding correction to the point-contact junction resistance. In this sense the result obtained resembles inelastic scattering of electrons across a boundary. However, the analogy is not complete. We can easily see by analyzing the point-contact spectrum in the case $\kappa \ll |p_z - p_z'|$ that the scattering of

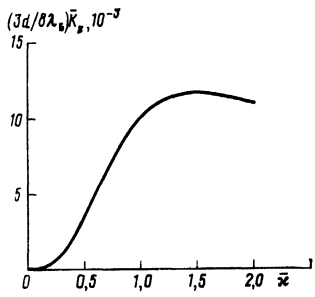


FIG. 2. Dependence of the averaged (over the momentum components perpendicular to the plane of the defect) K_s factor on the reciprocal of the damping distance of surface oscillations $\kappa = \bar{\kappa}\lambda_B$.

electrons occurs near their semiclassical motion and can be regarded as retardation of the electron flux because of a change in the momentum component \mathbf{p}_{\parallel} parallel to the barrier. Figure 2 shows the result of a calculation of the average form factor

$$\overline{K_s(\mathbf{n}, \mathbf{n}')} = \int_0^1 dn_z \int_0^1 dn_z' K_s(\mathbf{n}, \mathbf{n}') \quad (24)$$

as a function of κ . It is clear [see also Eq. (23)] that in the limit $\bar{\kappa} \rightarrow 0$ we have $\overline{K_s} \rightarrow 0$, and in general we must include in Eq. (22) the next terms of the expansion in D . These terms govern the correction to the point-contact spectrum that depends on the applied magnetic field:

$$\begin{aligned} \delta K_s(\mathbf{n}, \mathbf{n}') &= \frac{9}{2\pi^2} \frac{l_D \lambda_B}{d^2} \theta(n_z) \theta(n_z') \bar{\kappa} \Delta^2 (n_z - n_z') \\ &\times (\mathbf{n}_{\parallel} - \mathbf{n}'_{\parallel})^2 \frac{1 - (\Omega\tau_i)^2}{1 + (\Omega\tau_i)^2}, \end{aligned} \quad (25)$$

$\bar{\kappa} \ll 1, \quad \lambda_B = 1/p_F.$

We note that Eq. (25) does not include a term describing the scattering-induced change in the component of the momentum p_z perpendicular to the defect whose absolute value is conserved on reflection and tunneling of electrons apart from corrections of order $\lambda_B \kappa \ll 1$. In weak magnetic fields ($\Omega\tau_i < 1$) the form factor of Eq. (25) is positive, as in the

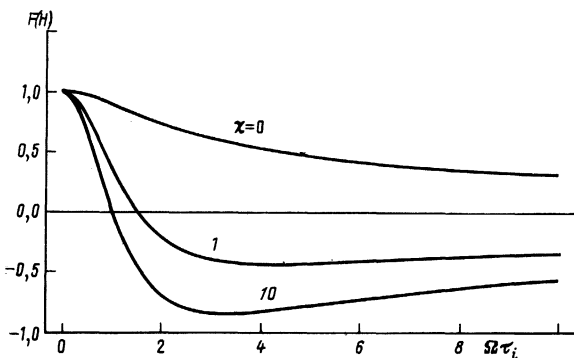


FIG. 3. Dependence of the averaged (over the Fermi surface) form factor K_s on the applied magnetic field (represented by the parameter $\Omega\tau_i$), plotted for different distances $\zeta = d\chi$ of the planar defect from the central plane of the junction in the case when $D \approx 1$ ($\theta = \pi/4$); $F(H) = \langle \langle K_s(H) \rangle \rangle / \langle \langle K_s(0) \rangle \rangle$.

case of the scattering by bulk phonons, and it is proportional to the barrier length l_D . The sign of $\delta K_s(\mathbf{p}, \mathbf{p}')$ changes as the field H increases ($\Omega\tau_i > 1$). This reflects the fact that the scattering of electrons characterized by a change in the momentum component \mathbf{p}_{\parallel} parallel to the boundary (and perpendicular to the vector \mathbf{H}) favors spreading of the electric current and reduces the resistance.

We now consider those defects which reflect electrons weakly ($D \rightarrow 1$). This case should clearly be encountered in the case of low-angle and twin boundaries in metals. We can easily see [see Eqs. (7), (12), and (13)] that if the planar defect is located at the center of the junction (in the $z = 0$ plane), the inelastic scattering processes make no contribution to the point-contact spectrum ($\partial\alpha^{(j)}/\partial x = \partial\alpha^{(j)}/\partial y = 0$ at $z = 0$). However, this corresponds to a random degeneracy associated with a high symmetry of the model. Since we are dealing with an asymmetric case, we shall regard the defect plane as shifted relative to the center of the junction by an amount ζ (Fig. 1). The form factor of the surface contribution of the defect to the point-contact spectrum considered in this geometry is

$$\begin{aligned} K_s(\mathbf{n}, \mathbf{n}') &= \frac{9}{32\pi} \frac{l_i \lambda_B}{d^2} \text{ctg} \frac{\theta'}{2} \frac{\theta(n_z) \theta(n_z')}{[1 + (\Omega\tau_i)^2]^{3/2}} \\ &\times \bar{\kappa} \left\{ 2[(n_z - n_z')^2 \Delta^2 (n_z - n_z') \right. \\ &+ (n_z + n_z')^2 \Delta^2 (n_z + n_z')] \ln \frac{1 + \chi^2}{\cos^4 \theta' + \chi^2} \\ &- (\mathbf{n}_{\parallel} - \mathbf{n}'_{\parallel})^2 \frac{1 - (\Omega\tau_i)^2}{1 + (\Omega\tau_i)^2} [\Delta^2 (n_z - n_z') \\ &+ \Delta^2 (n_z + n_z')] \left. \left[\ln \cos^4 \theta' + (1 + \chi^2) \ln \frac{1 + \chi^2}{\cos^4 \theta' + \chi^2} \right] \right\}, \end{aligned} \quad (26)$$

where $\chi = (2\zeta/d) \sin \theta'$ and the angle θ' is given by Eq. (11). The validity of Eq. (26) is limited to the range of fields in which point-contact spectroscopy can be performed [see the inequality of Eq. (3)]. It follows from Eq. (26) that for $H = 0$, the point-contact spectrum is positive for any value of $\bar{\kappa}$. This difference from the situation $D \ll 1$ discussed above is associated with a considerable difference between the electron states representing in the limit $D \rightarrow 1$ waves which are practically plane, and not almost standing as in the $D \ll 1$ case. Therefore, the destruction by phonons of the interference between the waves incident and reflected by a defect should not then occur. As expected, a point-contact spectrum corresponding to $D \approx 1$ depends strongly on the parameter $\Omega\tau_i$. This dependence is shown in Fig. 3 for the average form factor $F(H)$ in the quantum case defined by $\bar{\kappa} \gg 1$. For values of the parameter χ higher than a certain value $\chi_1 < 1$, we find that in strong magnetic fields the quantity $\langle \langle K_s \rangle \rangle$ changes its sign and the surface contribution to a point-contact spectrum becomes negative.

