Resonant Kondo transparency of a barrier with quasilocal impurity states

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The resonant transparency of a barrier with randomly arranged quasilocal centers is calculated for conditions corresponding to the Kondo effect.

The standard formulation of the problem of resonant tunneling can be outlined as follows: An electron of energy ϵ is incident on a barrier which contains a quasilocal state with an energy ϵ_0. The transmission coefficient D is studied as a function of ϵ. The critical dependence $D(\epsilon)$ is described by the Breit-Wigner formula[1]

$$D(\epsilon) = \frac{4\Gamma_a \Gamma_b}{(\epsilon - \epsilon_0)^2 + (\Gamma_a + \Gamma_b)^2} , \tag{1}$$

where Γ_a and Γ_β are the widths of the quasilocal level associated with escape to respectively the left-hand and right-hand banks. In real situations, the role of the barrier is played by an insulating interlayer between two metals, and the energy of the incident electron is equal to the Fermi energy in the banks, ϵ_F. It follows from (1) that the only quasilocal states which participate in the resonant transmission are those whose energies lie in a narrow band near the Fermi level: $|\epsilon_f - \epsilon_0| \lesssim \Gamma_a \Gamma_b$. Expression (1) was derived in the single-particle approximation, which ignores collective effects in the electron system. At the same time, we know that collective effects are important in a homogeneous metal even for an impurity state which lies deep below the Fermi level ($\epsilon_F - \epsilon_0 \gg \Gamma$). At temperatures T below the Kondo temperature T_K these effects make the cross section for the scattering of an electron with an energy $\epsilon = \epsilon_F$ by an impurity on the order of the square of the wavelength of the electron (the unitary limit).[2] It is reasonable to suggest that collective effects are also important in the tunneling problem, since there is an intimate relationship between resonant tunneling and scattering by a quasilocal center in the single-particle approximation. Both effects stem from the virtual capture and subsequent liberation of a band electron. We show below that the interaction of electrons with spin-degenerate states which are localized at a barrier gives rise to an analog of the Kondo effect, consisting of an increase in the tunneling transparency of a barrier with decreasing temperature. This effect occurs because even those impurities which are not resonant in the sense of expression (1) are drawn into tunneling processes as a result of collective effects as T is lowered.

We write the Hamiltonian of a tunnel junction containing an impurity in a barrier in a form analogous to Anderson's Hamiltonian[3]:

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} b^+_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma} + \epsilon_0 \sum_{\sigma} d^+_{\sigma} d_{\sigma} + W d^+_{\sigma} d_{\sigma} d^+_{-\sigma} d_{-\sigma}$$
$$+ \sum_{\mathbf{k}\sigma} (V_a a^+_{\mathbf{k}\sigma} d_{\sigma} + V_a^* d^+_{\sigma} a_{\mathbf{k}\sigma}) + \sum_{\mathbf{k}\sigma} (V_b b^+_{\mathbf{k}\sigma} d_{\sigma} + V_b^* d^+_{\sigma} b_{\mathbf{k}\sigma}). \qquad (2)$$

Here $a^+_{\mathbf{k}\sigma}$, $b^+_{\mathbf{k}\sigma}$, and d^+_{σ} are operators which create an electron in a state with a spin σ in the left-hand and right-hand banks of the junction and at the impurity, respectively; $\epsilon_{\mathbf{k}}$ and ϵ_0 are the energies of an electron in these states; W is the Coulomb energy of the interaction of two electrons at a center; and V_a and V_b are constants of the hybridization of a state at a center with states in the banks. The widths Γ_a and Γ_b are related to V_a and V_b by $\Gamma_{a(b)} = \pi |V_{a(b)}|^2 \rho$, where ρ is the state density at the Fermi level in the banks. In the absence of a Coulomb interaction ($W = 0$), Hamiltonian (2) describes ordinary resonant tunneling with transmission coefficient (1). Under the condition $\epsilon_F - \epsilon_0 \gg \Gamma_a, \Gamma_b$, the correct value $D \propto |V_a|^2 |V_b|^2$ can be found in first-order perturbation theory in the parameters V_a and V_b. Here D contains the same exponentially small factor $\exp(-2d/\lambda)$ as is found in the probability for direct tunneling (d is the thickness of the barrier, and λ is the above-barrier wavelength of an electron with the Fermi energy).

Under the condition $W \gg \epsilon_F - \epsilon_0$, a lowering of the temperature is accompanied by an increase in the correlation of the spin states of electrons in the banks and at the center (the Kondo effect). This correlation makes it incorrect to use ordinary perturbation theory to calculate the tunnel current. As a result, the expression for D may change markedly. We will show that the problem of calculating the tunneling transparency can be reduced to the well-known problem of the conductivity of a metal under conditions corresponding to the Kondo effect. For this purpose, we use the relations

$$\alpha_{\mathbf{k}\sigma} = u a_{\mathbf{k}\sigma} + v b_{\mathbf{k}\sigma}, \qquad \beta_{\mathbf{k}\sigma} = u b_{\mathbf{k}\sigma} - v a_{\mathbf{k}\sigma},$$
$$u = V_a / V, \qquad v = V_b / V, \qquad V = (|V_a|^2 + |V_b|^2)^{1/2} \qquad (3)$$

to introduce the new Fermi operators $\alpha_{k\sigma}$ and $\beta_{k\sigma}$. It turns out that quasiparticles of only one type interact with a localized state in the new representation:

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \alpha^+_{k\sigma} \alpha_{k\sigma} + \sum_{k\sigma} \epsilon_k \beta^+_{k\sigma} \beta_{k\sigma} + \epsilon_0 \sum_\sigma d^+_\sigma d_\sigma + W d^+_\sigma d_\sigma d^+_{-\sigma} d_{-\sigma}$$

$$+ V \sum_{k\sigma} (\alpha^+_{k\sigma} d_\sigma + d^+_\sigma \alpha_{k\sigma}). \qquad (4)$$

