Resonant Josephson current through Kondo impurities in a tunnel barrier

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The Josephson current in a junction containing resonant impurity levels in the tunnel barrier is calculated. Depending on the relation between the superconducting transition temperature and the width of these levels, the Coulomb repulsion of electrons at impurities will either suppress the Josephson current or stimulate it, by virtue of the Kondo effect.

The conductivity of a tunnel junction is very sensitive to the presence of impurity states in the barrier separating the metal banks. A resonant tunneling through these states provides the major component of the current beginning at extremely low impurity concentrations.[1] In real materials, the impurity states generally have a small radius $a \gtrsim 10$ Å, so there is a strong Coulomb repulsion, $U \gtrsim 0.1$ eV, of two electrons that occupy one level. This repulsion does not lead to a substantial change in the normal current, since it is a consequence of the tunneling of individual electrons. In the absence of a Coulomb interaction the Josephson current may also flow through resonant states.[2] The Josephson current, however, stems from a correlated tunneling of pairs of electrons, not single electrons, and it can be suppressed by Coulomb repulsion.

The role played by the Coulomb interaction varies with the relation between two time scales: that for the tunneling of a Fermi electron, which is the same as the reciprocal width Γ^{-1} of the resonant impurity state, and the correlation time of the electrons in a Cooper pair, T_c^{-1} (T_c is the superconducting transition temperature). If the tunneling time is long ($\Gamma < T_c$), the resonant Josephson current at $U = 0$ is dominated by processes in which the two electrons of a pair are simultaneously at a center. The Coulomb repulsion, $U \gg T_c$, also prohibits such processes and leads to a strong suppression of the Josephson current. In the case of a large level width, $\Gamma \gg T_c$, the processes by which the two electrons of a pair tunnel are separated in time, and the magnitude of the Josephson current is determined by the tunneling amplitudes of the individual electrons. As in the case of a junction with nonsuperconducting banks, the one-electron amplitude is not suppressed by Coulomb repulsion. Furthermore, thanks to the formation of a collective Kondo resonance at the Fermi level, the Coulomb repulsion increases the probability for a tunneling through deep impurity levels. Accordingly, as we will show below, under the condition $T_c < \Gamma$ the Coulomb interaction leads to an increase in the Josephson current.

We describe a Josephson junction with an impurity in the tunnel barrier by the Hamiltonian

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$$H = H_0 + H_i + H_\Delta + H_T ,$$

$$H_0 = \sum_{k\sigma} \xi_k (a^+_{k\sigma} a_{k\sigma} + b^+_{k\sigma} b_{k\sigma}), \qquad H_i = \sum_\sigma \epsilon_0 d^+_\sigma d_\sigma + U d^+_\uparrow d_\uparrow d^+_\downarrow d_\downarrow , \tag{1}$$

$$H_\Delta = \sum_k (\Delta_1 a^+_{k\uparrow} a^+_{-k\downarrow} + \Delta_1^* a_{-k\downarrow} a_{k\uparrow} + \Delta_2 b^+_{k\uparrow} b^+_{-k\downarrow} + \Delta_2^* b_{-k\downarrow} b_{k\uparrow}),$$

$$H_T = \sum_{k\sigma} [\, t_1 (a^+_{k\sigma} d_\sigma + d^+_\sigma a_{k\sigma}) + t_2 (b^+_{k\sigma} d_\sigma + d^+_\sigma b_{k\sigma}) \,] .$$

Here a^+, b^+, and d^+ are the operators which create an electron in the left bank, in the right bank, and at the impurity; the energies ξ_k and ϵ_0 are reckoned from the Fermi level ($U \to \infty$); t_1 and t_2 are the tunneling matrix elements which link an impurity with the left and right banks; and Δ_1 and Δ_2 are the superconducting order parameters in the banks. The current in the junction is given by

$$I = e \langle \frac{d}{dt} \sum_{k\sigma} a^+_{k\sigma} a_{k\sigma} \rangle = 2e \,\mathrm{Im} \sum_{k\sigma} t_1 \langle a^+_{k\sigma} d_\sigma \rangle . \tag{2}$$