b) Effects of renormalization of the carrier mass

The effects of renormalization of the electron spectrum are represented by the contributions of virtual electron transitions to the transport current. The corresponding component of the point-contact junction current is [see Eq. (19) and Appendix I]

$$I_s^{(2)} = \frac{2e}{(2\pi)^3} \int_{\mathbf{q} \in \sigma} d^3\rho \int d^3p \theta(p_z) \int d^3p' \theta(p'_z) \times \sum_{j, k, l=1}^2 \alpha_{\mathbf{p}_j, \mathbf{p}_{zj}}^{(j)}(\rho, -\mathbf{H}) \times \sum_{\gamma} |V_{\mathbf{p}_j - \mathbf{p}'_j, \gamma}|^2 \frac{\kappa^{-1}}{\pi} M_{kl}^{(j)}(\mathbf{p}, \mathbf{p}') \times \left[\frac{\Gamma_{lk}(\mathbf{p}', \mathbf{p})}{\epsilon_{\mathbf{p}'} - \epsilon_{\mathbf{p}} - \omega_{\mathbf{p}_j - \mathbf{p}'_j, \gamma}} - \frac{\Gamma_{kl}(\mathbf{p}, \mathbf{p}')}{\epsilon_{\mathbf{p}'} - \epsilon_{\mathbf{p}} + \omega_{\mathbf{p}_j - \mathbf{p}'_j, \gamma}} \right], \quad (27)$$

where the functions $M_{kl}^{(j)}(\mathbf{p}, \mathbf{p}')$ and $\Gamma_{kl}(\mathbf{p}, \mathbf{p}')$ are given by Eqs. (I.14) and (I.13) in Appendix I. Substituting in Eq. (27) the zeroth-approximation distribution functions of Eq. (5) and differentiating Eq. (27) twice with respect to the voltage V , we readily obtain an expression for the correction to the value of $R^{-1}(dR/dV)$ of Eq. (20), which describes an additional background in the point-contact spectrum due to the EPI in the quantum vicinity of the junction barrier. The corresponding term (identified by the index bg) in the normalized second derivative of the current-voltage characteristic of the point-contact junction at the temperature $T = 0$ is

$$\left[\frac{1}{R(0)} \frac{dR(V)}{dV} \right]_{bg} = \frac{16ed}{3v_F} \left(\int \frac{dS_{\mathbf{p}}}{v} \right)^{-1} \sum_{\gamma} \int \frac{dS_{\mathbf{p}}}{v} \int \frac{dS_{\mathbf{p}'}}{v'} \times |V_{\mathbf{p}_j - \mathbf{p}'_j, \gamma}|^2 K_s^{bg}(\mathbf{p}, \mathbf{p}') \frac{2\omega_{\mathbf{p}_j - \mathbf{p}'_j, \gamma}}{(eV)^2 - \omega_{\mathbf{p}_j - \mathbf{p}'_j, \gamma}^2}, \quad (28)$$

where

$$K_s^{bg}(\mathbf{p}, \mathbf{p}') = \frac{3\pi\kappa^{-1}}{32d} \theta(n_z) \theta(n'_z) \left(\int_{\mathbf{q} \in \sigma} d^3\rho \langle n_z \alpha_{\mathbf{p}}^{(j)}(\rho) \rangle \right)^{-1} \times \sum_{j, k, l=1}^2 M_{kl}^{(j)} \int_{\mathbf{p} \in \sigma} d^3\rho \alpha_{\mathbf{p}_j, \mathbf{p}_{zj}}^{(j)}(\rho, -\mathbf{H}) [\alpha_{\mathbf{p}_j, \mathbf{p}_{zk}}^{(k)}(\rho, \mathbf{H}) + \alpha_{\mathbf{p}_j, \mathbf{p}_{zl}}^{(l)}(\rho, \mathbf{H}) - 2\alpha_{\mathbf{p}_j, \mathbf{p}_{zk}}^{(k)}(\rho, \mathbf{H}) \alpha_{\mathbf{p}_j, \mathbf{p}_{zl}}^{(l)}(\rho, \mathbf{H})]. \quad (29)$$

Since the matrix $M_{kl}^{(j)}$ contains only the off-diagonal components of $D_{sk}^{(j)}$ and, consequently, is proportional to the product of the quantum reflection R and tunneling T coefficients [see Eqs. (I.14) and (I.19) in the Appendix I], the component of the point-contact spectrum given by Eq. (28) is small both for tunnel junctions with a transparency $D \ll 1$ and for junctions with direct conduction ($D \approx 1$). Using the expres-

sions for the probabilities $\alpha_{\mathbf{p}}^{(j)}$ in Eqs. (7) and (12), we can show that in the case of symmetric contacts we have $K_z^{bg} = 0$. However, any deviation from the junction symmetry gives a nonzero value of K_s^{bg} . For example, when a tunnel barrier of transparency $l_i/d \ll D \ll 1$ separates metals of different purity ($l_i^{(2)} < l_i^{(1)}, l_i^{(j)}$ is the elastic mean free path of carriers in the j th metal), we have

$$K_s^{bg}(\mathbf{n}, \mathbf{n}') = \frac{9\pi\kappa^{-1}l_i^{(2)}}{d^2} \theta(n_z) \theta(n'_z) (n_z n'_z)^2 \Delta^2(n_z - n'_z) \Delta^2(n_z + n'_z). \quad (30)$$

Beyond the boundary of the phonon spectrum ($eV > \omega_D$) the quantum background of Eq. (28) is positive and it decreases as a function of V proportionally to V^{-2} .

