Features of tunneling in microjunctions

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We develop a theory in which a consistent account is taken both of the change of the initial spectrum of a sample by interaction with the tip of a tunnel microscope and of the relaxation time of the nonequilibrium electrons. We show that in many investigations of electron systems of low dimensionality tunneling between the banks of the junction lead to formation of a localized bound state that makes an additional contribution to the tunnel current.

INTRODUCTION

Contemporary developments in scanning tunnel microscopy (STM) call for descriptions of phenomena outside the scope of standard tunneling theory. Thus, an important role can be played in a tunneling microjunction by localized states due to various impurities and defects, or else to the presence of an adsorbate, etc., and not only by the states of the continuum. In STM and STS (scanning tunnel spectroscopy) investigations of samples, even individual localized states influence substantially the image obtained in the experiment, in contrast to macroscopic junctions whose contribution to the tunnel current is small if the density of the localized states is low.[1,2] In studies of tunnel microjunctions in the presence of localized states, as well as investigations of semiconductors and of poorly conducting samples by the STM method, it is necessary to take into account various relaxation processes that lead to the onset of a stationary distribution of the electron density.[3] The expression customarily used for the tunnel current is[4]

$$I\sim 2\pi e\int d\varepsilon\, V^2\rho_p(\varepsilon)\rho_k(\varepsilon)\,[n_p^0(\varepsilon)-n_k^0(\varepsilon-eU)], \qquad (1)$$

where V is the tunneling amplitude, $\rho_p(\varepsilon)$ and $\rho_k(\varepsilon)$ are the densities of the electron states at the edges of the tunnel junction, and $n_p^0(\varepsilon)$ and $n_k^0(\varepsilon-eU)$ are the Fermi functions of the electron distribution.

This expression "works" well for metals when the relaxation rate Γ is large:

$$\Gamma\gg V^2\rho_{p,(k)}.$$

This relation is far from always satisfied for semiconductors.

Allowance for the finite relaxation rate changes the tunnel current even in the absence of localized states. Starting with a self-consistent system of kinetic equations with a relaxation term, the following expression can be obtained for the tunnel current:

$$I\sim 2\pi e\int\frac{(n_p^0(\varepsilon)-n_k^0(\varepsilon-eU))\,V^2\rho_k(\varepsilon)\rho_p(\varepsilon)\Gamma_p\Gamma_k}{V^2\rho_p\Gamma_p+V^2\rho_k\Gamma_k+\Gamma_p\Gamma_k}d\varepsilon, \qquad (2)$$

where $\Gamma_{p,(k)}$ are the relaxation rates on the banks of the junction.

If

$$\Gamma_{p,(k)}\gg V^2\rho_{p,(k)}$$

this expression goes over into the standard equation (1).

It is important in addition to take into account in tunnel microjunctions also the spectrum renormalization due to the interaction between the electron states at the banks, since the distances between the electrodes are comparable with the interatomic distances. Such an interaction can produce in the energy gap of one of the electrodes collective localized electronic states which contribute to the tunnel current in the presence of relaxation (of interaction with the heat reservoir). An attempt to take into account the manifestation of a bound state in an interaction between an STM tip and a sample was made in Ref. 5. The use of inconsistent methods, however, made it impossible to obtain there a correct description of the tunnel microjunction.

We need thus a self-consistent description of the tunneling, with simultaneous account of the electron relaxation processes and the renormalization of the spectrum via the interaction of the electronic states on the banks. This is indicated also by recent experiments in which current mappings of surfaces of nonconducting samples was obtained at a junction voltage on the order of several mV, considerably lower than the band gap, and also experimental observation of dielectric molecules with energy levels significantly below the Fermi level.

DESCRIPTION OF MODEL AND MAIN RESULTS

1. Consider a situation in which the sample's electronic-states spectrum has a gap on the boundary of which the state density has a singularity (does not vanish). In addition, an impurity state exists near the surface of the tip or of the sample, with an energy located in the valence band (see Fig. 1). Such a system can be described by the Hamiltonian

$$\hat H=\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}^{+}c_{\mathbf{k}\sigma}+\varepsilon_d\sum_{\sigma}d_\sigma^{+}d_\sigma+\sum_{\mathbf{p}'\sigma}\varepsilon_{\mathbf{p}'}c_{\mathbf{p}'\sigma}^{+}c_{\mathbf{p}'\sigma}+\hat H_1,$$

$$\hat H_1=g_d\sum_{\mathbf{p}'\sigma}d_\sigma^{+}c_{\mathbf{p}'\sigma}+V\sum_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}^{+}d_\sigma+\text{ H.a.}, \qquad (3)$$

where $c_{\mathbf{k}\sigma}^{+}$ and $c_{\mathbf{p}'\sigma}^{+}$ are the electron creation operators in the states $(\mathbf{k},\sigma)$ and $(\mathbf{p}',\sigma)$ on the different banks of the junction, d_σ^{+} is the operator of electron production on an impurity, and V is the tunnel matrix element of a transition between the states d_σ and $(\mathbf{k},\sigma)$.

We assume for simplicity that the second bank of the junction is in thermodynamic equilibrium and serves as a heat reservoir for the states (d_σ), while g_d is the corresponding matrix element of the interaction.

