Transport properties of conductors with electron-phonon interaction at resonance scattering centers

L. I. Glazman, I. F. Itskovitch, I. O. Kulik, and R. I. Shekhter

The Institute of Problems in Microelectronic and Ultrapure Materials Technology, USSR Academy of Sciences

(Submitted 21 March 1988)
Zh. Eksp. Teor. Fiz. **94**, 309–320 (October 1988)

A theory of resonance scattering of electrons is formulated by taking into account the formation of polariton-type electron-phonon states at the impurity center. A formula is derived for the resonance scattering cross section with an arbitrary value of the electron-phonon interaction at the center. The possibility of point-contact spectroscopy of the electron-phonon interaction function in quasilocal electron states is demonstrated. The conclusions of the theory are compared with experiments employing mixed valence heterojunctions ($CeNi_5$–Cu).[13]

1. INTRODUCTION

The extensive investigation of mixed valence systems, heavy-fermion and metal-oxide compounds has recently generated special interest in the problem of localized electron states in metals. Since the presence of such states near the Fermi level causes substantial changes in the thermodynamics and kinetics of the metal, it is important to investigate their interaction with the vibrational degrees of freedom of the crystal. This interaction will produce a polaron shift and a band of coupled electron-phonon states at the center. It is important to note that conventional optical spectroscopic techniques used to investigate analogous states in semiconductors[1] are less effective in the case of metals due to the skin effect. One promising approach in these conditions is to investigate the transport properties, which are sensitive to the structure of the localized electron states due to resonance scattering.

We will demonstrate in the present study that electron-phonon interaction (EPI) at the center has a substantial influence on the resonance scattering picture, as it determines its inelastic nature and the temperature dependence of the cross section. The most promising method for investigation of this scattering process is analysis of the point-contact electrical conductivity.[2,3] As we will demonstrate the first derivative of the I-V characteristic is proportional to the total scattering cross section and in many cases can be used to recover the EPI function in local states.

A model taking into account the hybridization of the band and localized states and the EPI in the localized states will be formulated in the next section. The problem of resonance scattering at an empty center is solved exactly for electron-phonon interaction of arbitrary magnitude, and expressions are derived for the partial and total scattering cross sections.

Section 3 demonstrates the possibility of point-contact spectroscopy of EPI at the centers. It is demonstrated that the first derivative of the I-V characteristic of the heterojunction, one of whose junctions contains resonance scattering centers, is proportional to the total scattering cross section and allows determination of the position of the resonance level and the extent of electron-phonon interaction at the center. Unlike regular point-contact spectroscopy[2,3] an appropriately normalized first derivative of the I-V characteristic is proportional (in the case of weak EPI) to the thermodynamic (and not the point-contact) EPI function in the localized state.

2. HYBRIDIZATION HAMILTONIAN AND THE EVOLUTION OF ELECTRON-PHONON STATES AT THE CENTER; SCATTERING CROSS SECTIONS AT AN EMPTY CENTER

We will consider the localized electron state as a distinct degree of freedom (operators c^+, c) corresponding to energy ε_0. In this case the hybridization of such a state with the band states characterized by the operators $a_p{}^+$, a_p can be described by means of Anderson's Hamiltonian.[4] Consistent with the discussion in the Introduction, the Hamiltonian must be augmented to account for the interaction of the localized state with the phonons (the operators $b_q{}^+$, b_q correspond to these). Below we will not take into account the interaction of the band electrons with the phonons. This is possible since the phonon renormalizations of the band electron energies are small compared to analogous renormalizations for localized states by a factor $\omega_D/q_D v \sim s/v \ll 1$ (s is the speed of sound; v is the electron velocity, ω_D and q_D are the Debye frequency and momentum).

The Hamiltonian of the model takes the following form:

$$H=H_b+H_s+H_{bs}, \tag{1}$$

$$H_b=\sum_p \varepsilon_p a_p{}^+ a_p,$$

$$H_s=c^+c\Big[\varepsilon_0+\sum_q \alpha_q(b_q{}^+-b_q)\Big]+\sum_q \omega_q b_q{}^+ b_q, \tag{2}$$

$$H_{bs}=g\sum_p (a_p{}^+c+c^+a_p). \tag{3}$$

Here ε_p is the dispersion law of the band electrons, ω_q is the phonon frequency. The EPI matrix element α_q is related in the normal manner to the deformation interaction constant Λ of the localized electrons (V, NM/V are the crystal volume and density):

$$\alpha_q=-i\Lambda q(NM\omega_q)^{-1/2}. \tag{4}$$

 0038-5646/88/102134-07$04.00

We will henceforth assume that the hybridization constant g is small on the scale of characteristic electron energies of the metal:

$$g \ll \varepsilon_0. \tag{5}$$

In order to solve the problem of band electron scattering at the center it is necessary to analyze its hybridization dynamics with the set of local electron-phonon states described by the Hamiltonian H_s. We will introduce the probability amplitudes $\hat{u}_\mathbf{p}$ and $\hat{v}$ of a transition from the initial state $a_k^+|0\rangle$ to the states $a_\mathbf{p}^+|0\rangle$ and $c^+|0\rangle$. The one-electron wave function can be represented as

$$\psi(t) = \Big[\sum_\mathbf{p} \hat{u}_\mathbf{p}(t) a_\mathbf{p}^+ + v(t) c^+\Big]|0\rangle \tag{6}$$

