Josephson current in unconventional superconductors through an Anderson impurity

Y. Avishai*
Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva, Israel
and Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan

A. Golub†
Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva, Israel

(Received 28 December 1999)

Josephson current for a system consisting of an Anderson impurity weakly coupled to two unconventional superconductors is studied and shown to be driven by a surface zero energy (midgap) bound state. The repulsive Coulomb interaction in the dot can turn a π junction into a 0 junction. This effect is more pronounced in p-wave superconductors while in high-temperature superconductors with $d_{x^2-y^2}$ symmetry it can exist for rather large artificial centers at which tunneling occurs within a finite region.

Recently, the Josephson effect in unconventional superconductors have attracted a considerable attention.[1–6] Measurements of direct Josephson current yield valuable information on the symmetry of the order parameter which is essential for understanding the mechanisms of superconductivity in these complex materials. Phase interference experiments[7] definitely suggest the presence of d-wave symmetry of the order parameter in high-T_c superconductors, while the recent discovery of superconductivity in Sr_2RuO_4 (Ref. 8) implies the existence of a peculiar system for which the pair potential has a triplet (p wave) symmetry.[9]

p- and d-wave symmetries of the order parameter have in common a property which reflects the variation of the pair potential across the Fermi surface. This results in a strong sensitivity to inhomogeneities which, in turn, influences the Josephson effect. In particular, an anomalous temperature dependence of a single Josephson junction at low temperatures[3–6] and an induced crossover from a usual (0 junction) to a π junction on approaching the critical temperature were observed.

Tunneling in a Josephson junction consisting of conventional (s-wave) superconductors and a dynamical impurity (Anderson and Kondo) was considered sometime ago.[10–13] In a recent work[14] the tunneling current was calculated at zero temperature and was shown to be strongly dependent on the Coulomb interaction which, in some cases, may cause a sign change of the current. The experimental observations described above motivate us to study the same device albeit with unconventional superconductors at finite temperatures. As will be demonstrated, the underlying physics is remarkably different.

The main focus here is the influence of Coulomb interaction on the low temperature behavior of the current in a 2D Josephson junction consisting of left (L) and right (R) superconductors with either p or $d_{x^2-y^2}$ symmetry of the order parameter weakly coupled to a quantum dot (via identical hoping matrix elements $t_L = t_R = t$). The dot is represented by a finite U Anderson impurity whose energy $\epsilon_0 < 0$ lies below the Fermi energy. Usually, the inequalities $U > -\epsilon_0 > 0$ are maintained so that the ground state of the disconnected ($t = 0$) dot is singly occupied. We use the nonperturbative scheme suggested in Ref. 14 (extended for finite temperature) and elucidate the low-temperature behavior of the Josephson current and its dependence on U, t, and the phase of the order parameter Δ.

Since Δ is not isotropic, it is useful at this point to specify the underlying geometry. Each superconductor has the shape of half a plane defined as $-\infty < y < \infty$ and $x < 0$ ($x > 0$) for the left (right) superconductor. The dot is located at the origin $\mathbf{r} = 0$ and tunneling is described by zero-range hoping between the impurity and the superconductors along the x axis. For d-wave superconductors we choose the nodal line of the pair potential on the Fermi surface to coincide with the tunneling direction, such that $\Delta = v_\Delta p_F \sin 2\alpha$ where p_F is the Fermi momentum. For spin-triplet superconducting states the pair potential is an odd vector function of momentum and a 2×2 matrix in spin space. We chose to represent it by the time reversal symmetry breaking state[9] which is off-diagonal in spin indices with the order parameter approximately given as $\Delta = \Delta_0 \exp i\alpha$. In this junction geometry α is the azimuthal angle in the x-y plane.

The physical implication of this geometrical construction for d- and p-wave superconductors can be described as follows: The pair potential pertaining to electronlike excitations has different values (and signs) depending on whether they propagate along the direction α or reflected along the direction π-α (see Fig. 1). This fact significantly affects the scattering process and causes the formation of a zero energy (midgap) bound state centered at the boundary. Another ge-

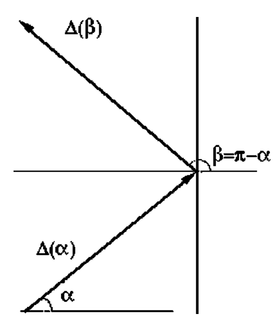

FIG. 1. Schematic geometry of the junction. Incoming and reflected electronlike excitations are moving in an angle-dependent pair potential which can have different signs for these quasiparticles.

ometry which has been used recently is that of a mirror junction,[3] in which the barrier is a reflection-symmetry plane for the superconducting electrodes.