A correct description of the tunnel phenomena in such a system calls for a self-consistent account of both the renormalization of the electron spectrum and of the relaxation. We introduce to this end into the Hamiltonian an additional interaction with the heat reservoir:

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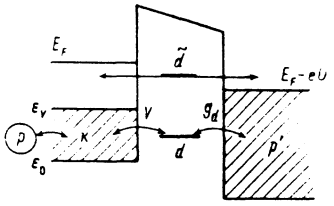

FIG. 1. Diagram of states in a microjunction: d—impurity state, $\tilde{d}$—renormalized collective state, k. p'—states of continuum on the banks of the junction, p—states of heat reservoir, V—tunnel matrix element.

$$\hat{H}_2 = \sum_{\mathbf{kp}\sigma} g(\mathbf{k}-\mathbf{p}) c_{\mathbf{k}\sigma}^{+} b_{\mathbf{p}\sigma} + \text{H.a.}, \tag{4}$$

where

$$g(\mathbf{k}-\mathbf{p}) = \frac{1}{L^d}\int d\mathbf{r}\, g(\mathbf{r}) \exp[i(\mathbf{k}-\mathbf{p})\mathbf{r}],$$

$g(\mathbf{r})$ is the effective potential of the interaction with the heat reservoir, $g(\mathbf{r}) \to 0$ in the region of the tunnel barrier and on its boundaries, and $b_{\mathbf{p},\sigma}^{+}$ is the creation operator of a heat-reservoir electron in a state $(\mathbf{p},\sigma)$. The heat reservoir is in an equilibrium state that is not altered by the perturbation $g(\mathbf{r})$.

For a self-consistent description of the tunneling in such a system we use the diagram technique for nonequilibrium processes.[6] We take the perturbation to be

$$\hat{W} = \hat{H}_1 + \hat{H}_2.$$

Note that in this technique the Green's functions are matrices over temporal indices. The equations for $\hat{G}^r$ yield the renormalized spectrum and the density of states of the system, while the equations for $\hat{G}^{-+}$ yield the system of kinetic equations from which one can determine the tunnel current. The interaction $\hat{W}$ does not intermix the spin indices, which can therefore be omitted. Taking standard Fourier transforms with respect to the fast variables, the corresponding equations acquire the form

$$\begin{aligned}
G_{\mathbf{kk}'}^{r} &= G_{\mathbf{kk}'}^{0r} + G_{\mathbf{kk}}^{0r} V G_{d\mathbf{k}'}^{r} + G_{\mathbf{kk}}^{0r} (\hat{\Sigma}^r \hat{G}^r)_{\mathbf{kk}'}, \\
G_{d\mathbf{k}'}^{r} &= G_{dd}^{0r} V \sum_{\mathbf{k}} G_{\mathbf{kk}'}^{r} + G_{dd}^{0r} \Sigma_{dd}^{r} G_{d\mathbf{k}'}^{r}, \\
G_{\mathbf{k}d}^{r} &= G_{\mathbf{kk}}^{0r} V G_{dd}^{r} + G_{\mathbf{kk}}^{0r} (\hat{\Sigma}^r \hat{G}^r)_{\mathbf{k}d}, \\
G_{dd}^{r} &= G_{dd}^{0r} + G_{dd}^{0r} V \sum_{\mathbf{k}} G_{\mathbf{k}d}^{r} + G_{dd}^{0r} \Sigma_{dd}^{r} G_{dd}^{r}.
\end{aligned} \tag{5}$$

For $\hat{G}^{-+}(\omega,t)$ we obtain the system of kinetic equations

$$\begin{aligned}
&i\frac{\partial}{\partial t} G_{dd}^{-+} = V \sum_{\mathbf{k}} (G_{\mathbf{k}d}^{-+} - G_{d\mathbf{k}}^{-+}) + (\hat{\Sigma}_{dd}\hat{G}_{dd})^{-+} + (\hat{G}_{dd}\hat{\Sigma}_{dd})^{-+}, \\
&i\frac{\partial}{\partial t} G_{\mathbf{kk}'}^{-+} + (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) G_{\mathbf{kk}'}^{-+} \\
&\quad = V(G_{d\mathbf{k}'}^{-+} - G_{\mathbf{k}d}^{-+}) + (\hat{\Sigma}\hat{G})_{\mathbf{kk}'}^{-+} + (\hat{G}\hat{\Sigma})_{\mathbf{kk}'}^{-+}, \\
&i\frac{\partial}{\partial t} G_{\mathbf{k}d}^{-+} + (\varepsilon_{\mathbf{k}} - \varepsilon_d) G_{\mathbf{k}d}^{-+} \\
&\quad = V\Big(G_{dd}^{-+} - \sum_{\mathbf{k}'} G_{\mathbf{kk}'}^{-+}\Big) + (\hat{G}\hat{\Sigma})_{\mathbf{k}d}^{-+} + (\hat{\Sigma}\hat{G}_{\mathbf{k}d})^{-+},
\end{aligned} \tag{6}$$

$$\begin{aligned}
&i\frac{\partial}{\partial t} G_{d\mathbf{k}}^{-+} + (\varepsilon_d - \varepsilon_{\mathbf{k}}) G_{d\mathbf{k}}^{-+} \\
&\quad = V\Big(\sum_{\mathbf{k}'} G_{\mathbf{kk}'}^{-+} - G_{dd}^{-+}\Big) + (\hat{G}\hat{\Sigma})_{d\mathbf{k}}^{-+} + (\hat{G}\hat{\Sigma})_{d\mathbf{k}}^{-+}.
\end{aligned}$$

In these equations $\hat{\Sigma}$ is the self-energy part due to the interaction with the heat reservoir $\hat{H}_2$ and is, just as $\hat{G}$, a matrix in temporal indices:

$$\hat{\Sigma}_{xy} = \begin{vmatrix} \Sigma_{xy}^{--} & \Sigma_{xy}^{-+} \\ \Sigma_{xy}^{+-} & \Sigma_{xy}^{++} \end{vmatrix},$$

$$\begin{aligned}
\Sigma_{\mathbf{kk}'}^{\alpha\beta} &= \sum_{\mathbf{p}} g(\mathbf{k}-\mathbf{p}) g(\mathbf{k}'-\mathbf{p}) G_{\mathbf{pp}}^{\alpha\beta_0}(\omega), \\
\Sigma_{dd}^{\alpha\beta} &= \sum_{\mathbf{p}'} |g_d|^2 G_{\mathbf{p}'\mathbf{p}'}^{\alpha\beta_0}(\omega), \quad \alpha,\beta = -,+, \\
\Sigma_{dd}^{r} &= i|g_d|^2 \nu_{p'}(\omega) = i\Gamma_d(\omega),
\end{aligned} \tag{7}$$

where $\nu_{p'}(\omega)$ is the density of the electronic states p'.