($\hat{u}_\mathbf{p}$, $\hat{v}$ operate on the phonon variables). The Schrödinger equation $\psi(t)$ determines the time dependence of the operators $\hat{u}_\mathbf{p}$ and $\hat{v}$:

$$i\frac{\partial \hat{u}_\mathbf{p}}{\partial t} = \varepsilon_\mathbf{p}\hat{u}_\mathbf{p} + g\hat{v},$$

$$i\frac{\partial \hat{v}}{\partial t} = \Big\{\varepsilon_0 + \sum_\mathbf{q} \alpha_\mathbf{q}[b_\mathbf{q}^+ \exp(i\omega_\mathbf{q} t) - b_\mathbf{q} \exp(-i\omega_\mathbf{q} t)]\Big\} v + g\sum_\mathbf{p} \hat{u}_\mathbf{p}. \tag{7}$$

The initial conditions on Eqs. (7) in accordance with the scattering problem at the empty center we are treating take the form

$$\hat{u}_\mathbf{p}(t=0) = \delta_{\mathbf{pk}}, \quad \hat{v}(t=0) = 0. \tag{8}$$

We will focus on the formal analogy between this problem and the problem of resonance tunneling involving phonons.[5] The Hamiltonian (1) differs from the tunnel Hamiltonian in that the localized states undergo hybridization only with a single "kind" of band electron. Hence only a single kind of amplitude $\hat{u}_\mathbf{p}$ will figure into the scattering problem. It is possible to simplify equation Eq. (7) in the case of low levels of energy transfer:

$$|\varepsilon_\mathbf{p} - \varepsilon_\mathbf{k}| \ll \varepsilon_\mathbf{k} \sim \varepsilon_0, \tag{9}$$

for which the density of states in the band may be taken as fixed: $N(\varepsilon) = N(\varepsilon_0)$. This allows introduction of damping of the local electron states, which gives the level Γ a finite width:

$$\Gamma = \pi g^2 \sum_\mathbf{p} \delta(\varepsilon_\mathbf{p} - \varepsilon_0) = \pi g^2 N(\varepsilon_0). \tag{10}$$

It follows from (7) that

$$i\frac{\partial \hat{u}_\mathbf{p}}{\partial t} = \varepsilon_\mathbf{p}\hat{u}_\mathbf{p} + g\hat{v},$$

$$i\frac{\partial v}{\partial t} = \Big\{\varepsilon_0 - i\Gamma + \sum_\mathbf{q} \alpha_\mathbf{q}[b_\mathbf{q}^+ \exp(i\omega_\mathbf{q} t) - b_\mathbf{q} \exp(-i\omega_\mathbf{q} t)]\Big\}\hat{v} + g\sum_\mathbf{p} \hat{u}_\mathbf{p}(0)\exp(-i\varepsilon_\mathbf{p} t). \tag{11}$$

The solution of system (11) for $\hat{u}_\mathbf{p}(t)$ can be represented as

$$\hat{u}_\mathbf{p}(t) = [\delta_{\mathbf{pk}} \hat{I} + \hat{U}_{\mathbf{k}\to\mathbf{p}}(t)]\,\hat{u}_\mathbf{k}(0).$$

In analyzing transport phenomena the probability of resonance scattering at a single center must be averaged over the states of the phonon system. Assuming an equilibrium phonon system we will define the transition probability per unit time $W_{\mathbf{k}\to\mathbf{p}}$ in the following manner:

$$W_{\mathbf{k}\to\mathbf{p}} = \lim_{t\to\infty} \frac{1}{t} \mathrm{Sp}\Big\{\exp\Big[-\beta\sum_\mathbf{q} \omega_\mathbf{q} b_\mathbf{q}^+ b_\mathbf{q}\Big] \hat{U}^\pm_{\mathbf{k}\to\mathbf{p}}(t)\,\hat{U}_{\mathbf{k}\to\mathbf{p}}(t)\Big\} \Big/ \mathrm{Sp}\Big\{\exp\Big[-\beta\sum_\mathbf{q} \omega_\mathbf{q} b_\mathbf{q}^+ b_\mathbf{q}\Big]\Big\}.$$

Using the results from Ref. 5 we have

$$W_{\mathbf{k}\to\mathbf{p}} = g^4 \int_{-\infty}^{\infty} dt_1 \exp[i(\varepsilon_\mathbf{p} - \varepsilon_\mathbf{k})t_1] \times \int_0^\infty dt_2 \exp[-i(\varepsilon_0^* - \varepsilon_\mathbf{k} - i\Gamma)t_2] \int_0^\infty dt_3 \times \exp[i(\varepsilon_0^* - \varepsilon_\mathbf{k} + i\Gamma)t_3] V(t_1, t_2, t_3), \tag{12}$$

$$V(t_1, t_2, t_3) = \exp\Big\{-\sum_\mathbf{q} \frac{|\alpha_\mathbf{q}|^2}{2\omega_\mathbf{q}^2}\Big\{|[1 - \exp(-i\omega_\mathbf{q} t_3)] + \exp(i\omega_\mathbf{q} t_1) \times [\exp(-i\omega_\mathbf{q} t_2) - 1]|^2 \operatorname{cth}\frac{\omega_\mathbf{q}}{2T} + [\exp(i\omega_\mathbf{q} t_2) + \exp(-i\omega_\mathbf{q} t_3) + \exp(i\omega_\mathbf{q} t_1)(1 - \exp(i\omega_\mathbf{q} t_3))(\exp(-i\omega_\mathbf{q} t_2) - 1) - \text{c.c.}]\Big\}\Big\}. \tag{13}$$