3. POINT-CONTACT SPECTRUM OF THE BULK ELECTRON-PHONON INTERACTION IN THE PRESENCE OF A PLANAR DEFECT

If we assume $\hat{W}_j = 0$ in the boundary condition (1) and include in the transport equation (2) the electron-phonon collision integral I_{ep} using perturbation theory, we obtain the correction to the electron distribution function which can then be used to calculate the bulk contribution to the inelastic current through a point-contact junction.⁶ The corresponding term in the normalized second derivative of the current with respect to the voltage applied to a point-contact junction [see Eq. (20)] contains the EPI function in the bulk of the metal

$$G_V(\omega) = \left(\int \frac{dS_{\mathbf{p}}}{v} \right)^{-1} \sum_{\tau} \int \int \frac{dS_{\mathbf{p}} dS_{\mathbf{p}'}}{(2\pi)^3 v v'} \times W_{\mathbf{p}-\mathbf{p}', \tau} K_V(\mathbf{p}, \mathbf{p}') \delta(\omega - \omega_{\mathbf{p}-\mathbf{p}', \tau}), \quad (31)$$

where $W_{\mathbf{p}-\mathbf{p}', \tau}$ is the square of the absolute value of the EPI matrix element. The dependence of the point-contact spectrum on the magnetic field, on the geometry of the point-contact junction, and on the transparency D of a planar defect is concentrated in the factor K , which can be expressed in terms of the probability $\alpha_{\mathbf{p}}^{(j)}(\mathbf{r})$:

$$K_V(\mathbf{p}, \mathbf{p}') = \frac{3\pi}{32d} \sum_{j=1}^2 \frac{\int d^3r [\alpha_{\mathbf{p}}^{(j)}(\mathbf{r}, \mathbf{H}) - \alpha_{\mathbf{p}'}^{(j)}(\mathbf{r}, \mathbf{H})][\alpha_{\mathbf{p}}^{(j)}(\mathbf{r}, -\mathbf{H}) - \alpha_{\mathbf{p}'}^{(j)}(\mathbf{r}, -\mathbf{H})]}{\int d^3\rho \langle n_z \alpha_{\mathbf{p}}^{(j)} \rangle} \theta[(-1)z]. \quad (32)$$

Further analysis of Eq. (31) can be carried out conveniently as in the preceding section in the two limiting cases $D \rightarrow 1$ and $D \ll 1$.

a) Point-contact junction with direct conduction

Substituting the diffusion expansion of Eq. (7) for the functions $\alpha_{\mathbf{p}}^{(j)}$ in the limit $D \rightarrow 1$ [see Eqs. (12) and (13)], we obtain the following expression for the form factor of Eq.

(32) in the model of a point-contact junction in the shape of a hyperboloid of revolution:

$$K_V(\mathbf{n}, \mathbf{n}') = \frac{9\pi}{64} \frac{l_i}{d} \left\{ 2(n_z - n'_z)^2 \cos^2 \frac{\theta'}{2} + (\mathbf{n}_{\parallel} - \mathbf{n}'_{\parallel})^2 \frac{1 - (\Omega\tau_i)^2}{1 + (\Omega\tau_i)^2} \sin^2 \frac{\theta'}{2} \right\}. \quad (33)$$

The value of the K factor averaged over the directions of the electron momenta is

$$\langle\langle K_V \rangle\rangle = \frac{3\pi l_i}{16d} [1 + (\Omega\tau_i)^2]^{-1} \times \left\{ 1 + (\Omega\tau_i)^2 \frac{\cos\theta}{[1 + (\Omega\tau_i)^2 \sin^2\theta]^{1/2}} \right\}. \quad (34)$$

In the case of a junction in the form of an aperture ($\theta = \pi/2$) Eqs. (33) and (34) are identical with the results given in Ref. 12. It is worth noting that in strong magnetic fields when $\theta' \rightarrow \pi/2$ holds, so that the aperture model provides a satisfactory description of a point-contact junction, the contribution made to the point-contact spectrum by the scattering processes associated with the change in the momentum along the magnetic field \mathbf{H} is balanced out by the corresponding contribution when the momentum changes at right-angles to the field. However, the nature of the fall of $\langle\langle K_V \rangle\rangle$ as H increases is different for a junction in the form of an aperture ($\theta \approx \pi/2$) and for an extended contact ($\theta \ll 1$):

$$\langle\langle K_V \rangle\rangle = \frac{3\pi l_i}{16d} \begin{cases} (\Omega\tau_i)^{-2}, & \Omega\tau_i \gg 1, \quad \theta \approx \frac{\pi}{2} \\ (\theta\Omega\tau_i)^{-1}, & \theta\Omega\tau_i \gg 1, \quad \theta \ll 1 \end{cases}. \quad (35)$$

b) Planar defect with a low transparency

The use of the probabilities $\alpha_p^{(j)}$ for a point-contact tunnel junction of low transparency in the calculation of the K factor of Eq. (32) [Eqs. (7), (12), and (17)] gives the following result in the aperture model:

$$K_V(\mathbf{n}, \mathbf{n}') = \frac{3}{8} \frac{l_D}{d} [1 + (\Omega\tau_i)^2]^{1/2} \left[2(n_z - n_z')^2 + (\mathbf{n}_{\parallel} - \mathbf{n}'_{\parallel})^2 \frac{1 - (\Omega\tau_i)^2}{1 + (\Omega\tau_i)^2} \right]. \quad (36)$$

The value of the form factor averaged over the directions of the vectors \mathbf{n} and \mathbf{n}'

$$\langle\langle K_V(\mathbf{n}, \mathbf{n}') \rangle\rangle = \frac{1}{2} \frac{l_D}{d} \frac{1}{[1 + (\Omega\tau_i)^2]^{1/2}} \quad (37)$$

decreases as H^{-1} in strong magnetic fields ($\Omega\tau_i \gg 1$), in contrast to junctions with direct conduction, which are characterized by $\langle\langle K_V \rangle\rangle \propto H^{-2}$.