It is reasonable to assume that the heat reservoir is a system of scatterers randomly placed at points $\mathbf{R}_i$ [or that $g(\mathbf{r})$ is a random function]. Then

$$g(\mathbf{k}-\mathbf{p}) g(\mathbf{k}'-\mathbf{p}) = N^{-1} \sum_i g_i^2 \exp[i(\mathbf{k}-\mathbf{k}')\mathbf{R}_i].$$

For continuum states with a random distribution of such centers we have

$$\Sigma_{\mathbf{kk}'}^{\alpha\beta} = g_i^2 \bar{n} \delta_{\mathbf{kk}'} \sum_{\mathbf{p}} G_{\mathbf{p}}^{\alpha\beta}(\omega),$$

where $n(\mathbf{r}) = N_i/N$ is the average density of the scattering. With the heat reservoir so defined, a particular form is assumed by the kinetic equation for the relaxation of the occupation number $n_{\mathbf{k}}$ of each mode:

$$\frac{\partial n_{\mathbf{k}}}{\partial t} + iV \int d\omega\, (G_{d\mathbf{k}}^{-+}(\omega) - G_{\mathbf{k}d}^{-+}(\omega)) = -2\Gamma_{\mathbf{k}}(n_{\mathbf{k}} - n_{\mathbf{p}}^{0}),$$

$$\Gamma_{\mathbf{k}} = g_i^2 \bar{n} \nu_p(\omega),$$

$\nu_p(\omega)$ is the density of states of the heat reservoir p.

Since, however, we are mainly interested in the contribution made to the current by bound states localized near the microjunction, we can choose for the heat-reservoir model another limiting case, viz., local switching on of the heat reservoir. In this limiting case $\hat{\Sigma}_{\mathbf{kk}'}$ is independent of $\mathbf{k}$ and $\mathbf{k}'$, i.e.,

$$\Sigma_{\mathbf{kk}'}^{\alpha\beta} = g^2 \sum_{\mathbf{p}} G_{\mathbf{pp}}^{\alpha\beta_0}(\omega), \quad \Sigma_{\mathbf{kk}'}^{r} = ig^2 \nu_p(\omega) = i\Gamma_k(\omega).$$

We consider in greater detail the latter model. The results for the first model of the heat reservoir are given in Appendix 1.

The system (5) can be solved exactly and the explicit form of $\hat{G}^r$ can be obtained. For example:

$$\begin{aligned}
G_{dd}^{r}(\omega) &= (1-\Gamma)/Z(\omega), \\
Z(\omega) &= (1-\Gamma)(\omega - \varepsilon_d + i\Gamma_d(\omega)) - V^2 N(\omega),
\end{aligned}$$

where

$$N(\omega)=\sum_{\mathbf{k}} G_{\mathbf{kk}}^{r0}(\omega),$$
$$\Gamma=i\Gamma_k(\omega)\sum_{\mathbf{k}} G_{\mathbf{kk}}^{r0}(\omega). \tag{8}$$

Recall that

$$G_{\mathbf{kk}}^{r0}(\omega)=(\omega-\varepsilon_{\mathbf{k}}+i\delta)^{-1}.$$

$G^r_{\mathbf{kk}'}$, G^r_{kd}, and $G^r_{d\mathbf{k}}$ are similar in form. Explicit expressions for these functions are given in Appendix 2.

Note that the energies of all the states must be reckoned from a single level $E_f - eU$, where U is the applied potential. Therefore ε_d becomes $\varepsilon_d - eU$ in the presence of an applied voltage.

If ω is outside the boundaries of the $\varepsilon_{\mathbf{k}}$ spectrum, then $N(\omega)$ is pure real and $\Gamma(\omega)$ pure imaginary.

2. In the absence of relaxation ($\Gamma_d = 0$, $\Gamma = 0$), the energy of the collective bound state located in the band gap is given by the expression

$$\omega-\varepsilon_d-V^2N(\omega)=0 \tag{9}$$

or

$$\omega-\varepsilon_d-V^2\int d\varepsilon\rho_0(\varepsilon)(\omega-\varepsilon)^{-1}=0,$$

where $\rho_0 = dN/d\varepsilon$ is the nonrenormalized state density of the continuum. Equation (9) has a pure real solution in the regions $\omega > \varepsilon_v$ and $\omega < \varepsilon_0$, where ε_0 and ε_v are respectively the lower and upper boundaries of the $\varepsilon_{\mathbf{k}}$ spectrum. This value of ω corresponds to a localized state located in the band gap. The energy of this state depends on V and on the actual form of the nonrenormalized density of states $\rho_0(\varepsilon)$. For example, the onset of a localized state in the gap of the spectrum of a superconductor was investigated in Ref. 7.

If

$$\rho_0(\varepsilon)=(\varepsilon_v-\varepsilon_0)^{-1},$$

which is valid for a two-dimensional electronic system, we have in the region $\omega > \varepsilon_v$

$$\omega=\tilde{\varepsilon}_d=\omega_0+\varepsilon_v,$$
$$\omega_0=(\varepsilon_v-\varepsilon_0)\exp[-(\varepsilon_v-\varepsilon_0)(\tilde{\varepsilon}_d-\varepsilon_d)/V^2].$$

If $\rho_0(\varepsilon)$ is quasi-one-dimensional near the spectrum boundary

$$\tilde{\varepsilon}_d=\varepsilon_v+(V^2/(\varepsilon_v-\varepsilon_d))^2W_1^{-1}$$

(W_1 is the effective width of the quasi-one-dimensional region). It is easily seen that the amplitude of the wave function of a bound state ψ_0 directly in the junction region is determined by the residue of the function

$$G^r(\omega,0)=\sum_{\mathbf{kk}'} G^r_{\mathbf{kk}'}(\omega)$$

in point $\omega = \tilde{\varepsilon}_d$.