Here ε_0^* is the resonance level energy renormalized on account of the polaron shift:

$$\varepsilon_0^* = \varepsilon_0 - \varepsilon_\Pi, \quad \varepsilon_\Pi = \sum_\mathbf{q} |\alpha_\mathbf{q}|^2/\omega_\mathbf{q}. \tag{14}$$

The scattering cross-section is related to the quantity $W_{\mathbf{k}\to\mathbf{p}}$ by the relation

$$\sigma_{\mathbf{k}\to\mathbf{p}} = \frac{2\pi^2 N^2(\varepsilon_0)}{k_0^2} W_{\mathbf{k}\to\mathbf{p}}, \quad \frac{k_0^2}{2m} = \varepsilon_0. \tag{15}$$

Equations (12)–(15) make it possible to determine the energy dependence of the total scattering cross section:

$$\sigma_t(\varepsilon) = \int d\varepsilon'\,\sigma(\varepsilon \to \varepsilon') = \frac{2\pi\Gamma}{k_0^2} \int_{-\infty}^{\infty} dt \exp[-\Gamma|t| + i(\varepsilon - \varepsilon_0^*)t] \times \exp\Big\{-\sum_\mathbf{q} \frac{|\alpha_\mathbf{q}|^2}{\omega_\mathbf{q}^2}[(2n_\mathbf{q} + 1) - (n_\mathbf{q} + 1)\exp(-i\omega_\mathbf{q} t) - n_\mathbf{q} \exp(i\omega_\mathbf{q} t)]\Big\}, \tag{16}$$

where $n_\mathbf{q} = [\exp(\omega_\mathbf{q}/T) - 1]^{-1}$. It is clear from relation (16) that the EPI intensity is characterized by the dimensionless parameter λ:

$$\lambda = \sum_\mathbf{q} |\alpha_\mathbf{q}|^2/\omega_\mathbf{q}^2.$$

We can introduce the EPI function $g_{ph}(\omega)$ locally by analo-

gy to the EPI for band electrons by means of the relation

$$\lambda=\int_0^\infty \frac{d\omega}{\omega} g_{ph}(\omega), \quad g_{ph}(\omega)=\frac{1}{\omega}\sum_q |\alpha_q|^2\delta(\omega-\omega_q). \tag{17}$$

In the next section we will discuss the possibility of recovering this function from point-contact experiments.

The exponent in (16) can be expanded in this parameter $\lambda \ll 1$ (weak EPI). In this case the nth term of the expansion determines the scattering cross section involving n photons. Taking into account the contribution of the one-photon processes, we obtain

$$\sigma_t(\varepsilon)=(1-C)\sigma_{res}(\varepsilon-\varepsilon_0^*)+\sum_q [A_q\sigma_{res}(\varepsilon-\varepsilon_0^*-\omega_q) +B_q\sigma_{res}(\varepsilon-\varepsilon_0^*+\omega_q)], \tag{18}$$

$$\sigma_{res}(\varepsilon)=\frac{4\pi}{k_0^2}\frac{\Gamma^2}{\varepsilon^2+\Gamma^2}, \quad A_q=\frac{|\alpha_q|^2}{\omega_q^2}(n_q+1),$$

$$B_q=\frac{|\alpha_q|^2}{\omega_q^2}n_q, \quad C=\sum_q (A_q+B_q).$$

In the case $\lambda \gg 1$ (strong EPI) multiphoton contributions are significant. The integral (16) can be evaluated asymptotically by expanding the exponent in powers of $\omega_q t \sim \omega_q^2/|\alpha_q|^2 \ll 1$ up through quadratic terms. For

$$\Gamma^2 \ll \varepsilon_A^2(T)=\sum_q |\alpha_q|^2(2n_q+1) \tag{19}$$

we obtain

$$\sigma_t(\varepsilon)=\frac{(2\pi)^{1/2}}{k_0^2}\frac{\Gamma}{\varepsilon_A(T)}\exp\left\{-\frac{(\varepsilon-\varepsilon_0)^2}{2\varepsilon_A^2(T)}\right\}. \tag{20}$$

Expression (20) suggests that strong EPI produces significant resonance broadening. This is due to the activation of the inelastic scattering channels. It is interesting to note that such a change in the nature of the scattering does not alter the normalization of the function $\sigma_t(\varepsilon)$. Using relation (16) it is possible to directly determine the validity of the following sum rule:

$$\int d\varepsilon\, \sigma_t(\varepsilon)=4\pi^2\Gamma/k_0^2, \tag{21}$$

which holds with any value of the parameter λ.

The energy distribution that arises with resonance electron scattering is conveniently characterized by the partial inelastic scattering cross section $\sigma_i(\varepsilon\to\varepsilon')$. This quantity depends both on the departure from resonance $\varepsilon-\varepsilon_0$ and the energy transferred to the photons $E=\varepsilon-\varepsilon'$. In the case of strong EPI the cross section $\sigma_i(\varepsilon\to\varepsilon')$ is maximized for $|\varepsilon-\varepsilon_0|\leqslant\varepsilon_A(T)$ [see (20)]. The characteristic value of E is related to multiphoton processes and hence significantly exceeds ω_D. Using the saddle-point method to evaluate the integrals in (12) we obtain

$$\sigma_i(\varepsilon,E)=\frac{2\pi^{1/2}}{k_0^2}\frac{\Gamma\theta(E)}{\varepsilon_A(T)(\Delta\varepsilon E)^{1/2}}\exp\left\{-\frac{(\varepsilon-\varepsilon_0)^2}{2\varepsilon_A^2(T)}-\left(\frac{E}{\Delta\varepsilon}\right)^{1/2}\right\}, \tag{22}$$

where

$$\Delta\varepsilon=\frac{1}{\Gamma^2}\sum_q |\alpha_q|^2\omega_q, \tag{23}$$

$\theta(E)$ is the Heaviside step function.