Assuming that the tunneling width of the level is small, $\Gamma = \Gamma_1 + \Gamma_2 \ll T_c$, we can calculate the current by a perturbation theory in the tunneling Hamiltonian H_T (here $\Gamma_{1,2} = \pi \nu t^2_{1,2}$, where ν is the density of electron states in the banks). For brevity, we restrict the discussion to absolute zero. In calculating the current in the first nonvanishing approximation, we should evaluate the expectation value in (2) in terms of the wave function of the ground state, found to third order in H_T. As a result, we find

$$I = \lambda \frac{e}{\hbar} \frac{\Gamma_1 \Gamma_2}{\Delta} F\left(\frac{|\epsilon_0|}{\Delta}\right) \sin\varphi ,$$

$$F(x) = \frac{1}{\pi^2} \iint_{-\infty}^{+\infty} \frac{dt_1\, dt_2}{(\cosh t_1 + \cosh t_2)(x + \cosh t_1)(x + \cosh t_2)} , \tag{3}$$

where φ is the difference between the phases of the order parameters Δ_1 and Δ_2, $\lambda = 2$ at $\epsilon_0 > 0$, and $\lambda = -1$ at $\epsilon_0 < 0$. (The anomalous sign of the current stems from a localized spin in the barrier under the condition $\epsilon_0 < 0$; Ref. 3.) It can be verified that if there were no Coulomb repulsion ($U = 0$), the Josephson current through the resonant impurity would exceed (3) by a factor of $\Delta/\Gamma \gg 1$.

We now consider the opposite limit: $T_c \gg \Gamma_1, \Gamma_2$. In the absence of a superconductivity ($\Delta_1 = \Delta_2 = 0$), under the condition $\epsilon_0 < 0$, Hamiltonian (1) describes an impurity with a spin $S = 1/2$. The exchange interaction of the impurity spin with the band electrons in the banks leads, by virtue of the Kondo effect, to the formation of a collective resonant state at the Fermi level.[4] This state, which is formed by electrons from both banks, contributes to the amplitude for the tunneling of a Fermi electron. If the arrangement of the impurity in the barrier is symmetric, this contribution becomes the largest one and corresponds to the unitary limit. If $T_c \ll T_K$, the superconductivity does not disrupt the collective resonance, so the impurity contribution to the Josephson current also reaches its maximum value [here $T_K \sim \Gamma \exp(-\pi|\epsilon_0|/2\Gamma)$ is the Kondo temperature]. Impurities with negative values of ϵ_0 thus dominate the current.

To reduce the problem of the Josephson current through a single impurity to the problem of Kondo scattering, we rewrite Hamiltonian $\widetilde{H} = H_0 + H_i + H_T$ in terms of the new variables $A_{k\sigma} = (t_1 a_{k\sigma} + t_2 b_{k\sigma})/t$, $B_{k\sigma} = (t_2 a_{k\sigma} - t_1 b_{k\sigma})/t$, $t = (t_1^2 + t_2^2)^{1/2}$. As a result, $\widetilde{H}$ is represented as the sum of an Anderson Hamiltonian and a free-particle Hamiltonian:

$$\widetilde{H} = H_A + H_B,$$

$$H_A = \sum_{k\sigma} \xi_k A^+_{k\sigma} A_{k\sigma} + H_i + t \sum_{k\sigma} (A^+_{k\sigma} d_\sigma + d^+_\sigma A_{k\sigma}),$$

$$H_B = \sum_{k\sigma} \xi_k B^+_{k\sigma} B_{k\sigma}.$$

Hamiltonian H_A was studied by a numerical renormalization-group method in Ref. 5. Krishna-murthy *et al.*[5] showed that in states with energies $\epsilon \ll T_K$ the impurity spin is screened by band electrons, and at this energy scale H_A is equivalent to the Hamiltonian

$$H'_A = \sum_{k\sigma} \xi_k A^+_{k\sigma} A_{k\sigma} + (V/N) \sum_{kk'\sigma} A^+_{k\sigma} A_{k'\sigma}, \quad V \to \infty,$$

which does not contain dynamic variables of the impurity center. We are interested in the case $T_c \ll T_K$. We can therefore replace H_A by H'_A. After returning to the previous variables, we replace (1) by

$$H = H_0 + H_\Delta + \frac{V}{t^2 N} \sum_{kk'\sigma} (t_1 a^+_{k\sigma} + t_2 b^+_{k\sigma})(t_1 a_{k'\sigma} + t_2 b_{k'\sigma}). \tag{4}$$