This yields

$$|\psi_0|^2=\left[\int d\varepsilon\rho_0(\varepsilon)(\tilde{\varepsilon}_d-\varepsilon)^{-1}\right]^2 \Big/ \int d\varepsilon\rho_0(\varepsilon)(\tilde{\varepsilon}_d-\varepsilon)^{-2}. \tag{10}$$

In the case of a two-dimensional band

$$|\psi_0|^2=(\varepsilon_v-\varepsilon_d)^2W_2\omega_0V^{-4}, \tag{11}$$

where $W_2 = \varepsilon_v - \varepsilon_0$ is the width of the $2D$ band.

It turns out that even though the exponential decrease of the tails of the wave function takes place over a characteristic length

$$R_0\approx a(W/\omega_0)^{1/D},$$

where a is the lattice constant, the dimension of the effective localization region is determined not by R_0 but by the value of $a(|\psi_0|^{-2})^{1/D}$.

In the general case, when there is not one impurity state ε_d but two bands with a bounded spectrum

$$\varepsilon_{01}<\varepsilon_1<\varepsilon_{v1} \text{ and } \varepsilon_{02}<\varepsilon_2<\varepsilon_{v2},$$

localized states can also appear at the boundary of the spectrum. In this case one can obtain in lieu of Eq. (9) a more general equation for the energies of the localized states:

$$V^2\left[\int d\varepsilon_1\rho_{01}(\varepsilon_1)(\omega-\varepsilon_1)^{-1}\right]\left[\int d\varepsilon_2\rho_{02}(\varepsilon_2)(\omega-\varepsilon_2)^{-1}\right]=1. \tag{12}$$

Let $\rho_{01}(\varepsilon_1)$ have a singularity at $\varepsilon_1 = \varepsilon_{01}$ and $\varepsilon_1 = \varepsilon_{v1}$.

a) If $\varepsilon_{01} < \varepsilon_{02} < \varepsilon_{v2} < \varepsilon_{v1}$, two localized states are produced for any form of $\rho_{02}(\varepsilon_2)$ and for any value of V; one of them has an energy $\omega_1 > \varepsilon_{v1}$ and the other $\omega_2 < \varepsilon_{01}$.

b) If $\varepsilon_{02} < \varepsilon_{01} < \varepsilon_{v2} < \varepsilon_{v1}$ (or else $\varepsilon_{01} < \varepsilon_{02} < \varepsilon_{v1} < \varepsilon_{v2}$), there exists only one state with energy $\omega > \varepsilon_{v1}$ (or with energy $\omega < \varepsilon_{01}$) for any V. The second localized state in the region $\omega < \varepsilon_{02}$ (or $\omega > \varepsilon_{v2}$) occurs only if $V > V_{cr}$ if $\rho_{02}(\varepsilon_2)$ has no singularities in the density of states. If $\rho_{02}(\varepsilon_2)$ has a singularity at $\varepsilon = \varepsilon_{02}$ (or $\varepsilon = \varepsilon_{v2}$) the situation is similar to case a).

c) If $\varepsilon_{01} < \varepsilon_{v1} < \varepsilon_{02} < \varepsilon_{v2}$, while $\rho_{02}(\varepsilon_2)$ and $\rho_{01}(\varepsilon_1)$ have singularities at the spectrum boundaries, then two localized states are produced for any value of V, with energies $\omega < \varepsilon_{01}$ and $\omega > \varepsilon_{v2}$. Note that no localized states are produced in the band gap $\varepsilon_{v1} < \varepsilon < \varepsilon_{02}$.

When account is taken of the interaction with the heat reservoir, when $\Gamma_d(\omega)$ and $\Gamma_k(\omega)$ differ from zero, but $\Gamma_d(\tilde{\varepsilon}_d) < \tilde{\varepsilon}_d - \varepsilon_v$ and $\Gamma_k(\tilde{\varepsilon}_d) < \tilde{\varepsilon}_d - \varepsilon_v$, the split-off level $\tilde{\varepsilon}_d$ acquires a finite width γ:

$$\gamma=\frac{\Gamma_k(\tilde{\varepsilon}_d)(\tilde{\varepsilon}_d-\varepsilon_d)^2V^2+\Gamma_d(\tilde{\varepsilon}_d)}{1-V^2N'(\tilde{\varepsilon}_d)}. \tag{13}$$

In the specific case of a two-dimensional electron density

$$\gamma=\Gamma_k(\tilde{\varepsilon}_d)(\tilde{\varepsilon}_d-\varepsilon_d)^2(\tilde{\varepsilon}_d-\varepsilon_v)V^{-4}\rho_0^{-1}+\Gamma_d(\tilde{\varepsilon}_d)(\tilde{\varepsilon}_d-\varepsilon_v)V^{-2}\rho_0^{-1}.$$

The condition for the existence of a split-off state is

$$\gamma\ll\tilde{\varepsilon}_d-\varepsilon_v. \tag{14}$$

It should be noted that $\Gamma_k(\tilde{\varepsilon}_d)$ can be much smaller than $\Gamma_k(\omega)$ at $\omega < \varepsilon_v$ (the relaxation rate for the continuum states). In the selected heat-reservoir models the effective potential $g(r)$ tends to zero in the region of the tunnel barrier. In fact,

$$\Gamma_k(\omega)\sim\left|\int g(\mathbf{r})e^{i\mathbf{pr}}\psi_\omega(\bar{\mathbf{r}}-\bar{\mathbf{r}}_0)d\mathbf{r}\right|^2\nu_p(\omega).$$