Expression (22) holds when (19) is satisfied and for energy transfers satisfying $|E|\ll\varepsilon_T$. Hence for $\Delta\varepsilon\ll\varepsilon_T$ the characteristic energy transfer levels are determined by the value of $\Delta\varepsilon$. We can obtain an estimate for $\Delta\varepsilon$ by replacing the phonons with classical shifts. The polaron shift after the electron enters the localized state obeys the law

$$\varepsilon_T(t)\sim\sum_q\frac{|\alpha_q|^2}{\omega_q}(1-\cos\omega_q t). \tag{24}$$

If the time of the electron at the center is $t\sim\Gamma^{-1}\ll\omega_D^{-1}$, we obtain from (24):

$$\Delta\varepsilon\sim\varepsilon_T(t\sim\Gamma^{-1})\sim\varepsilon_T(\omega_D/\Gamma)^2, \tag{25}$$

which agrees (in terms of relevant parameters) with (23). In the inverse limiting case, $\Gamma\ll\omega_D$, the characteristic energy transfer levels are $E\sim 2\varepsilon_T$.

Finally, with regard to further applications of the theory to point-contact experiments, we will discuss the resonance scattering of hole excitations at filled local levels lying deep under the Fermi surface. Remaining within the framework of our model we will go from the electron creation operators to the hole excitation creation operators in the Hamiltonian (1)–(3):

$$\hat{\alpha}_p^+=a_p, \quad \gamma^+=c. \tag{26}$$

In this case it is necessary to take into account the crystal deformation arising from electron occupation of the local state and resulting in renormalization of the phonon operators

$$\beta_q=b_q+\alpha_q/\omega_q. \tag{27}$$

Using these operators and dropping the insignificant constant terms we write the Hamiltonian in the form of (1), where

$$H_b=-\sum_p\varepsilon_p\hat{\alpha}_p^+\hat{\alpha}_p,$$

$$H_s=-\gamma^+\gamma\left[\varepsilon_0^*-\sum_q\alpha_q(\beta_q^+-\beta_q)\right]+\sum_q\omega_q\beta_q^+\beta_q, \tag{2a}$$

$$H_{bs}=-g\sum_p(\hat{\alpha}_p^+\gamma+\gamma^+\hat{\alpha}_p). \tag{3a}$$

Here $\varepsilon_0^*=\varepsilon_0-\varepsilon_T$ is the resonance level energy for a hole at a filled center. After this transformation we can analyze resonance scattering of the hole at the deep filled center in the same manner as was done previously for an electron. Specifically, the wave function of the hole takes the form

$$\psi(t)=\Big[\sum_{\mathbf{p}}\hat{u}_{\mathbf{p}}(t)\hat{a}_{\mathbf{p}}^{+}+\hat{v}(t)\gamma^{+}\Big]|0\rangle_h,$$

$$\hat{u}_{\mathbf{p}}(t=0)=\delta_{\mathbf{pk}}\hat{I},\quad \hat{v}(t=0)=0. \tag{6a}$$

We note that the completely filled states in the band and at the center correspond to the hole excitation vacuum $|0\rangle_h$. By comparing Eqs. (2a), (3a), and (6a) with (2), (3), and (6) we see that a formal transformation from the results of the scattering problem for an electron to the corresponding results for a hole is achieved by the substitution.

$$\varepsilon_{\mathbf{k}}\to-\varepsilon_{\mathbf{k}},\quad \varepsilon_{\mathbf{p}}\to-\varepsilon_{\mathbf{p}},\quad \varepsilon_0\to-\varepsilon_0^{*},\quad \alpha_{\mathbf{q}}\to\alpha_{-\mathbf{q}}.$$

Thus the transition probability for the hole $W^h_{\mathbf{k}\to\mathbf{p}}$ is related to the scattering probability $W_{\mathbf{k}\to\mathbf{p}}$ for an electron [see (12), (13)] by

$$W^h_{\mathbf{k}\to\mathbf{p}}(\varepsilon_{\mathbf{k}},\varepsilon_{\mathbf{p}},\varepsilon_0^{*})=W_{\mathbf{k}\to\mathbf{p}}(-\varepsilon_{\mathbf{k}},-\varepsilon_{\mathbf{p}},-\varepsilon_0^{*}). \tag{28}$$

3. POINT-CONTACT SPECTROSCOPY OF EPI AT IMPURITY CENTERS

Point-contact spectroscopy is an effective method of investigating the energy relaxation of current carriers in metals. Unlike conventional application it is quite unique for investigating resonance scattering in elastic and inelastic channels, since, as we have seen, the scattering cross section depends not only on energy transferred to the phonons but also on the absolute electron energy. This relation is determined by the proximity of the energy to the resonance scattering level and may be quite steep. We will demonstrate below that in the limit $\Gamma\ll\omega_D$ this steepness is responsible for the features of the EPI function appearing as early as the first derivative of the I-V characteristic of the point-contact. Heterojunctions containing scattering centers on only one of the junction boundaries (the "dirty" boundary) are the most sensitive to resonance scattering emission. A specific asymmetry of the nonlinear I-V characteristic will appear in such structures and this will make it possible, in addition to the EPI intensity, to also determine the position of the resonance level with respect to the Fermi surface.

