Josephson Transport through a Hubbard Impurity Center

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(Received 20 December 2002; published 4 June 2003)

We investigate the Josephson transport through a thin semiconductor barrier containing impurity centers with the on-site Hubbard interaction u of an arbitrary sign and strength. We find that in the case of the repulsive interaction the Josephson current changes sign with the temperature increase if the energy of the impurity level ε (measured from the Fermi energy of superconductors) falls in the interval $(-u, 0)$. We predict strong temporal fluctuations of the current if only a few centers are present within the junction. In the case of the attractive impurity potential ($u < 0$) and at low temperatures, the model is reduced to the effective two level Hamiltonian allowing thus a simple description of the nonstationary Josephson effect in terms of pair tunneling processes.

DOI: 10.1103/PhysRevLett.90.226805 PACS numbers: 73.63.–b, 73.23.–b, 74.50.+r

Josephson transport through a semiconductor barrier containing resonance impurity centers is a subject of intense current theoretical and experimental interest. Being a coherent current of Cooper pairs, the Josephson current flowing through the impurity center is extremely sensitive to the presence of on-site impurity interaction [1,2]. This offers a possibility of using the Josephson effect as a unique spectroscopic tool for measurements of impurities' energy states and calls for a theoretical study of Josephson transport through an impurity level with arbitrary strength and sign of the on-site interaction.

The on-site Coulomb repulsion makes the occupation of an impurity center by a Cooper pair unfavorable. Thus, one would expect that the Josephson current flowing through an impurity level is considerably suppressed (unlike the normal current via a resonance state). However, recent analysis of the hopping magnetoresistance data for different semiconductors revealed a presence of a comfortable transmission channel via the double-occupied level (related to the states of the upper Hubbard band) [3] with the very low, as compared to the naively expected value, repulsion energy. Such a repulsion reduction may result from the polaronic effect, which sometimes can even "overscreen" the Coulomb repulsion, reverting it to the effective *attraction* at the site. The so-called D^X centers in semiconductors formed by substitutional dopants in GaAs and AlGaAs alloys (see, e.g., [4,5]) represent an example of those attractive impurities. The zero temperature Josephson transport through a Hubbard center with the infinite on-site repulsion was considered in the pioneering work [1].

In this Letter we investigate the finite temperature Josephson transport through a semiconductor barrier containing impurity centers of the arbitrary strength and sign. We restrict ourselves to a sufficiently low impurity concentration and assume that the semiconductor film is thin enough, so that its width is less than the average distance between the impurity centers: in this case the transport is indeed determined by the tunneling through a single impurity rather than by hopping over a chain of resonant impurities' levels.

Given the on-site interaction strength, u, the occupancy of the impurity level is controlled by the level energy ε. For $u > 0$ (repulsion), the impurity level is double occupied if $\varepsilon < -u$. It is single occupied when $-u < \varepsilon < 0$, and, finally, the impurity state is empty if $\varepsilon > 0$. In the case of a very strong repulsion, $u \to \infty$, and zero temperature, the Josephson current changes sign abruptly as soon as the transition from the empty state to a single-occupied state occurs; in the latter case a so-called π junction is realized [1]. We show that this effect holds and that the jump of the Josephson current becomes even more pronounced for any finite positive interaction u. At finite temperatures in the regime $-u < \varepsilon < 0$ the double and zero occupied states that carry positive Josephson currents become excited. We demonstrate that it results in nonmonotonic dependence of the Josephson current on temperature: the current first increases from negative to positive values and then decreases.

In the case of an attracting center, the impurity level is either double occupied if $\varepsilon < |u|/2$ or empty when $\varepsilon > |u|/2$. Close to the resonance, where $\varepsilon \approx |u|/2$, the main contribution to the Josephson current comes from pair tunneling processes, and the system can be described by the effective two level Hamiltonian that includes pair tunneling processes only [2]. Solution of this model gives two energy branches with energies $E_{\pm}(\phi)$ that depend on the phase difference $\phi = \phi_2 - \phi_1$ of the superconductors and correspond to exactly opposite Josephson currents (see Fig. 3 below). At finite temperatures the upper level is excited and the Josephson current depends on the temperature as $\tanh E(\phi)/2T$ with $E(\phi) = E_+(\phi) - E_-(\phi)$. This model also allows for a simple enough analysis of the nonstationary Josephson effect in the regime where the applied voltage $V \ll \min(\Delta, u)/e$. We will consider the simplest setup where the Josephson

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current is shunted by the resistor and show that in this regime the current-voltage dependence exhibits resonant peaks.