At $\omega = \tilde{\varepsilon}_d$ the function $\psi_\omega(\bar{\mathbf{r}}-\bar{\mathbf{r}}_0)$ describes a state localized in the region of the barrier, where $g(r)$ tends to zero, so that the effective-potential matrix element $g(r)$ which enters

in $\Gamma_k(\tilde{\varepsilon}_d)$ can be very small if $g(r)$ decreases rapidly enough, and the condition (14) will be met even if

$$\Gamma_k(\omega) \gg V^2\rho_0(\omega)$$

for the states of the continuum:

$$\varepsilon_0 < \omega < \varepsilon_v.$$

3. We proceed now to the kinetic equations (6) for the Green's functions $\hat{G}^{-+}$, which determine the tunnel current. We investigate the stationary case

$$\frac{\partial G^{-+}}{\partial t} = 0.$$

Recall that the $\hat{G}^{\alpha\beta}$ are related by

$$\hat{G}^{--} = \hat{G}^r + \hat{G}^{-+},$$
$$\hat{G}^{++} = -\hat{G}^a + \hat{G}^{-+}.$$

In the stationary state, furthermore, since we are interested in the contribution to the tunnel current from a bound state, we can assume that

$$G_{\mathbf{kk}'}^{-+}(\omega) = 2n_1(\omega)\,\mathrm{Im}\,G_{\mathbf{kk}'}^r(\omega), \qquad (15)$$
$$G_{dd}^{-+}(\omega) = 2n_2(\omega)\,\mathrm{Im}\,G_{dd}^r(\omega),$$

where $n_1(\omega)$ and $n_2(\omega)$ are the occupation numbers for the states $\mathbf{k}$ and d, respectively.

After summation over $\mathbf{k}$, the equation for $G_{\mathbf{kk}}^{-+}$ yields

$$V\sum_{\mathbf{k}}(G_{d\mathbf{k}}^{-+} - G_{\mathbf{k}d}^{-+})$$
$$= -2i\Gamma_{\mathbf{k}}(\omega)\,\mathrm{Im}\,G^r(\omega,0)\,(n_1(\omega) - n_p^0(\omega)), \qquad (16)$$

where $n_p^0(\omega)$ is the Fermi distribution function for the states of the heat reservoir p with energy ω, while

$$\mathrm{Im}\,G^r(\omega,0) = \mathrm{Im}\,G^r(\omega,\mathbf{r})|_{r=0} = \mathrm{Im}\sum_{\mathbf{kk}'}G_{\mathbf{kk}'}^r(\omega).$$

From the stationary equation for G_{dd}^{-+} it follows that

$$V\sum_{\mathbf{k}}(G_{d\mathbf{k}}^{-+} - G_{\mathbf{k}d}^{-+}) = 2i\Gamma_d(\omega)\,\mathrm{Im}\,G_{dd}^r(n_2(\omega) - n_{p'}^0(\omega)), \qquad (17)$$

$n_{p'}^0(\omega)$ is the Fermi distribution function for the states p' with energy ω; $n_p^0(\omega)$ and $n_{p'}^0(\omega)$ have Fermi-level positions that differ by eU, where U is the applied voltage.

It follows from (16) and (17) that

$$\Gamma_d(\omega)\,\mathrm{Im}\,G_{dd}^r(\omega)\,(n_2(\omega) - n_{p'}^0(\omega)) = -\Gamma_k(\omega)\,\mathrm{Im}\,G^r(\omega,0)\,(n_1(\omega) - n_p^0(\omega)). \qquad (18)$$

From the stationary equations for $G_{d\mathbf{k}}^{-+}$ and $G_{\mathbf{k}d}^{-+}$ we obtain after summing over $\mathbf{k}$

$$V^2(\mathrm{Im}\,X(\omega)\,\mathrm{Im}\,G_{dd}^r n_2 - \mathrm{Im}\,Y(\omega)n_1) + 2\Gamma_d\,\mathrm{Im}\,\lambda(\omega)n_{p'}^0 - 2\Gamma_k\,\mathrm{Im}\,\beta(\omega)n_p^0 = -2\Gamma_d\,\mathrm{Im}\,G_{dd}^r(n_2 - n_{p'}^0), \qquad (19)$$

where we have introduced the notation

$$X(\omega) = \sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - \varepsilon_d + i\Gamma_d)^{-1}S(\omega),$$
$$S(\omega) = \left[1 - i\Gamma_k(\omega)\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - \varepsilon_d + i\Gamma_d)^{-1}\right]^{-1},$$
$$Y(\omega) = \sum_{\mathbf{kk}'}\mathrm{Im}\,G_{\mathbf{kk}'}^r(\omega)\,(\varepsilon_{\mathbf{k}} - \varepsilon_d + i\Gamma_d)^{-1}S(\omega),$$
$$\lambda(\omega) = \sum_{\mathbf{k}}VG_{\mathbf{k}d}^r(\omega)\,(\varepsilon_{\mathbf{k}} - \varepsilon_d + i\Gamma_d)^{-1}S(\omega),$$
$$\beta(\omega) = \sum_{\mathbf{k}}V\left(\sum_{k'}G_{\mathbf{k}'d}^a(\omega)\right)(\varepsilon_{\mathbf{k}} - \varepsilon_d - i\Gamma_d)^{-1}S(\omega).$$

After rather unwieldy transformations we obtain for $\omega > \varepsilon_v$

$$V^2\,\mathrm{Im}\,X(\omega)\,\mathrm{Im}\,G_{dd}^r(\omega) = V^2\rho_0\,\mathrm{Im}(Z(\omega))^{-1},$$
$$\mathrm{Im}\,\lambda(\omega) = \mathrm{Im}(Z(\omega))^{-1}, \qquad (20)$$
$$\mathrm{Im}\,\beta(\omega) = \mathrm{Im}(Z(\omega))^{-1}f,$$
$$f = \mathrm{Re}\left(\sum_{\mathbf{k}}(\tilde{\varepsilon}_d - \varepsilon_d)\,(\varepsilon_{\mathbf{k}} - \varepsilon_d + i\Gamma_d)^{-1}\right),$$
$$V^2\,\mathrm{Im}\,Y(\omega) = \mathrm{Im}(Z(\omega))^{-1}(V^2\rho_0 + \Gamma_k f + \Gamma_d),$$

where $Z(\omega)$ is the denominator of G_{dd}^r.