From (3) and (4) we find the relationship which we have been seeking between the probability amplitudes for tunneling, $f^{a\to b}_{k\sigma \to k'\sigma'}$, and scattering, $f_{\alpha\to\alpha}$, in a single-band metal: $f^{a\to b}_{k\sigma\to k'\sigma'} = (V_a V^*_b / V^2) f_{\alpha\to\alpha}$. The transparency of the impurity, D, is proportional to $|f^{a\to b}|^2$. It is convenient to normalize D to the transparency (D_0) of an impurity with $\epsilon_0 = \epsilon_F$, located precisely at the middle of the barrier (an exact resonance). In this case we have

$$D = D_0 \frac{4\Gamma_a \Gamma_b}{(\Gamma_a + \Gamma_b)^2} \sin^2 \delta \ , \qquad (5)$$

where δ is the scattering phase shift, in terms of which the quantity $f_{\alpha\to\alpha}$ is expressed.[2] This phase shift depends on the relation between T and the Kondo temperature T_K, which is determined by the quantity $\pi V^2 \rho = \Gamma_a + \Gamma_b$ and by the renormalized level energy ϵ_0^{**}, according to Ref. 4:

$$T_K = \frac{2}{\pi} [2\epsilon_0^{**} (\Gamma_a + \Gamma_b)]^{1/2} \exp \left\{ - \frac{\pi \epsilon_0^{**}}{2(\Gamma_a + \Gamma_b)} \right\} ;$$

$$\epsilon_0^{**} + \frac{\Gamma_a + \Gamma_b}{\pi} \ln \frac{W}{4\epsilon_0^{**}} = \epsilon_F - \epsilon_0 , \quad W \gg \epsilon_0^{**} > (\Gamma_a + \Gamma_b). \qquad (6)$$

At $T \gg T_K$, and in the Born approximation, we have $\delta \sim (\Gamma_a + \Gamma_b)/(\epsilon_F - \epsilon_0) \ll 1$. The transparency is small, and estimate (5) for D agrees with the estimate made above in first-order perturbation theory. In the next higher order, a correction to $\delta \sim (\Gamma_a + \Gamma_b) 2\ln(\epsilon_F/T)/(\epsilon_F - \epsilon_0)^2$ which is singular in the temperature arises; correspondingly, a correction to D on the order of $D_0 \Gamma_a \Gamma_b (\Gamma_a + \Gamma_b) \ln(\epsilon_F/T)/(\epsilon_F - \epsilon_0)^3$ arises. The latter correction is the same as that found in Refs. 5 and 6. It is easy to see that this correction reaches a maximum value if the impurity is near one of the banks, and even in this case it contains a small factor $\exp(-2d/\lambda)$. On the other hand, at $T \ll T_K$ the phase shift tends toward $\pi/2$, and the transparency may reach a maximum value D_0.

Up to this point we have been examining the effect of a single impurity on the transparency of the barrier. We now move on to a calculation of the total transparency of the barrier, assuming that the impurities in it are distributed uniformly in both the energy and the position (x) with respect to the middle of the barrier (Fig. 1). It is important to note that the value of T_K depends, through the constants Γ_a and Γ_b, exponentially strongly on x and equally strongly on ϵ_0^{**}. Consequently, impurities with those values of ϵ_0^{**} and x for which the relation $T_K(\epsilon_0^{**}, x) > T$ holds contribute

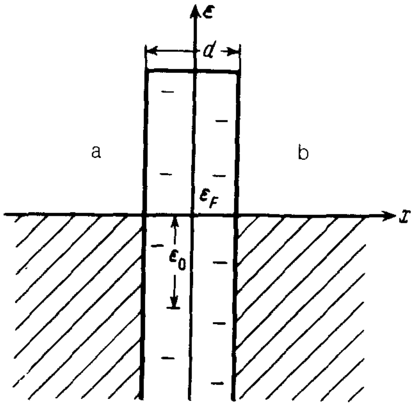

FIG. 1.

to the transparency. In the limit $W \gg \epsilon_F - \epsilon_0 \gg \Gamma_a + \Gamma_b$, the latter condition can be put in the form

$$\frac{4}{\pi}\Gamma_0 \lesssim \epsilon_0^{**} < \frac{4\Gamma_0}{\pi}\left(\mathrm{ch}\frac{2x}{\lambda}\right)\ln\left(\frac{\Gamma_0}{T}\mathrm{ch}^{1/2}\frac{2x}{\lambda}\right), \tag{7}$$

where $\Gamma_0 = (\Gamma_a \Gamma_b)^{1/2} \propto \exp(-d/\lambda)$ is the width of the level of an impurity at $x = 0$. In deriving (7) we used (6) and the x dependence of the constants Γ_a and Γ_b. We see from (5) that the transparency of impurities which satisfy condition (7) is $D = D_0/\cosh^2(2x/\lambda)$. Summing the contributions from the individual impurities, we find the definitive expression for the transparency:

$$D = \frac{2\widetilde{D}}{\pi^2}\ln(\Gamma_0/T) \qquad T \ll \Gamma_0, \tag{8}$$

where $\widetilde{D} = \pi^2 Sg\lambda\Gamma_0 D_0$ is the resonant transparency calculated without consideration of collective effects ($D \approx \widetilde{D}$ at $T \gtrsim \Gamma$), S is the area of the barrier, and g is the impurity-state density. It can be seen from (8) that the Kondo effect leads to an increase in the transparency as the temperature is lowered. This increase is limited at temperatures $T \sim U$, where U is the bias voltage applied to the junction. In this case we should replace T by U in (8).

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