For illustrative purposes we will consider the case of the electrical conductivity of a point contact in ballistic conditions when the mean free path l of the electron exceeds the contact dimensions d:

$$l\gg d,\quad l\sim(n_0\sigma_t)^{-1} \tag{29}$$

(n_0 is the concentration of resonance impurities). In investigating the electrical conductivity it is important to take into account the additional carrier scattering on the contact surface of the metals forming the heterojunction. When the transmission coefficient of the electrons through the surface is small, the resistance is largely produced by these scattering processes, while the applied voltage V is principally applied at the contact boundary.[6] Current flow in this system is accompanied by injection of carriers with excess energy distributed in the interval from 0 to eV to the metallic boundaries. The diffusion of these carriers in the solid boundaries accompanied by scattering at the centers determines the nonlinear addition to the I-V characteristic which may be calculated using the standard method for point-contact spectroscopy. In solving the kinetic equation it is necessary to use the collision integral of the carriers with the resonance scattering centers:

$$S\{f_{\mathbf{p}}\}=\frac{n_0}{(2\pi)^3}\int d\mathbf{p}'\{W_{\mathbf{p}'\to\mathbf{p}}f_{\mathbf{p}'}(1-f_{\mathbf{p}})-W_{\mathbf{p}\to\mathbf{p}'}f_{\mathbf{p}}(1-f_{\mathbf{p}'})\}. \tag{30}$$

Without energy relaxation at each point in the metal the current carriers can be divided into two groups: those that have and those have not passed through the contact. We will introduce the probability $\omega_{\mathbf{p}}(\mathbf{r})$ of elastic electron arrival from the dirty metal at point $\mathbf{r}$ with momentum $\mathbf{p}$. In the absence of resonance scattering the trajectory classification given above can then be taken into account by representing the carrier distribution function[7,8] as

$$f_{\mathbf{p}}(\mathbf{r})=w_{\mathbf{p}}(\mathbf{r})n_F(\varepsilon_{\mathbf{p}}+e\varphi+eV/2)+[1-w_{\mathbf{p}}(\mathbf{r})]n_F(\varepsilon_{\mathbf{p}}+e\varphi-eV/2). \tag{31}$$

We note that with this selection of $f_{\mathbf{p}}$ the potential φ in the dirty metal will differ from the limit $-V/2$ by a value proportional to the low transparency of the contact boundary. When (29) holds, the current in the point contact can be calculated using perturbation theory in the collision integral (30); the function $f_{\mathbf{p}}(\mathbf{r})$ (31) of the elastic approximation must be substituted into (30). As a result the nonlinear correction determining the "return current" in the point contact[9] can be represented as[8]

$$\delta I=\frac{2e}{(2\pi)^3}\int d\mathbf{r}\int d\mathbf{p}\, w_{-\mathbf{p}}(\mathbf{r})S\{f_{\mathbf{p}}(\mathbf{r})\}, \tag{32}$$

where under ballistic conditions

$$w_{\mathbf{p}}(\mathbf{r})=\begin{cases}0, & \mathbf{v}\in\Omega(\mathbf{r})\\ D_{\mathbf{p}}, & \mathbf{v}\in\Omega(\mathbf{r})\end{cases},$$

$\Omega(\mathbf{r})$ is the solid angle of observation of the aperture from the point $\mathbf{r}$ in the point contact, and $D_{\mathbf{p}}$ is the transparency of the contact boundary between the metals (Fig. 1).

We can observe a qualitative picture of the electrical conductivity by considering an example where the resonance level in the metal is above the Fermi level. Figure 1 shows a diagram corresponding to carrier injection from the point-contact. The figure clearly reveals a qualitative difference of the electron scattering patterns in the two different voltage polarities. When a positive potential is applied to the dirty metal (Fig. 1, b) the nonequilibrium electrons are injected to the energy band above the Fermi level. Their possible scattering at the resonance center determines the nonlinear behavior of the I-V characteristic. In the absence of EPI the scattering of electrons with a boundary energy ε_F+eV is maximized for $eV=\varepsilon_0-\varepsilon_F$. Weak EPI is responsible for the inelastic resonance scattering processes and will produce an additional I-V characteristic reflecting phonon duplications of resonance. In the opposite polarity (Fig. 1, c) nonequilibrium holes are injected to the energy band under the Fermi surface, there is no resonance scattering, and the I-V characteristic contains no resonance features.

It is quite evident that if the resonance level lies below the Fermi surface, the I-V features will appear with a negative potential across the dirty metal. These features correspond to resonance scattering of the hole excitations at a filled center (see Sec. 2).