From Eqs. (18)–(20) we can determine $n_1(\omega)$ and $n_2(\omega)$. The tunnel current is then determined by the expression

$$I = \int d\omega\{2\Gamma_d(\omega)\,\mathrm{Im}\,G_{dd}^r(\omega)\,[n_2(\omega) - n_{p'}^0(\omega)]\}. \qquad (21)$$

Taking into account the explicit form of $n_2(\omega)$, we obtain

$$I = \int d\omega 4\Gamma_d\Gamma_k\,\mathrm{Im}(Z^{-1})\,[(\Gamma_d\,\mathrm{Im}\,\lambda - V^2\,\mathrm{Im}\,X\,\mathrm{Im}\,G_{dd}^r)n_{p'}^0 - (\Gamma_k\,\mathrm{Im}\,\beta - V^2\,\mathrm{Im}\,Y)n_p^0][2V^2(\mathrm{Im}\,G_{dd}^r/\mathrm{Im}\,G^r(\omega,0))\,\mathrm{Im}\,Y\Gamma_d + (2V^2\Gamma_k\,\mathrm{Im}\,X + 4\Gamma_d\Gamma_k)\,\mathrm{Im}\,G_{dd}^r]^{-1}.$$

We have to notice that Eqs. (18)–(20) can be written in the following form:

$$\Gamma_2 n_2 + \Gamma_1 n_1 + \gamma_0' n_2^0 + n_1^0\gamma_0 = -\gamma_2(n_2 - n_2^0),$$
$$\gamma_1(n_1 - n_1^0) = -\gamma_2(n_2 - n_2^0), \qquad (22)$$

where $n_2^0 = n_{p'}^0$, $n_1^0 = n_p^0$. The tunnel current is given by

$$I \sim \int d\omega\,|\gamma_1\gamma_2|\,(\Gamma_1 + \gamma_0)\,(n_{p'}^0 - n_p^0)\,(|\gamma_2\Gamma_1| + |\gamma_1\Gamma_2| + |\gamma_1\gamma_2|)^{-1}. \qquad (23)$$

Note that it suffices to determine only one of the coefficients, of $n_{p'}^0$ or of n_p^0, since the current depends only on the difference between the occupation numbers. The following relation is then satisfied:

$$\Gamma_1 + \gamma_0 = -(\Gamma_2 + \gamma_0'),$$

which can be verified by direct substitution of the explicit expressions for Γ_1, Γ_2, γ_0, and γ_0' from (18)–(20).

We are interested in the contribution made to the tunnel current by a localized state, i.e., when $\omega \sim \tilde{\varepsilon}_d$. It can therefore be assumed that

$$Z(\omega)=Z'(\tilde{\varepsilon}_d)(\omega-\tilde{\varepsilon}_d+i\gamma).$$

For the specific case of a two-dimensional system of electrons, recognizing that for $\omega\sim\tilde{\varepsilon}_d$ we have

$$\sum_{kk'} \operatorname{Im} G^r_{kk'}(\omega)=\operatorname{Im} G^r_{dd}(\omega)(\varepsilon_v-\varepsilon_d)^2V^{-2},$$

we obtain for the tunnel current the expression

$$I\sim\frac{4\Gamma_d\Gamma_k(V^2\rho_0+2\Gamma_d)[n_p{}^0(\tilde{\varepsilon}_d)-n_{p'}{}^0(\tilde{\varepsilon}_d)]}{\{V^2\rho_0[2\Gamma_dV^2(\varepsilon_v-\varepsilon_d)^{-2}+2\Gamma_k]+4\Gamma_d\Gamma_k\}Z'(\tilde{\varepsilon}_d)}, \quad (24)$$

where

$$[Z'(\tilde{\varepsilon}_d)]^{-1}=(V\rho_0)^{-2}\exp[-(\varepsilon_v-\varepsilon_d)\varepsilon_vV^{-2}].$$

When $V^2\rho_0\gg\Gamma_d$, Γ_k, it follows from (24) that

$$I\sim\frac{2\Gamma_d\Gamma_k(n_p{}^0(\tilde{\varepsilon}_d)-n_{p'}{}^0(\tilde{\varepsilon}_d))}{Z'(\tilde{\varepsilon}_d)(\Gamma_dV^2(\varepsilon_v-\varepsilon_d)^{-2}+\Gamma_k)}. \quad (25)$$

The values of Γ_d and Γ_k in (24) and (25) are defined for $\omega=\tilde{\varepsilon}_d$. If $\tilde{\varepsilon}_d$ is located between E_f and E_f-eU, the tunnel current differs from zero because of the appearance of a new collective state $\tilde{\varepsilon}_d$.

Recall once more that the position of $\tilde{\varepsilon}_d$ relative to the band boundary depends on the applied voltage U, since the difference of all the characteristic energies is changed additionally by an amount eU.