The quantity $\langle\langle K_V \rangle\rangle$ represents the total intensity in a point-contact spectrum. In an anisotropic material a situation may arise in which the dominant contribution to the spectrum at some particular energy is made by the EPI processes involving changes in the electron momentum components longitudinal (p_z) or transverse (\mathbf{p}_{\parallel}) relative to the magnetic field vector \mathbf{H} . Then in strong magnetic fields the intensities of the individual peaks in the spectrum increase linearly with the field H . The part of the spectrum corresponding to the emission of phonons with a modified value of \mathbf{p}_{\parallel} (these processes represent the spreading of the current) has the negative sign. An increase in the intensities of the individual peaks in the point-contact spectrum in a magnetic field is due to an increase, with H , in the size of the region of

the strong interaction between electrons and phonons, which coincides with the region in which the current is concentrated.

CONCLUSIONS

Our analysis shows that single planar defects have a considerable influence on the nonlinear electrical conductivity of point-contact junctions, giving rise to an additional term G_s (eV) in the point-contact spectrum. This term is due to the inelastic scattering of electrons by phonons localized near the defect. The intensity and sign of the point-contact spectrum characterized by the average value of the form factor $\langle\langle K_s \rangle\rangle$ depend on the defect transparency D to carriers and on the ratio of the de Broglie wavelength λ_B to the characteristic damping depth κ^{-1} of surface phonons ($\omega = eV$). In the case of a low-transparency defect, we have

$$\langle\langle K_s \rangle\rangle \approx \begin{cases} -\frac{\kappa^{-1}}{d} (\kappa\lambda_B)^{-2}, & \lambda_B \gg \kappa^{-1} \\ D \frac{\lambda_B}{d} \frac{1 - (l_i/r_H)^2}{1 + (l_i/r_H)^2}, & \lambda_B \ll \kappa^{-1} \end{cases}. \quad (38)$$

In the quantum case defined by $\lambda_B \gg \kappa^{-1}(\omega)$, typical of intervalley relaxation in semimetals and semiconductors, when the scattering processes occur at distances κ^{-1} from a barrier smaller than λ_B the intensity in the point-contact spectrum is independent of the bulk relaxation lengths of electrons and of the applied magnetic field, whereas the sign of the average K_s factor is negative. This is due to "bleaching" of the barrier because of suppression (by inelastic surface processes) of the interference between the incident and reflected electron waves. In the semiclassical case when the depth at which surface phonons are damped out is considerable ($\kappa^{-1} > \lambda_B$), the point-contact spectrum is positive for $H = 0$ and becomes negative in a strong magnetic field ($r_H < l_i$) perpendicular to the defect plane. Reversal of the sign in the spectrum in this case is due to the processes that are accompanied by a change in the carrier momentum projection perpendicular to the vector \mathbf{H} .

When the defect is highly transparent, so that $D \rightarrow 1$ and the interference between the electrons incident and reflected by the barrier is negligible, the dependence of $\langle\langle K_s \rangle\rangle$ on l_i and r_H is retained in the quantum and semiclassical cases:

$$\langle\langle K_s \rangle\rangle \approx \frac{l_i \lambda}{d^2} \mathcal{F}\left(\frac{l_i}{r_H}\right), \quad \lambda = \min\{\kappa^{-1}, \lambda_B\}. \quad (39)$$

Behavior of the function $\mathcal{F}(\xi)$ [$\mathcal{F}(0) = 1$ —see Fig. 3] in strong magnetic fields ($\xi = l_i/r_H \gg 1$) depends on the position of the defect in the junction, which governs the ratio of the contributions made to the scattering spectrum and accompanied by changes in the momentum along and at right-angles to the magnetic field. In the most natural (from the experimental point of view) situation when the plane defect is located at a distance of order d from the center of the junction, we have

$$\mathcal{F}(\xi) \approx -(1/\xi) \ln \xi, \quad \xi \gg 1. \quad (40)$$

We may find from Eqs. (38) and (39) that the point-contact spectrum of surface oscillations obtained for the phonon momentum range $q \approx \kappa^{-1} \gg \lambda_B$ is characterized by a "quantum" smallness λ_B/d compared with the contribu-

tion of the bulk EPI. However, the absence of integration of the third component of the phonon momentum from $G_s(\omega)$ [see Eq. (21)] suppresses the effects of the smallness of the K factor and the relative intensity of the surface EPI in the point-contact spectrum when $q \ll p_F$ is governed by the parameter q^{-1}/d .

The contribution of the bulk EPI processes to the point-contact spectrum of a junction in the form of an aperture with tunnel conduction across a planar defect is always proportional to the transparency coefficient $D \ll 1$ and falls linearly with increasing magnetic field, but remains positive:

$$\langle\langle K_V \rangle\rangle \approx D(1 + l_i^2/r_H^2)^{-1/2}. \quad (41)$$

When the barrier transparency is close to unity, the dependence of $\langle\langle K_V \rangle\rangle$ on H is very sensitive to the shape of the junction:

$$\langle\langle K_V \rangle\rangle \approx \frac{l_i}{d} \left(1 + \frac{l_i L}{r_H d}\right) \left[1 + \left(\frac{l_i}{r_H}\right)^2\right]^{-1}, \quad (42)$$

so that in the aperture model (junction length $L = 0$) we have $\langle\langle K_V \rangle\rangle \propto r_H^2$, whereas for an extended junction ($L \gg d$), we obtain $\langle\langle K_V \rangle\rangle \propto r_H$.

It therefore follows that although the surface contribution to the point-contact spectrum contains the small parameter κ^{-1}/d , representing the smallness of the region of generation of two-dimensional phonons, this contribution can be distinguished from the background bulk effect. This is possible because of the different behavior of $\langle\langle K_s \rangle\rangle$ and $\langle\langle K_V \rangle\rangle$ in strong magnetic fields. The surface component $\langle\langle K_s \rangle\rangle$ changes sign in the range $r_H/l_i \ll 1$ and tends to a constant value for $D \ll 1$, as given by Eq. (38), or it falls as $(r_H/l_i) \ln(l_i/r_H)$ in the limit $D \rightarrow 1$, whereas the bulk component of the K factor $\langle\langle K_V \rangle\rangle$ remains positive and decreases at least as fast as $1/H$ for any value of D . It therefore follows that when the magnetic field is sufficiently strong, the surface contribution becomes dominant and can be investigated under the conventional conditions used in point-contact spectroscopy experiments. In the quantum case ($\kappa^{-1} \ll \lambda_B$) the point-contact spectrum of point-like tunnel junctions with a very low transparency $D < (\kappa^3 \lambda_B^2 d)^{-1}$ is negative and is governed by the interaction of electrons with the surface phonons even if $H = 0$.