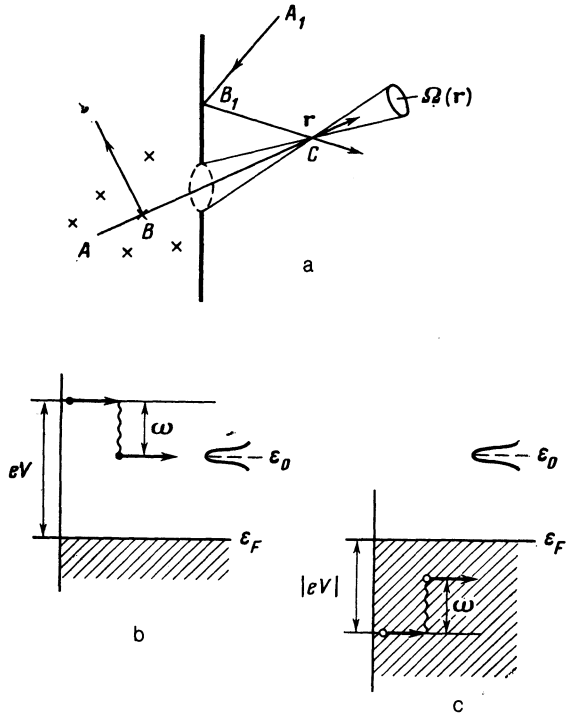

FIG. 1. Point-contact configuration: a—($\times s$: Resonance scattering centers; lines: Trajectories of impurity-scattered electron (ABC, A_1B_1C) and non-impurity-scattered electron) and energy relaxation diagram of carriers injected from the point-contact in two voltage polarities: b—Scheme of electrons undergoing subsequent scattering on the resonance level, c—hole scheme.

The calculations carried out by Eq. (32) subject to (15), (16) yield the following expression for the correction δR to the ballistic resistance R_0 of the contact:

$$\delta R/R_0 = d^*/l_T(eV); \tag{33}$$

here

$$d^* = (32/3\pi)\, d\langle\langle K\rangle\rangle, \tag{34}$$

d is the diameter of the point contact, $\langle\langle K\rangle\rangle$ is the form-factor of a heterojunction averaged over the directions of the momenta.[6] The quantity $l_T(\varepsilon)$ figuring into (33) is the mean free path of the electron with respect to resonance scattering by the impurities:

$$l_T^{-1}(\varepsilon) = n_0 \int \frac{d\varepsilon'}{4T} \operatorname{ch}^{-2}\left(\frac{\varepsilon'-\varepsilon-\varepsilon_F}{2T}\right) \sigma_t(\varepsilon'). \tag{35}$$

Expression (33) is valid for any EPI level if the actual values of electron energy during the scattering process are far from the Fermi surface. The corresponding criteria take the following form in the case of weak ($\lambda \ll 1$) and strong ($\lambda \gg 1$) EPI, respectively

$$\Gamma,\ \omega_D,\ T \ll \varepsilon_0 - \varepsilon_F,\quad \lambda \ll 1;$$

$$\Delta\varepsilon,\ \varepsilon_\Lambda,\ T \ll \varepsilon_0 - \varepsilon_F,\quad \lambda \gg 1.$$

The most direct relation between the EPI function and the nonlinearity of the I-V characteristic occurs in the case of weak EPI for Γ, $T \ll \omega_D$:

$$\frac{\delta R}{R_0} = \frac{d^*}{l_{T=0}(\varepsilon_0-\varepsilon_F)} \left\{ g_0(\omega) + \frac{\pi\Gamma}{\omega} g_{ph}(\omega) \right\} \Big|_{\omega=\varepsilon_F-\varepsilon_0+eV}. \tag{36}$$

Here the function $g_0(\omega)$ determines the position and shape of the line produced by scattering in the elastic channel:

$$g_0(\omega) = \frac{\Gamma^2}{4T} \int_{-\infty}^{\infty} \frac{d\varepsilon}{\varepsilon^2+\Gamma^2} \operatorname{ch}^{-2}\frac{\varepsilon-\omega}{2T}$$

$$= \begin{cases} \Gamma^2/(\omega^2+\Gamma^2), & T \ll \Gamma, \\ (\pi\Gamma/4T)\operatorname{ch}^{-2}(\omega/2T), & T \gg \Gamma. \end{cases} \tag{37}$$

Figure 2 provides a schematic representation of $\delta R/R_0$ plotted as a function of V. We note that the integral scattering intensity in the elastic channel is determined solely by Γ:

$$\int_{-\infty}^{\infty} d\omega\, g_0(\omega) = \pi\Gamma. \tag{38}$$

Taking into account that the total intensity of the phonon repetitions is small compared to (38) we obtain from (36) the capability to directly recover the EPI function based on experimental data[1)]:

$$g_{ph}(\omega) = \omega\delta R(eV=\omega+\varepsilon_0-\varepsilon_F) \Big/ \int d\omega\, \delta R(\omega), \quad \omega > \Gamma. \tag{39}$$

For $\Gamma \geqslant \omega_D$, the weak phonon repetitions are nondifferentiable against the principal peak $g_0(\omega)$ determining the position and width of the resonance level.

In the case of weak EPI the multiphonon processes cause significant smearing of the resonance scattering line [see (20)]. In this case the nonlinear correction (33) to the resistance will be determined by expression ($T \ll \varepsilon_\Lambda$)

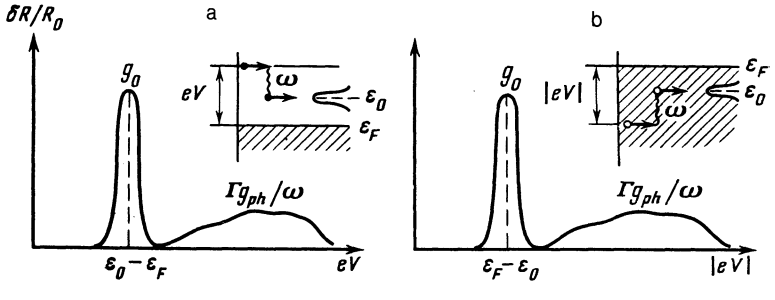

FIG. 2. Schematic representation of the nonlinear addition to the point-contact resistance as a function of the voltage in the case of weak EPI for a resonance level lying above: a—($\omega = eV + \varepsilon_F - \varepsilon_0$) and below: b—($\omega = |eV| + \varepsilon_0 - \varepsilon_F$) the Fermi surface. The inserts provide inelastic resonance scattering diagrams of electron (a) and hole (b) excitations.