Model.—We describe our system by the Hamiltonian of impurity level coupled with superconductors via weak tunneling matrix elements t_1 and t_2,

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_0 + \sum_{k=1,2} t_k [\hat{\psi}^\dagger_{k\alpha}(0)\,\hat{d}_\alpha + \hat{d}^\dagger_\alpha \psi_{k\alpha}(0)],$$

where H_1 and H_2 are the BCS Hamiltonians of the superconductors and H_0 is the impurity Hamiltonian $\hat{H}_0 = \varepsilon \hat{d}^\dagger_\alpha \hat{d}_\alpha + u\, \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow$.

Perturbation theory in tunneling matrix elements.—The current flowing through the impurity can be found as the expectation value of the current operator $\hat{I}_1 = t_1 e i[\hat{\psi}^\dagger_{1\alpha}(0)\hat{d}_\alpha - \hat{d}^\dagger_\alpha \hat{\psi}_{1\alpha}(0)]$ flowing between the superconductor 1 and the impurity. In the second order perturbation theory in t_1 the current $I = \langle I_1 \rangle$ is

$$I = -4iet_1^2 \,\mathrm{Im} \int_0^\beta d\tau_1 F^\dagger_{1\psi}(\tau) F_d(-\tau), \tag{1}$$

where $F_{1\psi}(\tau)$ is the local anomalous Green function of the superconductor 1, $F_{1\psi}(\omega) = \pi \nu_1 \Delta_1/\sqrt{|\Delta_1|^2 + \omega^2}$, where ν_1 is the density of states. The anomalous Green function of the impurity center $F_d(\tau_1, \tau_2) = \langle d_\uparrow(\tau_1) d_\downarrow(\tau_2)\rangle$ is found by the second order perturbation theory in t_2 and the current I becomes

$$I = -4iet_1^2 t_2^2 \int d\tau d\tau_3 d\tau_4 F^\dagger_{1\psi}(\tau) K(0, \tau, \tau_3, \tau_4) \times F_2(\tau_4 - \tau_3), \tag{2}$$

where the correlation function

$$K(\tau_1, \tau_2, \tau_3, \tau_4) = \langle d_\uparrow(\tau_1) d_\downarrow(\tau_2) d^\dagger_\downarrow(\tau_3) d^\dagger_\uparrow(\tau_4)\rangle_d, \tag{3}$$

is defined with respect to impurity Hamiltonian H_0. Assuming for simplicity that $|\Delta_1| = |\Delta_2| = \Delta$ we arrive at the final answer for the current in the form

$$I = I_0(\phi)(i_0 + i_1 e^{-\beta\varepsilon} + i_2 e^{-\beta\varepsilon_2}) Z^{-1}, \tag{4}$$

where $\varepsilon_2 = 2\varepsilon + u$ is the energy of double-occupied state,

$$I_0(\phi) = 4\pi^2 e (t_1 t_2)^2 \nu_1 \nu_2 \sin(\phi), \tag{5}$$

the impurity partition function $Z = 1 + 2e^{-\beta\varepsilon} + e^{-\beta\varepsilon_2}$, and the terms i_0 and i_2 are

$$i_0 = \frac{1}{\varepsilon_2} A^2(\varepsilon) + \frac{1}{\Delta} B(\varepsilon),$$

$$i_2 = \frac{-1}{\varepsilon_2} A^2(\varepsilon - \varepsilon_2) + \frac{1}{\Delta} B(\varepsilon - \varepsilon_2),$$

with functions A and B defined by

$$A(\epsilon) = 2T \sum_\omega \frac{\epsilon}{\epsilon^2 + \omega^2} \frac{\Delta}{\sqrt{\Delta^2 + \omega^2}}, \tag{6}$$

$$B(\epsilon) = -\Delta A^2(\epsilon)/2\epsilon + T \sum_\omega \frac{1}{\epsilon^2 + \omega^2} \frac{\Delta}{\Delta^2 + \omega^2}.$$