When the contribution of the EPI at a planar defect is not the dominant term, reversal of its sign in the range $\kappa^{-1}(\omega) \gtrsim \lambda_B$ should result in an effective reduction of the hf part of the overall spectrum and should enhance the lf part. It should be noted that this enhancement of the lf part of the spectrum should be much stronger because the effective volume $\propto d^2 \kappa^{-1}(\omega)$ of the region where surface phonons are generated increases as the frequency decreases. This may account for the "softening" of the EPI spectrum reported for point-contact junctions of tin containing twin boundaries.⁸ It is worth noting the appearance of a specific quantum background in the point-contact spectrum (as demonstrated by the experimental results reported in Ref. 8), which is associated with the energy-dependent effect of the renormalization of the electron mass because of the interaction with strongly localized surface phonons. The anomalously strong background in the experiments of Ref. 8 is of such quantum nature.

Reliable identification of macroscopic defects in a

point-contact junction and identification of their contribution to the point-contact spectrum of the EPI requires that the experiments be carried out in a magnetic field which above all provides an opportunity¹³ to determine the tunnel barrier transparency in the point-contact junction from the dependence $R(H)$.

The authors are deeply grateful to I. O. Kulik for his constant interest and valuable comments.

APPENDIX I. BOUNDARY CONDITION FOR THE SEMICLASSICAL DISTRIBUTION FUNCTION OF ELECTRONS INTERACTING WITH OSCILLATIONS LOCALIZED NEAR A PLANAR DEFECT

The derivation of the boundary condition (1) involves calculation of the Wigner distribution function

$$f_{\mathbf{p}}^W(\mathbf{r}, t) = -i \int d\mathbf{r}' e^{-i\mathbf{p}\mathbf{r}'} G_{12}\left(\mathbf{r} + \frac{\mathbf{r}'}{2}, t; \mathbf{r} - \frac{\mathbf{r}'}{2}, t\right). \quad (I.1)$$

The electron Green's function $G_{jk}(x_1, x_2)$ [$x \equiv (\mathbf{r}, t)$] satisfy the following matrix equation¹⁴

$$\hat{G}(x_1, x_2) = \hat{G}^{(0)}(x_1, x_2) + \int dx dx' \hat{G}^{(0)}(x_1, x) \hat{\Sigma}(x, x') \hat{G}(x', x_2). \quad (I.2)$$

To lowest order of perturbation theory in the Hamiltonian H_{int} representing the interaction between electrons and surface phonons, we can modify the right-hand side of Eq. (I.2) by replacing the functions G_{jk} with the functions $G_{jk}^{(0)}$ that correspond to $H_{\text{int}} = 0$ and by writing the components of the matrix of the self-energy functions Σ_{jk} in the form

$$\Sigma_{jk}(x_1, x_2) = (-1)^{j+k} i G_{jk}^{(0)}(x_1, x_2) D_{kj}(x_2, x_1), \quad (I.3)$$

where $\hat{D}(x_1, x_2)$ is the matrix Green's function of the surface phonons that includes the potential of their interaction with electrons.

We expand the field electron operators $\Psi(x)$ in terms of a complete system of the electron wave functions $\Psi_{jk}(\mathbf{r})$ in the case when a barrier is located near the $z = 0$ plane:

$$\Psi(x) = \sum_{j=1}^2 \sum_{\mathbf{k}} a_{jk} \Psi_{jk}(\mathbf{r}) \exp(-i\varepsilon_{kj}t), \quad (I.4)$$

where a_{jk} is the annihilation operator for an electron in a state with a momentum \mathbf{k} and a total energy ε_{kj} , where the index $j = 1$ and 2 labels the half-spaces to the left ($j = 1$) and to the right ($j = 2$) of the barrier. In calculating the relevant matrix elements accurate apart from corrections of order eV/ε_F , we can regard the electron momentum p_{zj} as conserved after tunneling and outside the barrier region we can describe the wave functions as follows:

$$\psi_{jk}(\mathbf{r}) = \frac{1}{(2\pi)^{1/2}} \exp(i\mathbf{k}_{\parallel}\mathbf{r}_{\parallel}) \psi_{k_{zj}}(z), \quad (I.5)$$

$$\psi_{k_{zj}}(z) = \begin{cases} T \exp(ik_z|z|), & \text{sign } z = (-1)^{j-1} \\ \exp(-ik_z|z|) + R \exp(ik_z|z|), & \text{sign } z = (-1)^j \end{cases}, \quad (I.6)$$

for $k_z > 0$ (R and T are the electron reflection and tunneling coefficients linked by the relationship $|T|^2 + |R|^2 = 1$).

We expand the phonon operators $\Phi(x)$ as follows:

$$\Phi(x) = \frac{1}{2\pi} \sum_{\mathbf{q}, \gamma} [\Phi_{\mathbf{q}, \gamma}(\mathbf{r}) c_{\mathbf{q}, \gamma} \exp(-i\omega_{\mathbf{q}, \gamma} t) + \text{H.c.}], \quad (\text{I.7})$$

where

$$\Phi_{\mathbf{q}, \gamma}(\mathbf{r}) = (2\kappa)^{1/2} V_{\mathbf{q}, \gamma} \exp(i\mathbf{q}\mathbf{r}_{\parallel} - \kappa|z|). \quad (\text{I.8})$$

In Eq. (I.8) the notation is as follows: $c_{\mathbf{q}, \gamma}$ is the annihilation operator for a phonon of frequency $\omega_{\mathbf{q}, \gamma}$ with a two-dimensional wave vector $\mathbf{q} = (q_x, q_y, 0)$; γ labels the branches of the spectrum; $V_{\mathbf{q}, \gamma}$ is the matrix element of the interaction of electrons with oscillations damped out at a distance $\kappa^{-1}(\omega_{\mathbf{q}, \gamma})$ from a planar defect.