$$\frac{\delta R}{R_0} = \frac{d^*}{l_{T=0}(\varepsilon_0-\varepsilon_F)} \frac{\varepsilon_\Lambda(0)}{\varepsilon_\Lambda(T)} \exp\left[-\frac{(eV+\varepsilon_F-\varepsilon_0)^2}{2\varepsilon_\Lambda^2(T)}\right]. \quad (40)$$

We note that at any EPI intensity the integral intensity of the nonlinear additions $\int d\omega \delta R(\omega)/R_0$ is independent of λ and T, and is determined [in accordance with (21)] solely by the width of the level Γ.

The relations given above refer to the case of a resonance level lying below the Fermi surface. As discussed above in the opposite case the features of the I-V characteristic appear in the reverse polarity. In order to obtain the corresponding results it is necessary to analyze ballistic spreading of the holes and their resonance scattering [see (28)]. In this case it is necessary to carry out the simple substitution $V \to -V$ and to change the sign of the difference $\varepsilon_0 - \varepsilon_F$ in the final expressions (36), (39), and (40) for the cases of weak and strong EPI, see Fig. 2, b.

The nonlinear features of the I-V characteristic attributable to resonance scattering also occur for a symmetric homojunction with the boundaries consisting of the same dirty metal. However in this case the I-V characteristic is symmetric with respect to the voltage polarity and is independent of the sign of the difference $\varepsilon_0 - \varepsilon_F$. Moreover due to the lack of a contact boundary between the metals the electrostatic potential $\varphi(\mathbf{r})$ changes throughout the spreading region.[3] Hence the kinetic energy of the injected electrons depends on the coordinates and the resonance condition $\varepsilon \approx \varepsilon_0$ holds for any possible values of the voltage ($eV > |\varepsilon_0 - \varepsilon_F|$) even for electrons in a relative small fraction of the spreading region. As a result the intensity of the resonance features in the first derivative of the I-V characteristic is substantially reduced compared to the case of a heterojunction, while their decay law with increasing voltage diminishes. In the limit of weak EPI the elastic addition to the resistance of the contact for the circular hole model take the form ($T \ll \Gamma$)

$$\frac{\delta R}{R_0} = \frac{\pi\sqrt{2}}{20} \frac{d}{l_{T=0}(|\varepsilon_0-\varepsilon_F|)} \frac{\Gamma^{1/2}}{|\varepsilon_0-\varepsilon_F|^{1/2}} \tilde{g}_0(eV-|\varepsilon_0-\varepsilon_F|), \quad (41)$$

$$\tilde{g}_0(\omega) = \Gamma^{3/2}(\omega^2+\Gamma^2)^{-1/2}[(\omega^2+\Gamma^2)^{1/2}-\omega]^{-1/2}, \quad |\omega| \ll |\varepsilon_0-\varepsilon_F|,$$

while the phonon features appear clearly only in the second derivative of the I-V characteristic:

$$g_{ph}(\omega) = \frac{\omega}{e\delta R} \frac{d\delta R}{dV}\bigg|_{eV=\omega+|\varepsilon_0-\varepsilon_F|}, \quad \Gamma \ll \omega < |\varepsilon_0 - \varepsilon_F|. \quad (42)$$

In the case of strong EPI the nonlinear addition to resistance is determined by the relation ($T \ll \varepsilon_\Lambda$)

$$\frac{\delta R}{R_0} = \frac{\pi\sqrt{2}}{20} \frac{d}{l_{T=0}(|\varepsilon_0-\varepsilon_F|)} \frac{\varepsilon_\Lambda(0)}{(\varepsilon_\Lambda(T)\,|\varepsilon_0-\varepsilon_F|)^{1/2}}$$
$$\times \exp\left[-\frac{(eV-|\varepsilon_0-\varepsilon_F|)^2}{4\varepsilon_\Lambda^2(T)}\right] D_{-1/2}\left(\frac{|\varepsilon_0-\varepsilon_F|-eV}{\varepsilon_\Lambda(T)}\right). \quad (43)$$

Here $D_{-1/2}(z)$ is a parabolic cylinder function having the asymptotic forms

$$e^{-z^2/4} D_{-1/2}(z) = \begin{cases} \sim z^{-1/2} e^{-z^2/2}, & z \gg 1, \\ \sqrt{2}\,|z|^{-1/2}, & -z \gg 1. \end{cases}$$

The analysis carried out in the present section referred to the case of ballistic charge transfer in the point contact ($l \gg d$). The electrical conductivity of the point contact in diffusion conditions ($l \ll d$) differs significantly from the electrical conductivity in the absence of resonance scattering. This can be attributed to the sharp energy dependence of the resonance scattering time which produces a sharp dependence in the coefficient of diffusion. In this case, as demonstrated in Ref. 10, the nonlinear portion of the resistance is determined by the relaxation processes that occur in a region far from the point contact over the total energy relaxation length. This will serve to amplify the intensity of the nonlinear features of the I-V characteristic and will produce multiphoton duplications (in the case $\lambda \ll 1$) in the $\delta R(V)$ relation. A detailed analysis of this issue lies beyond the scope of the present study.

