Coulomb correlations in the tunneling through resonance centers

L. I. Glazman and K. A. Matveev
L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR Institute of Problems in Technology of Microelectronics and Especially Pure Materials, Academy of Sciences of the USSR

(Submitted 30 August 1988)
Pis'ma Zh. Eksp. Teor. Fiz. **48**, No. 7, 403–406 (10 October 1988)

Two electrons cannot tunnel simultaneously through a center because of Coulomb repulsion at the center. Such a correlation in the resonance tunneling is revealed by the magnetic field B. This correlation leads to a universal dependence of the conductance, $G(B) = G_0F(\mu_B B/T)$, of the tunnel junction which contains quasilocal centers.

The conductance of a tunnel junction with a thin, amorphous insulating layer at low temperatures is a consequence of a resonant tunneling of electrons through quasilocal states. At moderately small thickness d of the layer, this mechanism dominates over the direct tunneling.[1] The distinctive feature of the resonance mechanism is the fact that the wave function of the tunneling electron has a sharp peak in the region of the quasilocal center. The Coulomb repulsion of electrons, which tunnel through one center, in this case is appreciable: The simultaneous transmission of electrons with opposite spins is suppressed. This circumstance is clearly seen in the plot of the conductance of the junction as a function of the applied magnetic field B. The magnetic impurities in a tunnel barrier can be described by using a Hamiltonian similar to the Anderson Hamiltonian

$$H = \sum_{k\sigma} \epsilon_{k\sigma} a^+_{k\sigma} a_{k\sigma} + \sum_{p\sigma} \epsilon_{p\sigma} a^+_{p\sigma} a_{p\sigma} + \sum_{\sigma} \epsilon_\sigma a^+_\sigma a_\sigma + U a^+_\sigma a_\sigma a^+_{-\sigma} a_{-\sigma}$$

$$+ \sum_{k\sigma} (T_k a^+_{k\sigma} a_\sigma + T^*_k a^+_\sigma a_{k\sigma}) + \sum_{p\sigma} (T_p a^+_{p\sigma} a_\sigma + T^*_p a^+_\sigma a_{p\sigma}). \tag{1}$$

Here $a^+_{k\sigma}$, $a^+_{p\sigma}$, and a^+_σ are the operators for the creation of an electron in the state with a spin σ at the left edge and the right edge of the junction and in the impurity, respectively; $\epsilon_{k\sigma}$, $\epsilon_{p\sigma}$ and ϵ_σ are the energies of the electron in these states, U is the Coulomb repulsion energy, and T_k and T_p are the constants of hibridization of the state at the center with the states at the edges. We assume that the Coulomb energy U is reasonably large, $U \gg T, \Gamma_l, \Gamma_r$, where T is the temperature, and Γ_l and Γ_r are the widths of the impurity level, which are associated with the tunneling at the left edge and the right edge of the contact, respectivley., We also assume that $T \gg \Gamma = \Gamma_l + \Gamma_r$ (otherwise, the Kondo effect would be appreciable[2,3]). Because of the width of the impurity level is small ($\Gamma \ll T$), we were able to calculate the current in terms of the impurity by using the kinetic equations for the average filling of the center $\langle n_\sigma \rangle = \langle a^+_\sigma a_\sigma \rangle$ and for the probability of a double filling of the center $\langle n_\sigma n_{-\sigma} \rangle$:

$$\frac{d}{dt}\langle n_\sigma\rangle = \sum_k 2\pi |T_k|^2 [f_{k\sigma}\langle(1-n_\sigma)(1-n_{-\sigma})\rangle - (1-f_{k\sigma})\langle n_\sigma(1-n_{-\sigma})\rangle]\delta(\epsilon_\sigma-\epsilon_{k\sigma})$$
$$+\sum_p 2\pi|T_p|^2[f_{p\sigma}\langle(1-n_\sigma)(1-n_{-\sigma})\rangle-(1-f_{p\sigma})\langle n_\sigma(1-n_{-\sigma})\rangle]\delta(\epsilon_\sigma-\epsilon_{p\sigma})$$
$$+\sum_k 2\pi|T_k|^2[f_{k\sigma}\langle(1-n_\sigma)n_{-\sigma}\rangle-(1-f_{k\sigma})\langle n_\sigma n_{-\sigma}\rangle]\delta(\epsilon_\sigma+U-\epsilon_{k\sigma})$$
$$+\sum_p 2\pi|T_p|^2[f_{p\sigma}\langle(1-n_\sigma)n_{-\sigma}\rangle-(1-f_{p\sigma})\langle n_\sigma n_{-\sigma}\rangle]\delta(\epsilon_\sigma+U-\epsilon_{p\sigma}), \tag{2}$$

$$d/_{dt}\langle n_\sigma n_{-\sigma}\rangle = \sum_{k\sigma} 2\pi|T_k|^2[f_{k\sigma}\langle(1-n_\sigma)n_{-\sigma}\rangle - (1-f_{k\sigma})\langle n_\sigma n_{-\sigma}\rangle]\delta(\epsilon_\sigma+U-\epsilon_{k\sigma})$$
$$+\sum_{p\sigma} 2\pi|T_p|^2[f_{p\sigma}\langle(1-n_\sigma)n_{-\sigma}\rangle - (1-f_{p\sigma})\langle n_\sigma n_{-\sigma}\rangle]\delta(\epsilon_\sigma+U-\epsilon_{p\sigma}). \tag{3}$$