The contribution i_1 in (4) is

$$i_1 = \frac{A^2(\varepsilon) - A^2(\varepsilon - \varepsilon_2)}{\varepsilon_2} - \frac{B(-\varepsilon) + B(\varepsilon_2 - \varepsilon)}{\Delta} + 4T \sum_\omega \frac{\varepsilon(\varepsilon_2 - \varepsilon) + \omega^2}{(\varepsilon^2 + \omega^2)[(\varepsilon_2 - \varepsilon)^2 + \omega^2]} \frac{\Delta^2}{\Delta^2 + \omega^2}. \tag{7}$$

Repulsive Hubbard center.—In the case of repulsive interaction at zero temperature Eq. (4) simplifies to

$$I = I_0(\phi) \times \begin{cases} i_2, & \varepsilon < -u, \\ i_1/2, & -u < \varepsilon < 0, \\ i_0, & \varepsilon > 0, \end{cases} \tag{8}$$

which describes double-occupied, single-occupied, and unoccupied contributions, respectively. The dependence of the Josephson current on ε given by Eq. (8) is discontinuous (see Fig. 1) with the jumps at points $\varepsilon = 0$ and $\varepsilon = -u$ where the Josephson current changes sign. The maximal values of the Josephson current $I_{\max}/I_0(\phi) = 1/u + (2/\pi - 1/2)/\Delta$ grow as $1/u$ when $u \to 0$ such that for $u < t^2\nu$ the perturbation theory in hopping elements at $\varepsilon \approx 0, -u$ becomes inapplicable. In the region $-u < \varepsilon < 0$ the Josephson current does not exhibit a singular behavior because occupation of the impurity level by one electron prevents the resonant pair current flow even in the case of small u. Thus the height of the jumps of the Josephson current at points $\varepsilon = 0$ and $\varepsilon = -u$ decreases with the increase of the interaction strength u.

At finite temperatures the dependence of the Josephson current on ε becomes continuous (Fig. 1) and, eventually, at high enough T the Josephson current becomes positive for all ε. Thus for ε laying within the interval $(-u, 0)$ the Josephson current changes its sign as temperature grows [Fig. 2(a)]. This can be understood as follows: At low temperatures the current is given by the single-occupied contribution i_1 which is negative, at finite temperature the zero and double-occupied states corresponding to positive

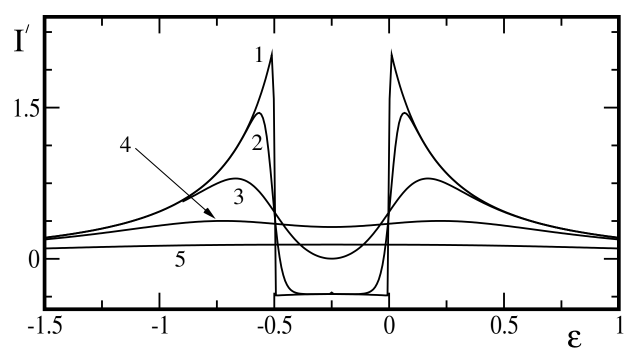

FIG. 1. The Josephson current $I' = I/I_0(\phi)$ as a function of the energy of the single-occupied impurity state ε for $u/\Delta = 0.5$ and different temperatures: $T' = T/\Delta = 0, 0.02, 0.04, 0.1, 0.2$ for plots 1–5, respectively.

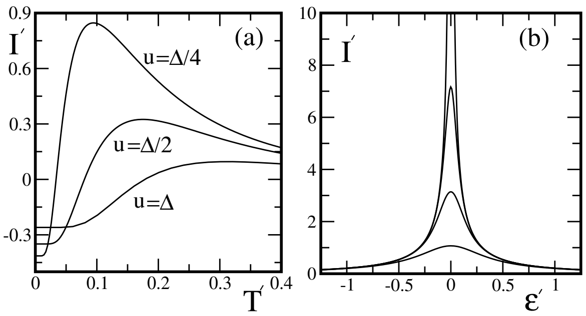

FIG. 2. (a) The Josephson current $I' = I/I_0(\phi)$ as a function of temperature $T' = T/\Delta$ for different positive interactions u and $\varepsilon = -u/2$. (b) Dependence of the Josephson current on $\varepsilon' = \varepsilon + u/2$ for $u/\Delta = -0.5$ and different temperatures: $T' = 0, 0.05, 0.1, 0.2$ (top to bottom).

currents are excited. Since the latter ones make larger contributions, the Josephson current eventually changes sign with the increase of temperature.