4. DISCUSSION OF RESULTS

As noted previously the area of particular interest is the application of these results to an analysis of the energy structure of mixed valence compounds. It is important to point out at the outset that this model contains a significant simplification and does not account for correlation effects. It applies to the case of a low concentration of scatterers, while the familiar systems take the form of concentrated solutions. Moreover an analysis of the electrical conductivity in terms of the scattering cross section can apply only to the so-called impurity (noncoherent) charge transfer regime in these compounds, where the resonance centers are distributed chaotically and there is no band motion over the ordered local states.[11] Nonetheless we believe that the relations obtained in the present study relating the point-contact electrical conductivity to the resonance scattering cross section can be used to estimate the configuration and width of the quasilocal levels in these compounds. In this regard we will cite research on YbCuAl, $CeNi_5$, $CeCu_2Si_2$ intermediate valence compounds by means of point contacts.[12-16] Experiments conducted in Ref. 12, 13 were carried out on heterojunctions and applied, in the opinion of their authors, to the ballistic mode of electrical conductivity. So-called thermal conditions in which the $R(V)$ relation of the point contact is similar to the $R(T)$ relation in a bulk metal with $T \approx eV/3.63$[17] is realized in other studies[15] due to the short scattering length. In emphasizing the experimentally observed asymmetry in the I-V characteristic the authors identify the variable nature of its nonlinear features. While a noticeable nonlinearity of the I-V characteristic was identified in Ref. 12, 14 together with a minimum appearing in the first voltage derivative of the current, an analogous structure was observed in the second derivative of the I-V characteristic. In this case the features correlate well with the position and width of the levels of the quasilocal states of rare-earth ions obtained from other experiments. The analysis carried out in the present study makes it possible to attribute the difference in the two experiments to the possible role of electron scattering on the adjoining surface of the contact metals. If this scattering is substantial, a near-tunneling situation occurs and the features associated with resonance scattering appear as early as the first derivative of the I-V characteristic. If scattering at

the contact boundary is rather weak, the inhomogeneity of the electrostatic potential distribution in the spreading region is significant, and the corresponding features in the nonlinear I-V characteristic are smoothed out.

Unfortunately the distance of the resonance level from the Fermi surface was shorter than the characteristic phonon frequencies for the compounds used as test specimens in Refs. 12–14. This made it impossible to differentiate the point-contact contributions from the EPI on the quasilocal level and in the conduction band (as noted in Sec. 3, these contributions will be shifted along the energy axis by a magnitude equal to the distance of the level from the Fermi surface). It is also important to consider the temperature dependence of the width of the peaks on the nonlinear I-V characteristic of the point contact in investigating the EPI intensity in localized states. However the literature contains no such data at present.

[1)] We note that the features of the I-V characteristic related to EPI at the resonance center are shifted by $\varepsilon_0 - \varepsilon_F$ along the eV axis with respect to the phonon spectrum for the band electrons. In the case $\varepsilon_0 - \varepsilon_F > \omega_D$ this makes it possible to reliably differentiate the corresponding contributions.

[1] *Light Scattering in Solids*, edited by J. L. Birman, H. Z. Cummin, and K. K. Rebane, N.Y., Plenum Press, 1979.

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

[3] 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)].

[4] P. W. Anderson, Phys. Rev. **124**, 41 (1961).

[5] L. I. Glazman and R. I. Shekhter, Zh. Eksp. Teor. Fiz. **94**, No. 1, 292 (1988) [Sov. Phys. JETP **67**, 163 (1988)].

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

[7] I. O. Kulik and I. K. Yanson, Fiz. Nizk. Temp. **4**, 1267 (1978) [Sov. J. Low Temp. Phys. **4**, 596 (1978)].

[8] I. O. Kulik, R. I. Shekhter, and A. G. Shkorbatov, Zh. Eksp. Teor. Fiz. **81**, 2126 (1981) [Sov. Phys. JETP. **81**, 1130 (1981)].

[9] A. G. M. Jansen, A. P. Van Gelder, and P. Wyder, J. Phys. **13**, 6073 (1980).

[10] I. F. Itskovich and R. I. Shekhter, Fiz. Nizk. Temp. **10**, 437 (1984) [Sov. J. Low Temp. Phys. **10**, 229 (1984)].

[11] D. I. Khomskiy, Usp. Fiz. Nauk. **129**, 443 (1979) [Sov. Phys. Usp. **129** (1979)].

[12] B. Bussian, J. Frankowski and D. Wohlleben, Phys. Rev. Lett. **49**, 1026 (1982).

[13] A. I. Akimenko, N. M. Ponomarenko, and I. K. Yanson, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 235 (1985) [JETP Lett. **41**, 285 (1985)].

[14] J. Jguchi, T. Yasuda, Y. Onuki, and T. Komatsubara, Phys. Rev. B **35**, 8873 (1987).

[15] Yu. G. Naydyuk, N. N. Gribov, A. A. Lysykh *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 325 (1985) [JETP Lett. **41**, 399 (1985)].

[16] I. K. Yanson and O. I. Shklyarevskiy, Fiz. Nizk. Temp. **12**, 899 (1986) [Sov. J. Low Temp. Phys. **12**, 509 (1986)].

[17] I. F. Itskovich, M. Z. Moskalets, R. I. Shekhter and I. O. Kulik, Fiz. Nizk. Temp. **13**, 1034 (1987) [Sov. J. Low Temp. Phys. **13**, 588 (1987)].

Translated by Kevin S. Hendzel