The terms with $\delta(\epsilon_\sigma - \epsilon_{k(p)\sigma})$ correspond to the transitions between the states of the zero-filled and singly filled centers and the terms with $\delta(\epsilon_\sigma + U - \epsilon_{k(p)\sigma})$ correspond to the transitions between the states of the singly and doubly filled centers. The distribution functions $f_{k\sigma} = f_l(\epsilon_{k\sigma})$ and $f_{p\sigma} = f_r(\epsilon_{p\sigma})$ at the left edge and the right edge of the contact are Fermi distributions. The difference in the corresponding Fermi levels, $E_F^l - E_F^r = eV$, is determined by the voltage V across the junction and is assumed to be small in comparison with U. A resonant tunneling occurs only if the energy of the electron at the center (ϵ_σ or $\epsilon_\sigma + U$, depending on the filling) is close to the Fermi level. Using the tunneling through broken bonds in an a-Si barrier as a guideline, we assume[1)] that $|\epsilon_\sigma + U - E_F| \sim T$ (the transitions between the singly and doubly filled states are allowed). Since $U \gg T$, we have $f_l(\epsilon_\sigma) = f_r(\epsilon_\sigma) = 1$ and in the steady-state regime it follows from Eqs. (2) and (3) that

$$[f_l(\epsilon_\sigma+U)\langle n_{-\sigma}\rangle - \langle n_\sigma n_{-\sigma}\rangle]\Gamma_l + [f_r(\epsilon_\sigma+U)\langle n_{-\sigma}\rangle - \langle n_\sigma n_{-\sigma}\rangle]\Gamma_r = 0, \tag{4}$$

$$1-\langle n_\sigma\rangle - \langle n_{-\sigma}\rangle + \langle n_\sigma n_{-\sigma}\rangle = 0. \tag{5}$$

Here the level widths are defined by the relations

$$\Gamma_l = \pi\sum_k |T_k|^2\,\delta(\epsilon_\sigma+U-\epsilon_{k\sigma}), \qquad \Gamma_r = \pi\sum_p |T_p|^2\,\delta(\epsilon_\sigma+U-\epsilon_{p\sigma}).$$

Equation (5) reflects the fact that the probability of the zero-fold filling of the impurity $\langle(1-n_\sigma)(1-n_{-\sigma})\rangle$ is zero. The solution of Eqs. (4) and (5) is

$$\langle n_\sigma\rangle = \frac{\nu_\sigma}{\nu_\sigma+\nu_{-\sigma}-\nu_\sigma\nu_{-\sigma}}, \qquad \langle n_\sigma n_{-\sigma}\rangle = \frac{\nu_\sigma\nu_{-\sigma}}{\nu_\sigma+\nu_{-\sigma}-\nu_\sigma\nu_{-\sigma}}, \tag{6}$$

where

$$\nu_\sigma = \frac{\Gamma_l}{\Gamma} f_l(\epsilon_\sigma + U) + \frac{\Gamma_r}{\Gamma} f_r(\epsilon_\sigma + U). \tag{7}$$

Substituting the solutions of (6) and (7) into the expression for the current given in terms of the impurity

$$I = e\sum_{p\sigma}\dot{n}_{p\sigma} = 2e\Gamma_r\sum_\sigma(\langle n_\sigma n_{-\sigma}\rangle - f_r(\epsilon_\sigma+U)\langle n_{-\sigma}\rangle).$$

we find

$$I = 2e\frac{\Gamma_l\Gamma_r}{\Gamma}\frac{[f_l(\epsilon_\sigma+U)-f_r(\epsilon_\sigma+U)]\nu_{-\sigma}+[f_l(\epsilon_{-\sigma}+U)-f_r(\epsilon_{-\sigma}+U)]\nu_\sigma}{\nu_\sigma+\nu_{-\sigma}-\nu_\sigma\nu_{-\sigma}}. \tag{8}$$

As was noted above, we will consider the effects associated with the external magnetic field applied to the sample. These effects are implicitly incorporated in Eqs. (1)–(8) in terms of the quantity ϵ_σ:

$$\epsilon_\sigma = \epsilon_0 + 2\sigma\mu_B B, \qquad \sigma = \pm 1/2, \tag{9}$$

where ϵ_0 is the energy of the impurity state at $B=0$. We have ignored the magnetic-field-related change in the orbital states of the electron at the edges and at the center. This is justifiable in the case of "dirty" edges ($\omega_c\tau\ll 1$, where ω_c is the cyclotron frequency, and τ is the mean-free time) and localized states with a small radius a ($a\ll\sqrt{c\hbar/eB}$; in a-Si the radius $a\lesssim 10$ Å).