It is shown in Appendix 1 that the results are qualitatively unchanged when another limiting case is chosen for the model of the heat reservoir, when

$$\Sigma^r_{kk'}(\omega)\sim\delta_{kk'}g_i{}^2\bar{n}\nu_p(\omega).$$

POSSIBLE GENERALIZATIONS OF THE INVESTIGATED MODEL

It is possible to take into account the direct interaction of the electronic states in different banks of the junction:

$$H'=V_1\sum_{k\sigma p'}c_{k\sigma}{}^+c_{p'\sigma}+\text{H.a.} \quad (26)$$

The situation does not change here if $V_1\ll V$, except that it is necessary to replace $\Gamma_k(\tilde{\varepsilon}_d)$ by $\Gamma'_k(\tilde{\varepsilon}_d)$ in expressions (21)–(25) for the tunnel current:

$$\Gamma_k'(\tilde{\varepsilon}_d)=\Gamma_k(\tilde{\varepsilon}_d)+V_1{}^2\nu_{p'}(\tilde{\varepsilon}_d).$$

We have considered thus far a finite relaxation rate of the continuum spectrum in only one bank of the junction. The relaxation in the other bank can also be taken into account by introducing an additional interaction with the heat reservoir for the states p':

$$\hat{H}_3=\sum_{qp'\sigma}\alpha_{p'}c_{p'\sigma}c_{q\sigma}+\text{H.a.} \quad (27)$$

The interaction $\hat{H}_3$ is analogous to $\hat{H}_2$, and $\alpha_{p'}$ is the analog of $g(\mathbf{k}-\mathbf{p})$. The energy and width of the localized level are now determined by the equation

$$(1+\Gamma_{p'}\nu_{p'})(1-i\Gamma_kN(\omega))(\omega-\varepsilon_d)-V^2N(\omega)-i\Gamma_d=0, \quad (28)$$

where

$$\Gamma_{p'}(\omega)=\alpha_{p'}{}^2\nu_q(\omega),$$

and $\nu_q(\omega)$ is the density of state of the heat reservoir q. $\Gamma_k(\omega)$ and $\Gamma_d(\omega)$ were defined earlier in Eq. (7).

The energy of the new bound state can be found from the condition

$$\omega-\varepsilon_d-V^2N(\omega)(1+\Gamma_{p'}\nu_{p'})^{-1}=0, \quad (29)$$

that is to say, allowance for the relaxation in the other bank of the junction leads to effective renormalization of the interaction-matrix element

$$V^2 \text{ на } V^2(1+\Gamma_{p'}\nu_{p'})^{-1}.$$

For a wide enough band $\Gamma_{p'}$, however, $\nu_{p'}\ll 1$, therefore $\tilde{\varepsilon}_d$ decreases only insignificantly. When $\Gamma_{p'}$ is taken into account in expression (25) for the tunnel junction, Γ_d must be replaced by Γ'_d:

$$\Gamma_d'(\tilde{\varepsilon}_d)=\Gamma_d(\tilde{\varepsilon}_d)\Gamma_{p'}(\tilde{\varepsilon}_d)[\Gamma_d(\tilde{\varepsilon}_d)+\Gamma_{p'}(\tilde{\varepsilon}_d)]^{-1}.$$

Note that the equation for the resonant tunneling without allowance for a finite rate of electron-density relaxation at

$$eU\gg\Gamma_l,\ \Gamma_r,$$

where Γ_l and Γ_r are tunneling widths of the resonant level due to the interaction with the left- and right-hand banks of the junction, takes the form

$$I\sim\Gamma_l\Gamma_r(\Gamma_l+\Gamma_r)^{-1}(n_k-n_{p'}).$$

In our case Γ_l corresponds to $V^2\rho_0$, and Γ_r corresponds to Γ_d. When relaxation is taken into account, Γ_l must be replaced by $\Gamma_l\Gamma_k(\Gamma_l+\Gamma_k)^{-1}$, and Γ_r by $\Gamma_r\Gamma_{p'}(\Gamma_r+\Gamma_{p'})^{-1}$. As a result we obtain

$$I\sim\frac{V^2\rho_0\Gamma_d\Gamma_k\Gamma_{p'}[n_p{}^0(\tilde{\varepsilon}_d)-n_q{}^0(\tilde{\varepsilon}_d)][Z'(\tilde{\varepsilon}_d)]^{-1}}{V^2\rho_0\Gamma_d(\Gamma_k+\Gamma_{p'}V^2(\varepsilon_v-\varepsilon_d)^{-2})+\Gamma_k\Gamma_{p'}(V^2\rho_0+\Gamma_d)}.$$

This expression agrees fully with the equation obtained for the tunnel current by directly substituting in (24) the value of $\Gamma'_d(\tilde{\varepsilon}_d)$ from (30).

Let us finally dwell briefly on one simpler special case. If the conduction band of the tunnel-microscope tip is regarded as quasi-one-dimensional, or if the electron spectrum of the investigated sample has a two-dimensional character, the appearance of tunnel transitions between the sample and the tip can lead to formation of a new bound state. Thus, we confine ourselves to the usual tunnel Hamiltonian:

$$\hat{H}=\sum_{k\sigma}\varepsilon_kc_{k\sigma}{}^+c_{k\sigma}+\sum_{p\sigma}\varepsilon_pc_{p\sigma}{}^+c_{p\sigma}+V_1\sum_{kp\sigma}c_{k\sigma}{}^+c_{p\sigma}+\text{H.a.}$$

We recognize, however, that the density of states of one of the bands has a singularity. Recall that the new state spectrum is determined by the poles of the Green's function (12), where ρ_{01} and ρ_{02} are the densities of the p- and k-states in the junction banks. If Eq. (12) leads to the appearance of a split-off bound state, then if account is taken of the relaxation in both banks of the junction this state makes an additional contribution to the tunnel current. A closed system of equations for the Green's function can be written in the form (22), which is convenient for the determination of $n_p(\omega)=n_1$ and $n_k(\omega)=n_2$. The quantities γ_1, γ_2, γ_0, and

Γ_1 needed to calculate the tunnel current are in this case given by

$$\gamma_1=\Gamma_p \operatorname{Im} G_{11}^r(\omega),$$
$$\gamma_2=\Gamma_k \operatorname{Im} G_{22}^r(\omega),$$
$$\gamma_0=V_1 \operatorname{Re} Z_0 \operatorname{Im} G_{12}^r(\omega)\Gamma_p,$$
$$\Gamma_1=V_1^2 \operatorname{Im} Z_0 \operatorname{Im} G_{11}^r(\omega),$$

where

$$\hat{G}_{\mu\nu}(\omega)=\sum_{pp'}\hat{G}_{\mu\nu}(\omega, p, p'), \qquad (31)$$
$$Z_0=\sum_{kp}[\varepsilon_k-\varepsilon_p+i(\Gamma_k+\Gamma_p)]^{-1}.$$