Using the expansions (I.5) and (I.7) for the matrices of the Green's functions $\hat{G}^{(0)}$ and \hat{D} , we obtain the following expressions:

$$\hat{G}^{(0)}(x_1, x_2) = i \sum_{j=1}^2 \sum_{\mathbf{k}} \theta(k_z) \hat{n}_{j\mathbf{k}}(t_1 - t_2) \times \exp[-i\epsilon_{\mathbf{k}j}(t_1 - t_2)] \psi_{j\mathbf{k}}(\mathbf{r}_1) \psi_{j\mathbf{k}}(\mathbf{r}_2), \quad (\text{I.9})$$

$$\hat{n}_{j\mathbf{k}}(t) = \begin{pmatrix} n_{j\mathbf{k}} - \theta(t) & n_{j\mathbf{k}} \\ n_{j\mathbf{k}} - 1 & n_{j\mathbf{k}} - \theta(-t) \end{pmatrix}, \quad n_{j\mathbf{k}} = \langle a_{j\mathbf{k}}^+ a_{j\mathbf{k}} \rangle,$$

$$\hat{D}(x_1, x_2) = -i \sum_{\mathbf{q}, \gamma} \{\Phi_{\mathbf{q}, \gamma}(\mathbf{r}_1) \Phi_{\mathbf{q}, \gamma}^*(\mathbf{r}_2) \times \exp[-i\omega_{\mathbf{q}, \gamma}(t_1 - t_2)] \hat{N}_{\mathbf{q}, \gamma}(t_1 - t_2) + \Phi_{\mathbf{q}, \gamma}^*(\mathbf{r}_1) \Phi_{\mathbf{q}, \gamma}(\mathbf{r}_2) \exp[i\omega_{\mathbf{q}, \gamma}(t_1 - t_2)] \hat{N}_{\mathbf{q}, \gamma}(t_2 - t_1)\},$$

$$\hat{N}_{\mathbf{q}, \gamma}(t) = \begin{pmatrix} N_{\mathbf{q}, \gamma} + \theta(t) & N_{\mathbf{q}, \gamma} \\ N_{\mathbf{q}, \gamma} + 1 & N_{\mathbf{q}, \gamma} + \theta(-t) \end{pmatrix},$$

$$N_{\mathbf{q}, \gamma} = \langle c_{\mathbf{q}, \gamma}^+ c_{\mathbf{q}, \gamma} \rangle, \quad (\text{I.10})$$

where $\tilde{N}_{\mathbf{q}, \gamma}$ is a matrix transposed relative to $\hat{N}_{\mathbf{q}, \gamma}$. Substituting the expressions of Eqs. (I.9) and (I.10) into Eq. (I.2), we can find, in the first nonvanishing order of perturbation theory in H_{int} , a correction to the function $G_{12}^{(0)}$ and thus calculate in the same approximation the Wigner distribution function $f_{\mathbf{p}}^W(\mathbf{r})$ of Eq. (I.1). After very involved calculations for electrons traveling away from a planar defect ($p_z = -p_{zj}$), we obtain the following expression if $|z| \gg \lambda_B$, κ^{-1} :

$$f_{\mathbf{p}_{\parallel}, -p_{zj}}^W = |T|^2 f_{\mathbf{p}}^{(1)} + |R|^2 f_{\mathbf{p}}^{(2)} + \tilde{W}_j \{f_{\mathbf{p}}^{(1)}, f_{\mathbf{p}}^{(2)}\}, \quad (\text{I.11})$$

$$\tilde{W}_j \{f_{\mathbf{p}}^{(1)}, f_{\mathbf{p}}^{(2)}\} = \frac{\theta(-p_{zj})}{|v_z|} \sum_{\gamma} \sum_{k, l=1}^2 \int \frac{dp_z' d^2q}{(2\pi)^3} \theta(p_z') |V_{\mathbf{q}, \gamma}|^2 \kappa^{-1} \times \{W_{kl}(p_z, p_z'; \mathbf{q}) [\Gamma_{lk}(\mathbf{p}', \mathbf{p}) \delta(\epsilon_{\mathbf{p}'l} - \epsilon_{\mathbf{p}k} - \omega_{\mathbf{q}, \gamma}) - \Gamma_{kl}(\mathbf{p}, \mathbf{p}') \delta(\epsilon_{\mathbf{p}'l} - \epsilon_{\mathbf{p}k} + \omega_{\mathbf{q}, \gamma})] + M_{kl}^{(j)}(p_z, p_z', \mathbf{q}) \left[\frac{\Gamma_{lk}(\mathbf{p}', \mathbf{p})}{\epsilon_{\mathbf{p}'l} - \epsilon_{\mathbf{p}k} - \omega_{\mathbf{q}, \gamma}} - \frac{\Gamma_{kl}(\mathbf{p}, \mathbf{p}')}{\epsilon_{\mathbf{p}'l} - \epsilon_{\mathbf{p}k} + \omega_{\mathbf{q}, \gamma}} \right]\}, \quad l \neq j, \quad (\text{I.12})$$

where

$$\Gamma_{kl}(\mathbf{p}, \mathbf{p}') = f_{\mathbf{p}}^{(k)} (1 - f_{\mathbf{p}'}^{(l)}) (N_{\mathbf{q}, \gamma} + 1) - f_{\mathbf{p}'}^{(l)} (1 - f_{\mathbf{p}}^{(k)}) N_{\mathbf{q}, \gamma},$$

$$\mathbf{p}' = \mathbf{p} + \mathbf{q}, \quad (\text{I.13})$$

$M_{kl}^{(j)}$ and $W_{kl}^{(j)}$ are real functions linked by the relationship

$$W_{kl}^{(j)} + iM_{kl}^{(j)} = \sum_{s=1}^2 D_{sk}^{(j)} A_{sl} A_{kl}^*, \quad (\text{I.14})$$

where

$$A_{sl} = \kappa_{\mathbf{q}, \gamma}^{1/2} \int_{-\infty}^{\infty} dz \psi_{p_{zs}}^*(z) \psi_{p_{zl}'}(z) \exp(-\kappa_{\mathbf{q}, \gamma} |z|), \quad (\text{I.15})$$

$$D_{sk}^{(j)} \approx \int_0^{\infty} dp_z' \int_{-\infty}^{\infty} dz' \exp(-ip_z z') \psi_{p_{zs}'} \left(z + \frac{z'}{\gamma} \right) \psi_{p_{zk}'}^* \left(z - \frac{z'}{2} \right). \quad (\text{I.16})$$