In the absence of a magnetic field we have $\epsilon_\sigma=\epsilon_{-\sigma}=\epsilon_0$, $\nu_\sigma=\nu_{-\sigma}=\nu$, and Eq. (8) can be rewritten in a simplified form

$$I|_{B=0} = 4e\frac{\Gamma_l\Gamma_r}{\Gamma}\frac{f_l(\epsilon_0+U)-f_r(\epsilon_0+U)}{2-\nu}. \tag{10}$$

An additional dependence on the occupation numbers at the edges, which appears in the denominator of Eq. (10), stems from the Coulomb interaction of electrons at the center. (In the absence of interaction we have $I=4e(\Gamma_l\Gamma_r/\Gamma)[f_l(\epsilon_0)-f_r(\epsilon_0)]$). Coulomb correlations give rise, in particular, to the dependence of the saturation current, expressed in terms of a single center with $\Gamma_l\neq\Gamma_r$, on the polarity of the applied voltage:

$$I_+ = 4e\Gamma_l\Gamma_r/(\Gamma_l+2\Gamma_r), \quad I_- = 4e\Gamma_l\Gamma_r/(\Gamma_r+2\Gamma_l).$$

In experiments with tunneling metal-oxide-semiconductor structures[4] peaks which are associated with the tunneling of electrons through individual resonance centers can be observed on the plot of the linear conductance of the contact G as a function of E_F. Analysis of Eqs. (8) and (10) shows that the width of the peak of $G(E_F)$ in our case is T. At $B=0$ the peak of $G(E_F)$ is asymmetric. With an increase in the field B, the peak does not split[2)] but instead shifts toward larger values of E_F and at $\mu_B B \gg T$ it becomes symmetrical, while the peak's tip is situated at the point $E_F=\epsilon_0+U+\mu_B B$. the peak's height is $G_0=4(\sqrt{2}-1)^2(e^2/\hbar)\Gamma_l\Gamma_r/\Gamma T$ when $B=0$ and with an increase in the field, it decreases to $G_\infty=(1/2)(e^2/\hbar)\Gamma_l\Gamma_r/\Gamma T$ when $\mu_B B \gg T$. The change in the peak's height, $G_0/G_\infty=1.37$, is thus universal and does not depend on the parameters of the mixture Γ_l and Γ_r. The inequality $G_\infty/G_0<1$ is the result of the "freezing out" of spin-flip tunneling processes in a strong field.

In experiments with tunnel junctions containing an amorphous semiconductor layer[1] the barrier usually contains many impurities, and so characteristics averaged over the impurity coordinates and energies are of interest. Taking an average over G, we note that $\Gamma_{l(r)} \propto \exp(-2z_{l(r)}/a)$ depends exponentially on the position z of the impurity relative to the edges (a is the radius of the impurity state). As a result, we find

$$\bar{G}(B) = \bar{G}(\infty)F\left(\frac{\mu_B B}{T}\right), \qquad \bar{G}(\infty) = \frac{\pi e^2}{\hbar} gSa\Gamma_0 , \tag{11}$$

$$F(x) = e^{2x}\ln(1-e^{-2x}) + e^{-2x}\ln(1+e^{2x}). \tag{12}$$

Here g is the density of the impurity states at the Fermi level, and $\Gamma_0 \propto \exp(-d/a)$ is the level width at $z=d/2$. The plot of $\bar{G}$ vs B is universal in nature in the same way as (12); $\bar{G}(0)/\bar{G}(\infty)=1.39$. The differential conductance $\bar{G}_V(B)=\partial I/\partial V$ manifests similar universality at $eV \gg T$:

$$\bar{G}_V(B) = \bar{G}(\infty)F_V\left(\frac{2\mu_B B}{eV}\right), \qquad F_V(x) = \begin{cases} \sqrt{2} & \text{for } x<1 \\ 1 & \text{for } x>1 \end{cases} .$$

We wish to emphasize that the dependences $\bar{G}(B)$ and $\bar{G}_V(B)$, which are attributable to the Coulomb correlations, vanish at $U=0$.

We note in conclusion that the variation of the magnetic field in the region $B>T/\mu_B$ is equivalent to the variation of the Fermi level and that it causes a change in the arrangement of the resonance centers. As a result, mesoscopic fluctuations can be observed at the junction with a constant value of E_F.

We wish to thank A. I. Larkin and A. B. Fowler for useful discussions.

[1)]All these results can easily be extended to the case $|\epsilon-E_F|\sim T$ by substituting in (1) the hole operators for the electron operators.

[2)]In the absence of a Coulomb correlation ($U=0$) we would have an ordinary Zeeman splitting of the peak.

[1]M. Naito and M. R. Beasley, Phys. Rev. **B35**, 2548 (1987).
[2]L. I. Glazman and M. É. Raĭkh, Pis'ma Zh. Eksp. Teor. Fiz. **47**, 378 (1988) [JETP Lett. **47**, 452 (1988)].
[3]T. K. Ng and P. A. Lee, Preprint MIT, 1988.
[4]A. B. Fowler, G. L. Timp, J. J. Wainer, and R. A. Webb, Phys. Rev. Lett. **57**, 138 (1986).

Translated by S. J. Amoretty