The calculation of the Josephson current with quadratic Hamiltonian (4) reduces to a simple but tedious procedure of finding the Green's function $G^{ba}_{kk'\sigma}(\tau - \tau') \equiv -\langle T_\tau b_{k\sigma}(\tau) a^+_{k'\sigma}(\tau')\rangle$,

$$I = -2 \frac{t_1 t_2}{t^2} \lim_{V \to \infty} \frac{V}{N} \sum_{kk'\sigma} \operatorname{Im} G^{ba}_{kk'\sigma}(\tau = 0).$$

Although momentum is not conserved in (4), the system of Green's-function equations can be solved exactly, since the matrix element V/N is independent of the momenta of the scattered particles, k and k'. As a result, we find

$$I = 2 \frac{e}{\hbar} \frac{\Gamma_1 \Gamma_2}{(\Gamma_1 + \Gamma_2)^2} \Delta(T) \frac{1}{f(\varphi)} \tanh \left(\frac{\Delta(T) f(\varphi)}{2T}\right) \sin\varphi,$$

$$f(\varphi) = \left(1 - \frac{4\Gamma_1 \Gamma_2}{(\Gamma_1 + \Gamma_2)^2} \sin^2 \frac{\varphi}{2}\right)^{1/2} \tag{5}$$

In the limit $T \to T_c$ the current is given by $I \propto \Delta^2(T) \sin\varphi$. With decreasing temperature, I increases. The magnitude of the current depends strongly on the position of the impurity, reaching a maximum when the impurity is at the middle of the barrier ($\Gamma_1 \approx \Gamma_2$). In this case, at $T = 0$, the behavior $I(\varphi)$ is very nonsinusoidal, since the electron states in the different banks are highly hybridized.

To calculate the current through the junction, we should sum expressions (3) and (5) over all of the impurity states in the barrier. In carrying out this summation, we assume that the impurities are distributed uniformly in coordinates and energy with a state density g, and we assume that the level widths depend exponentially on the distances from the corresponding banks: $\Gamma_{1,2} = E_0 \exp(-2r_{1,2}/a)$. For large thicknesses, at which the condition $T_c \gg \Gamma_0 \equiv E_0 \exp(-L/a)$ is satisfied, an averaging of (3) yields

$$\langle I \rangle \approx \frac{e}{\hbar} E_0^2 gS \left(L - a\ln \frac{E_0}{\Delta}\right) \exp\left(-\frac{2L}{a}\right) \sin\varphi , \tag{6}$$

where S is the area and L the thickness of the tunneling layer. At smaller thicknesses, under the conditon $T_c \ll \Gamma_0$, a collective resonance involving impurities with $\Gamma_1 \approx \Gamma_2$ is important. An impurity makes a resonant contribution (5) to the current under the condition $T_K(\epsilon_0) > T_c$, which holds for energies in the interval $-(2/\pi)\Gamma_0 \ln(\Gamma_0/\Delta) < \epsilon_0 < 0$. [By virtue of the Kondo effect, this interval is larger by a factor of $\ln(\Gamma_0/\Delta)$ than the width of the resonance in the problem without a Coulomb interaction.] The behavior $I(\varphi)$ remains anomalous at low temperatures:

$$\langle I \rangle = \frac{\pi\Delta}{2e} \left\langle \frac{1}{R} \right\rangle \cos\frac{\varphi}{2} \ln \frac{1 + \sin\left(\frac{\varphi}{2}\right)}{1 - \sin\left(\frac{\varphi}{2}\right)} , \quad T \to 0. \tag{7}$$

Here $\langle 1/R \rangle \approx (e^2/\hbar) gSaE_0 \ln(\Gamma_0/T_c) \exp(-L/a)$ is the conductance of the junction in the normal state at $T = T_c$, found with allowance for the Kondo effect.[6]

Comparison of (6) and (7) shows that a disruption of the resonance with increasing L leads to a replacement of the behavior $\langle I \rangle \propto \exp(-L/a)$ by the faster $\langle I \rangle \propto \exp(-2L/a)$, while the conductance remains proportional to $\exp(-L/a)$.

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