In the case of electrons traveling toward a plane defect ($p_z = p_{zj}$), we have

$$f_{\mathbf{p}_{\parallel}, p_{zj}}^W = f_{\mathbf{p}}^{(j)}. \quad (\text{I.17})$$

The explicit forms of the functions $M_{kl}^{(j)}$ and $W_{kl}^{(j)}$ depend on the nature of the changes in the barrier potential $V(z)$. For example, in the case of the δ -function potential in the plane of a defect [$V(z) = h\delta(z)$] the matrix elements of Eqs. (I.15) and (I.16) are given by

$$\kappa_{\mathbf{q}, \gamma}^{-1/2} A_{sl} = 2\delta_{sl} \left[\frac{\kappa_{\mathbf{q}, \gamma}}{\kappa_{\mathbf{q}, \gamma}^2 + (p_z - p_z')^2} - \frac{\kappa_{\mathbf{q}, \gamma}}{\kappa_{\mathbf{q}, \gamma}^2 + (p_z + p_z')^2} \right] + \frac{T^*(p_z)}{\kappa_{\mathbf{q}, \gamma} + i(p_z + p_z')} + \frac{T(p_z')}{\kappa_{\mathbf{q}, \gamma} - i(p_z + p_z')} + \frac{T^*(p_z)R(p_z') + T(p_z')R^*(p_z)}{\kappa_{\mathbf{q}, \gamma} + i(p_z - p_z')}, \quad (\text{I.18})$$

$$D_{sk}^{(j)}(p_z) = \begin{pmatrix} |R|^2 \delta_{sj} + |T|^2 (1 - \delta_{sj}) & T^* R \delta_{sj} + R^* T (1 - \delta_{sj}) \\ TR^* \delta_{sj} + RT^* (1 - \delta_{sj}) & |T|^2 \delta_{sj} + |R|^2 (1 - \delta_{sj}) \end{pmatrix}, \quad (\text{I.19})$$

where $p_z > 0$ and $p_z' > 0$, and δ_{sj} is the Kronecker delta.

Equations (I.11) and (I.17) for the Wigner function $f_{\mathbf{p}}^W$, which is identical with the semiclassical distribution function $f_{\mathbf{p}}$ at distances $|z| \gg \lambda_B$, κ^{-1} from a defect, represent the boundary condition which we require and which links the value of $f_{\mathbf{p}_{\parallel}, -p_{zj}}^{(j)}$ for electrons traveling away from the boundary of a defect to the value $f_{\mathbf{p}_{\parallel}, p_{zj}}^{(j)}$ for electrons traveling toward this boundary.

APPENDIX II. CALCULATION OF THE INELASTIC COMPONENT OF THE CURRENT THROUGH A POINT-CONTACT JUNCTION

The inelastic component I_s of the current through a point-contact junction is governed by a correction $f_{sp}^{(j)}$, due to the interaction of carriers with surface phonons, to the electron distribution function $f_{op}^{(j)}$ of Eq. (5):

$$I_s = \frac{2e}{(2\pi)^3} \int d^2\rho \int_{\rho \in \sigma} d^3p v_z f_{sp}^{(1,2)}(\rho). \quad (\text{II.1})$$

Using the boundary condition of Eq. (1) to express the distribution function of electrons scattered by a defect in terms of the distribution functions of carriers incident on the defect, we can rewrite Eq. (II.1) in the form

$$I_s = \frac{2e}{(2\pi)^3} \int_{\rho \in \sigma} d^2\rho \int d^3p v_z \left\{ D \sum_{j=1}^2 f_{sp}^{(j)}(\rho) \theta(p_{zj}) + \widehat{W}_j(\rho, \mathbf{p}) \right\}. \quad (\text{II.2})$$

Since the current on both sides of the defect is conserved, the integral

$$I_j = \frac{2e}{(2\pi)^3} \int_{\rho \in \sigma} d^2\rho \int d^3p v_z \widehat{W}_j(\rho, \mathbf{p}) = I_1 = I_2 \quad (\text{II.3})$$

is independent of the index j [see Eq. (I.12) in the Appendix I].

The correction $f_{sp}^{(j)}$ satisfies Eq. (2) with $I_{eo} = 0$. Its solution, which is subject to the boundary condition (1), can be expressed in terms of the Green's function $g_{pp'}^{(j)}$:

$$f_{sp}^{(j)}(\mathbf{r}) = \int_{\rho \in \sigma} d^2\rho \int d^3p' v_z g_{pp'}^{(j)}(\mathbf{r}, S) \widehat{W}_j(\rho, \mathbf{p}'). \quad (\text{II.4})$$

The equation and boundary conditions which apply in the $\mathbf{r} \in \sigma$ case to $g_{pp'}^{(j)}$ are obtained by substituting Eq. (II.4) into Eqs. (1) and (2) subject to the condition $I_{ep} = 0$. Then, substituting Eq. (II.4) into Eq. (II.2), we find that the current is described by

$$I_s = \frac{2e}{(2\pi)^3} \int_{\rho \in \sigma} d^2\rho \int d^3p v_z \sum_{j=1}^2 \widehat{W}_j(\rho, \mathbf{p}) [G_p^{(j)}(\rho) + \delta_{j1}]. \quad (\text{II.5})$$

The above equation contains a function defined as follows:

$$G_p^{(j)}(\mathbf{r}) = \int_{\rho \in \sigma} d^2\rho \int d^3p' D v_z' \theta(p_{zj}') g_{p'p}^{(j)}(\rho, \mathbf{r}). \quad (\text{II.6})$$

The equation for $G_p^{(j)}$ can be obtained as follows. We multiply the transport equation for the function $f_{sp}^{(j)}$ by $D v_z' \theta(p_{zj}') g_{p'p}^{(j)}(\rho, \mathbf{r})$, and integrate with respect to \mathbf{p} , \mathbf{p}' , \mathbf{r} , and ρ :

$$\sum_{j=1}^2 \int d^3p d^3r \theta[(-1)^j z] \int d^3p' d^2\rho D v_z' \theta(p_{zj}') g_{p'p}^{(j)}(\rho, \mathbf{r}) \left[v \frac{\partial f_{sp}^{(j)}}{\partial \mathbf{r}} + \frac{e}{c} [\mathbf{vH}] \frac{\partial f_{sp}^{(j)}}{\partial \mathbf{p}} - I_i \{ f_{sp}^{(j)} \} \right] = 0.$$