For bands that are not too narrow ($W>V_1$) in the vicinity of the energy $\varepsilon_v+\omega_0$ of the split-off state (ε_v is the position of the upper boundary of the band, with a singularity in the density of states) we have $\gamma_2,\gamma_1 \gg \Gamma_1,\gamma_0$. Integration of Eq. (23) over ω in the vicinity of $\varepsilon_v+\omega_0$ yields for the additional contribution to the current the value

$$I\sim 4\pi e V_1^2(\Gamma_k+\Gamma_p)\cdot|\psi_0|^2[n_1^0(\varepsilon_v+\omega_0)-n_2^0(\varepsilon_v+\omega_0)](\operatorname{Re} Z_0)^2,$$

where ψ_0 is defined by Eq. (10).

Cases are also possible in which the relative locations of the bands are such that in some interval of voltage only a bound state ensures the onset of a tunnel current. As a comparison, the usual tunnel current for overlapping initial bands would be equal to

$$I\sim 4\pi e V_1^2 U(\operatorname{Re} Z_0)^2.$$

Disregarding the change of the spectrum of the initial conduction bands, considering only the final rate of the relaxation of Γ_k and Γ_p, expressions (23) and (31) lead to the modified equation (2) given in the Introduction for the tunnel current.

CONCLUSION

Thus, when analyzing contemporary experiments on scanning tunnel microscopy (STM) and standard tunnel spectroscopy (STS) it is necessary to alter substantially the conventional description of tunnel junctions. It is no longer correct to state that the tunnel current is a measure of the initial density of states in the investigated material. Interaction of the sample with the nearby tip in the course of tunneling distorts the initial density of states, and produces new bound states that play a particularly important role in the case of dielectrics or surface bands in semiconductors. In this case a nonzero current can occur at a potential difference such that the initial bands do not overlap, and a contribution can be made to the current by impurities from energy levels deep below E_f. The fact that the location of the bound state depends on the tunnel matrix element V should lead to a nonexponential (and sometimes also nonmonotonic) dependence of the tunnel current on the distance to the sample in the regions of potentials corresponding to the energies of such states.

Since the tip of a tunnel microscope can be located at distances on the order of interatomic from the surface of the investigated sample, the tunnel matrix element may not differ strongly from the hop-over integral that sets the widths of the energy bands in the sample itself. For the case of $1D$ and $2D$ bands, the level splitting can then be comparable with the width of the band itself.

An estimate of the actual values of the introduced relaxation constants is in general quite complicated. We can point only to one qualitative effect. In samples containing thin layers (for example in superlattices), the rate of relaxation from a bound state should increase abruptly if the layer thickness of the investigated material is less than the localization radius of this state.

APPENDIX 1

Note for a heat-reservoir model for which

$$\Sigma_{kk'}^{\alpha\beta}=\delta_{kk'}\bar{n}g_i^2\sum_p G_p^{\alpha\beta},$$

where $\bar{n}$ is the average number of the scatterers per unit cell, the Green's functions $\hat{G}^r$ take the form

$$G_{dd}^r=\left[\omega-\varepsilon_d+i\Gamma_d-V^2\sum_k(\omega-\varepsilon_k+i\Gamma_k)^{-1}\right]^{-1},$$

$$G_{kk'}^r=\delta_{kk'}(\omega-\varepsilon_k+i\Gamma_k)^{-1}$$
$$+V^2(\omega-\varepsilon_k+i\Gamma_k)^{-1}(\omega-\varepsilon_{k'}+i\Gamma_{k'})^{-1}G_{dd}^r,$$
$$G_{kd}^r=G_{dk}^r=V(\omega-\varepsilon_k+i\Gamma_k)^{-1}G_{dd}^r.$$

The changes mean in fact that the effective width of an energy level γ of a bound-state level is expressed somewhat differently in terms of the initial constants Γ_d and Γ_k:

$$\gamma\to\gamma'=\left[\Gamma_d+\Gamma_k V^2\sum_k(\omega-\varepsilon_k)^{-2}\right][1-V^2N'(\tilde{\varepsilon}_d)]^{-1}.$$

In contrast to Eqs. (18)–(21), in which the tunnel current is determined by the rate of relaxation of the local electron density

$$I\sim\int d\omega\, g^2\nu_p(\omega)\operatorname{Im} G^r(\omega,0)[n_1(\omega)-n_p^0(\omega)], \qquad (A1)$$

the tunnel current now sets the rate of change of the total number of particles:

$$I\sim\int d\omega\, g^2\bar{n}\nu_p(\omega)[n_1(\omega)-n_p^0(\omega)]\operatorname{Im}\sum_k G_{kk}^r(\omega). \qquad (A2)$$

It turns out that expressions (A1) and (A2) differ near the energy of the split-off level by an amount $\bar{n}|\psi_0|^{-2}$, where ψ_0 is the amplitude of the wave function of the bound state at the point $\mathbf{r}=0$. Thus, if the density $\bar{n}$ of the relaxation centers is such that within the region of localization of the bound state ($S\sim|\psi_0|^{-2}$) there is located on the average one such center, then the two expressions for the tunnel current simply coincide. Expressions of the type (18)–(23) for the tunnel current remain in any case, but the dependences of Γ_d and Γ_k on the initial constants g may differ.

APPENDIX 2

The Green's functions take the form:

$$G_{dd}^r=(1-\Gamma)/Z(\omega),$$
$$G_{dk}^r=G_{kd}^r=VG_{kk}^{0r}/Z(\omega),$$
$$G_{kk'}^r=G_{kk'}^{r0}+V^2G_{kk}^{r0}G_{k'k'}^{r0}/Z(\omega).$$

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