The temperature dependence in question implies the statistical averaging over impurity centers. If only a few centers are present, one expects significant temporal fluctuations of the critical current. These fluctuations can be observed, for example, by including the Josephson junction in a superconducting loop. The energy of such a loop in the absence of an external magnetic field can be written as a function of magnetic flux $\Phi = LI$, with L being the inductance of the loop, as $E_l(\Phi) = -I_c \cos(2\pi\Phi/\Phi_0) + \Phi^2/2L$, where I_c is the critical current defined by Eqs. (4) and (5) and Φ_0 is the magnetic flux quantum. Assuming $I_c L \gg \Phi_0$ we see that for positive I_c the minimal solution corresponds to $\Phi = 0$ while for $I_c < 0$ the solution corresponds to $\Phi = \Phi_0/2$. Transitions between different states of the impurity center lead to fluctuations of the magnetic flux through the loop. Change in the occupation number requires a quasiparticle tunneling from the leads to the center or vice verse. Thus, if $T < \Delta$ the characteristic fluctuation time is $\tau \sim (\hbar/t^2\omega_0\nu)\exp(\Delta/T)$. Here ω_0 is the attempt rate which is estimated bearing in mind that the processes of the center recharge are inelastic and related to phonon-assisted tunneling. Thus the value of ω_0 includes the parameter of the electron-phonon coupling. The characteristic times spent in the empty, single-occupied, and double-occupied states are then given as τZ, $\tau Z\exp(\beta\epsilon)$, and $\tau Z\exp(\beta\epsilon_2)$, respectively.

Attractive Hubbard center.—At $u < 0$ the dependence of the Josephson current on the level energy ε shows the resonance at values $\varepsilon \approx |u|/2$, where the energy of the double-occupied state ε_2 approaches zero [see Fig. 2(b)]. Near the resonance Eq. (4) can be simplified, leaving only the terms that demonstrate singular behaviors as of $1/\varepsilon_2$:

$$I = \frac{I_0(\phi)}{\varepsilon_2}\frac{A^2[(\varepsilon_2 + |u|)/2] - A^2[(\varepsilon_2 - |u|)/2]e^{-\beta\varepsilon_2}}{1 + e^{-\beta\varepsilon_2}}.$$

For $T \ll \Delta$ the maximal value of the current $I_{\max} = I_0(\phi)A^2(|u|/2)/2T$ diverges at very low temperatures $T < t^2\nu$ where the approach based on the perturbation theory in tunneling elements becomes inapplicable.

Effective low temperature model.—In the case of the attractive interaction the Josephson current obtained by the perturbation theory in t_1 and t_2 has a form of the Gibbs average of two terms corresponding to unoccupied- and double-occupied states. This holds as long as $T \ll u$, and the system in this regime can be described by the effective Hamiltonian [2,6]

$$\hat{H}_{\text{eff}} = \varepsilon_2 \hat{b}^\dagger \hat{b} + \tilde{t}_1[\hat{b}^\dagger e^{i\phi_1} + \hat{b}e^{-i\phi_1}] + \tilde{t}_2[\hat{b}^\dagger e^{i\phi_2} + \hat{b}e^{-i\phi_2}],$$

where $\hat{b} = \hat{d}_\downarrow \hat{d}_\uparrow$ is the hard-core boson operator satisfying $[\hat{b}, \hat{b}^\dagger] = 1 - 2\hat{b}^\dagger\hat{b}$, $\hat{b}^\dagger\hat{b}^\dagger = 0$. An eigenfunction of the Hamiltonian $\hat{H}_{\text{eff}}$ can be written as $\psi = \alpha|0\rangle + \beta|1\rangle$, where $|0\rangle$ is the empty state and $|1\rangle$ is the double-occupied (one pair) state. The operator of the current flowing through the impurity is

$$\hat{I} = 2ei\tilde{t}_1\langle\psi|\hat{b}e^{-i\phi_1} - b^\dagger e^{i\phi_1}|\psi\rangle. \tag{9}$$