Transforming the terms containing the derivatives of the function $f_{sp}^{(j)}$ by integration by parts and by altering the order of integration with respect to the momentum in the term containing the elastic collision integral $I_i \{ f_{sp}^{(j)} \}$, we obtain

$$\sum_{j=1}^2 \int d^3p v_z \left\{ (-1)^j \int_{\rho \in \sigma} d^2\rho G_p^{(j)}(\rho) f_{sp}^{(j)}(\rho) - \int d^3r \theta[(-1)^j z] \times f_{sp}^{(j)} \left[v \frac{\partial G_p^{(j)}}{\partial \mathbf{r}} + \frac{e}{c} [\mathbf{vH}] \frac{\partial G_p^{(j)}}{\partial \mathbf{p}} + I_i \{ G_p^{(j)} \} \right] \right\} = 0. \quad (\text{II.7})$$

Separating the first integral with respect to \mathbf{p} in Eq. (II.7) into a sum of integrals with respect to the momentum of electrons traveling toward the boundary of a defect and away from it, we can easily show by application of the

boundary condition (1) that if for $\mathbf{r} = \rho \in \sigma$ the function $G_p^{(j)}(\rho)$ satisfies the conditions

$$G_{p_{\parallel}, p_{zj}}^{(j)}(\rho) = (1-D) G_{p_{\parallel}, -p_{zj}}^{(j)}(\rho) + D G_{p_{\parallel}, -p_{zk}}^{(k)}(\rho) - (-1)^j D \theta(p_{zj}), \quad (\text{II.8})$$

then the first term in the braces of Eq. (II.7) vanishes. Since the remaining integral vanishes for any function $f_{sp}^{(j)}$, it follows that $G_p^{(j)}$ satisfies

$$v \frac{\partial G_p^{(j)}}{\partial \mathbf{r}} + \frac{e}{c} [\mathbf{vH}] \frac{\partial G_p^{(j)}}{\partial \mathbf{p}} + I_i \{ G_p^{(j)} \} = 0. \quad (\text{II.9})$$

Far from the constriction in the junction the function $G_p^{(j)}$ satisfies the obvious condition

$$G_p^{(j)}(\mathbf{r} \rightarrow \infty) = 0, \quad (\text{II.10})$$

which is a consequence of the requirement of recovery of an equilibrium in the electron system in the banks of the junction.

Comparing the boundary-value problem of Eqs. (II.8)–(II.10) with the boundary-value problem for the probabilities $\alpha_p^{(j)}$ (see Sec. 1), we can establish the equality

$$G_p^{(j)}(\mathbf{r}, \mathbf{H}) = \alpha_{-p}^{(j)}(\mathbf{r}, -\mathbf{H}) - \theta(z). \quad (\text{II.11})$$

Substituting Eq. (II.11) into Eq. (II.5) for the current and allowing for Eq. (II.3), we finally obtain

$$I_s = \frac{2e}{(2\pi)^3} \sum_{j=1}^2 \int_{\rho \in \sigma} d^2\rho \int d^3p \alpha_{-p}^{(j)}(\rho, -\mathbf{H}) \widehat{W}_j(\rho, \mathbf{p}). \quad (\text{II.12})$$

¹¹ The contributions to a point-contact spectrum representing the inelastic surface scattering of electrons on the boundary of a point-contact junction was investigated earlier.¹¹

² The expression for $K_s(p, p')$ can be obtained for a barrier of arbitrary shape [see Eq. (22) and the relationships (I.15) and (I.16) in the Appendix I]. However, the analysis of a specific case can be carried out conveniently using the model of a δ -function barrier, which is characterized by the minimum number of parameters.

¹ M. S. Khaikin and I. N. Khlyustikov, Pis'ma Zh. Eksp. Teor. Fiz. **33**, 167 (1981) [JETP Lett. **33**, 158 (1981)].

² I. N. Khlyustikov and A. I. Buzdin, Usp. Fiz. Nauk **155**, 47 (1988) [Sov. Phys. Usp. **31**, 409 (1988)].

³ Yu. V. Sharvin and D. Yu. Sharvin, Zh. Eksp. Teor. Fiz. **77**, 2153 (1979) [Sov. Phys. JETP **50**, 1033 (1979)].

⁴ Yu. A. Kolesnichenko and M. A. Lur'e, Fiz. Nizk. Temp. **7**, 1267 (1981) [Sov. J. Low Temp. Phys. **7**, 614 (1981)].

⁵ Yu. A. Kolesnichenko and V. G. Peschanskii, Fiz. Nizk. Temp. **10**, 1141 (1984) [Sov. J. Low Temp. Phys. **10**, 595 (1984)].

⁶ I. O. Kulik, A. N. Omel'yanchuk, and R. I. Shekhter, Fiz. Nizk. Temp. **3**, 1543 (1977) [Sov. J. Low Temp. Phys. **3**, 740 (1977)].

⁷ I. K. Yanson, Fiz. Nizk. Temp. **9**, 676 (1983) [Sov. J. Low Temp. Phys. **9**, 343 (1983)].

⁸ A. V. Khotkevich, I. K. Yanson, M. B. Lazareva *et al.*, Zh. Eksp. Teor. Fiz. **98**, 1672 (1990) [Sov. Phys. JETP **71**, 937 (1990)].

⁹ R. I. Shekhter and I. O. Kulik, Fiz. Nizk. Temp. **9**, 46 (1983) [Sov. J. Low Temp. Phys. **9**, 22 (1983)].

¹⁰ I. O. Kulik, M. V. Moskalets, R. I. Shekhter, and I. K. Yanson, Pis'ma Zh. Eksp. Teor. Fiz. **49**, 42 (1989) [JETP Lett. **49**, 50 (1989)].

¹¹ Yu. A. Kolesnichenko and R. I. Shekhter, Poverkhnost' No. 8, 49 (1990).

¹² E. N. Bogachek, I. O. Kulik, and R. I. Shekhter, Zh. Eksp. Teor. Fiz. **92**, 730 (1987) [Sov. Phys. JETP **65**, 411 (1987)].

¹³ M. V. Moskalets and R. I. Shekhter, Fiz. Nizk. Temp. **16**, 195 (1990) [Sov. J. Low Temp. Phys. **16**, 108 (1990)].

¹⁴ E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics*, Pergamon Press, Oxford (1981).