Solving the Schrödinger equation $\hat{H}_{\text{eff}}\psi = E\psi$ we find two eigenstates with energies

$$E_\pm(\phi) = \varepsilon_2/2 \pm \sqrt{\delta^2 + E_0^2[\cos(\phi) + 1]}, \tag{10}$$

where $\delta^2 = \varepsilon_2^2/4 + (\tilde{t}_1 - \tilde{t}_2)^2$, $E_0^2 = 2\tilde{t}_1\tilde{t}_2$. The currents corresponding to these two states are

$$I_\pm(\phi) = \mp\frac{eE_0^2\sin(\phi)}{\sqrt{\delta^2 + E_0^2[\cos(\phi) + 1]}} = 2e\frac{dE_\pm(\phi)}{d\phi}. \tag{11}$$

Dependences of the energies $E_\pm$ and currents $I_\pm$ on the phase ϕ are shown in Fig. 3. Comparing the current I_- given by Eq. (11) with the result of perturbation theory in t_1, t_2 we find the effective tunneling matrix elements $\tilde{t}_{1,2} = \pi t_{1,2}^2 \nu_{1,2} A(|u|/2)$. At $T \ll u$ the summation in (6) can be reduced to the integration resulting in

$$A(\epsilon) = \begin{cases} \frac{1-(2/\pi)\arcsin(\epsilon/\Delta)}{\sqrt{1-\epsilon^2/\Delta^2}}, & 0 < \epsilon < \Delta, \\ \frac{\Delta}{\pi\sqrt{\epsilon^2-\Delta^2}}\ln\frac{\epsilon+\sqrt{\epsilon^2-\Delta^2}}{\epsilon-\sqrt{\epsilon^2-\Delta^2}}, & \epsilon > \Delta. \end{cases} \tag{12}$$

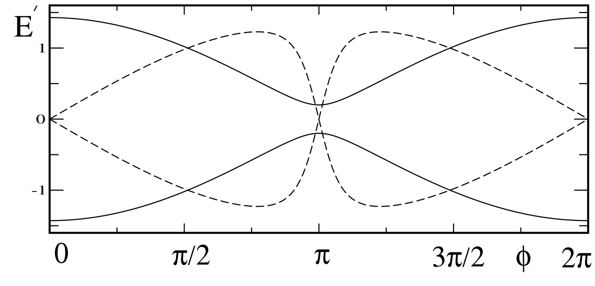

FIG. 3. Impurity energy $E' = (E - \varepsilon_2/2)/E_0$ as a function of the phase $\phi = \phi_1 - \phi_2$ (solid lines) and the corresponding Josephson currents $I'_\pm = I_\pm/(eE_0)$ (dashed lines).

At finite temperatures the Josephson current is given by the thermodynamic average of the two states $I(\phi) = I_-(\phi)\tanh E(\phi)/2T$ with $E(\phi) = E_+(\phi) - E_-(\phi)$. Analogously to the case of the repulsive interaction we expect strong temporal fluctuations of the current in the junctions containing only a few centers, since the critical currents for two branches have opposite signs.

Nonstationary regime.—Let us consider the simplest experimental setup (see Fig. 4): Superconductor contacts are shunted by the resistor while the potential of the superconductor 1 and the current I_0 are fixed. The potential of the superconductor 2, V_2, is determined by the current conservation equation

$$V_2/R + I_2(t) = I_0, \tag{13}$$

where $I_2(t)$ is the current flowing between the impurity center and the superconductor 2

$$I_2(t) = -2eit_2\,\mathrm{Im}\{\alpha^*\beta e^{-i\phi_2}\}. \tag{14}$$

The phase ϕ_2 is related to the voltage V_2 by

$$\dot{\phi}_2 = -2eV_2. \tag{15}$$

To close the system of Eqs. (13)–(15) we write the Schrödinger equation for the amplitudes α, β

$$i\dot{\alpha} = \beta\tilde{t}_1 + \beta\tilde{t}_2 e^{-i\phi_2}, \tag{16}$$

$$i\dot{\beta} = \beta\epsilon_i + \alpha\tilde{t}_1 + \alpha\tilde{t}_2 e^{i\phi_2}. \tag{17}$$

The Cooper pair energy on the impurity site ε_i has a contribution from the potential of the superconductor 2 $\varepsilon_i = \varepsilon_2 + 2keV_2$ where $k = l_1/(l_1 + l_2)$ and l_1, l_2 are the distances between the impurity center and superconductors 1 and 2, respectively. Equations (13)–(17) can be easily solved numerically. Solutions for $k = 0$, $\epsilon_2/E_0 = 0.5$, $\tilde{t}_1/E_0 = 2.0$, $\tilde{t}_2/E_0 = 0.5$, and different shunting resistors are shown in Fig. 4 along with approximate adiabatic solutions shown by the dashed lines. The adiabatic approximation is valid in the low voltage regime where the phase ϕ_2 changes slowly and the current is given by

$$I_2(t) = -eE_0^2\sin(\phi_2 t)/\sqrt{\delta^2 + E_0^2[\cos(\phi_2 t) + 1]}, \tag{18}$$

corresponding to the lower energy branch $E_-(\phi_2)$. At higher voltages the effect of Landau-Zener tunneling between two energy branches cannot be neglected. As we see it from the numerical solution, transitions between the branches appear as resonances on the current-voltage dependence. Positions of these resonances can be easily estimated in case $t_1 \gg t_2$; taking $t_2 = 0$ in Eq. (10) we obtain that the energy levels are split by $\Delta E = 2\sqrt{\varepsilon_2^2/4 + \tilde{t}_1^2}$. Resonances arise when the frequency of the phase oscillations of the superconductor $2\omega = 2eV_2/\hbar$ is related with ΔE as $m\hbar\omega = \Delta E$. Shown in the inset of Fig. 4 is the differential resistance as a function of voltage. One clearly sees resonances satisfying the above conditions.

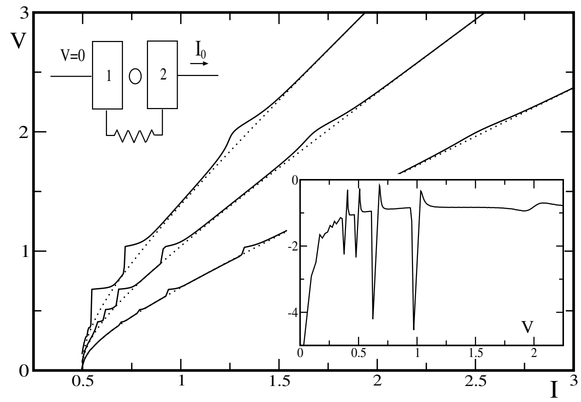

FIG. 4. Voltage-current dependence of the shunted Josephson contact for receptivities $Re^2/\hbar = 1.6, 1.2, 0.8$ (top to bottom). Upper inset shows the setup while the lower one shows the differential resistance (dV/dI) as a function of the applied voltage corresponding to the lower graph $(Re^2/\hbar = 0.8)$.

Conclusions.—In conclusion, we have investigated the Josephson transport through an impurity center for the cases of arbitrary sign and arbitrary strength of the Hubbard interaction. For repulsive centers we show that the Josephson current changes sign with temperature when the energy of single-occupied states ε lays within the interval $(-u, 0)$. If the junction contains only a few centers strong temporal fluctuations of the current are predicted. In the case of attractive centers we study the nonstationary Josephson effect with the help of the effective model that takes into account only pair tunneling processes. We consider the case of resistively shunted Josephson junction and show that the current-voltage characteristic has resonances associated with the transition between two states formed due to coupling of the impurity with one of the superconductors.

We thank Y. M. Galperin, A. E. Koshelev, and K. Matveev for useful discussions. This work was supported by the U.S. Department of Energy, Office of Science under Contract No. W-31-109-ENG-38.

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