To obtain the Josephson current we compute the partition function $Z=\int D[\overline{\psi}\psi\overline{c}c]\exp(-S)$ and the corresponding free energy of the system. The functional integration is performed over Grassmann fields in the superconductors and the quantum dot (see below for a precise definition). The Euclidean action can be written as a sum $S=S_L+S_R+S_{\rm tun}+S_{\rm dot}$, corresponding respectively to left, right, tunneling and dot parts. In the following, quantities pertaining to the right superconductor are obtained from those calculated for the left one by simply replacing $L\rightarrow R$. With obvious notations the actions read

$$S_L=T\sum_{\omega}\int dx\,dy\,\overline{\psi}_{L\omega}(xy)[i\omega+H_L^{\rm BDG}(\hat{p}_x,\hat{p}_y)]\psi_{L\omega}(xy), \tag{1}$$

$$S_{\rm tun}=-T\sum_{\omega}[t_L\overline{\psi}_{L\omega}(0)\tau_3c_\omega+t_L^*\overline{c}_\omega\tau_3\psi_{L\omega}(0)]+L\rightarrow R, \tag{2}$$

$$S_{\rm dot}=\int d\tau[\overline{c}\partial_\tau c+\tilde{\epsilon}\overline{c}\tau_3c-U(\overline{c}c)^2/2], \tag{3}$$

where $\tau_3=\mathrm{diag}(1,-1)$ being the Pauli matrix and $\tilde{\epsilon}=\epsilon_0+U/2$. The summation is taken over odd Matsubara frequencies $\omega=(2n+1)\pi T$, while $\overline{\psi}_{L\omega}(xy)\equiv[\overline{\psi}_{L\omega\uparrow}(xy)\psi_{L\omega\downarrow}(xy)],\overline{c}\equiv(\overline{c}_\uparrow c_\downarrow)$ and the corresponding conjugate fields are Grassmann variables of the superconductors and the impurity, respectively.

The Bogolubov-DeGennes Hamiltonian $H_L^{\rm BDG}$ acquires the form

$$H_L^{\rm BDG}(\hat{p}_x,\hat{p}_y)=\begin{pmatrix}\epsilon(\hat{p})-p_F^2/2m & \Delta(\hat{p})\exp(\phi_L)\\ \Delta(\hat{p})^*\exp(-\phi_L) & -\epsilon(\hat{p})+p_F^2/2m\end{pmatrix}, \tag{4}$$

where $\epsilon(\hat{p})$ denotes the kinetic energy operator with dispersion $\epsilon(p)$, and ϕ_L is the phase of the superconducting condensate. We take $\Delta_L=\Delta_R\equiv\Delta$ but $\phi_L\neq\phi_R$.

Since the pair potential is translation invariant in the y direction we employ Fourier transform and express the action in terms of fermion Grassmann variables $\psi_{L\omega k_y}(x)$ and BDG Hamiltonian $H_L^{\rm BDG}(\hat{p}_x,k_y)$ where $k_y=p_F\sin\alpha$. Accordingly, the available energy for the longitudinal motion (a renormalized chemical potential) is then $\mu_k\equiv(p_F^2-k_y^2)/2m\equiv k_0^2/2m$.

In computing the action (1) the integration over the fields can be carried out explicitly using the saddle point method (which is exact here, since the action is quadratic). The equation for the stationary fields is $G_{L\omega k_y}^{-1}\psi_{L\omega k_y}(x)=0$, with $G_{L\omega k_y}^{-1}=i\omega+H_L^{\rm BDG}(\hat{p}_x,k_y)$. The result of these manipulations is the following form for the action (1):

$$S_L=-T\sum_{\omega,k_y}\frac{1}{2m}\overline{\psi}_{L\omega k_y}(0)\tau_3\left(\frac{\partial}{\partial x}\psi_{L\omega k_y}(x)\right)_{x\rightarrow 0}. \tag{5}$$

Due to the zero-range nature of the tunneling matrix elements, the fields at $\mathbf{r}\neq 0$ (referred to as bulk fields) can be integrated out[14] yielding an effective action solely in terms of the boundary fields $\psi_{L\omega k_y}(0)$. To this end, we decompose $\psi_{L\omega k_y}(x)=\psi_{L\omega k_y}^{\rm bulk}(x)+\psi_{L\omega k_y}(0)$ in such a way that at the surface $\psi_{L\omega k_y}^{\rm bulk}(x)|_{x=0}=0$. The bulk fields $\psi_{L\omega k_y}^{\rm bulk}(x)$ are obtained by solving the inhomogeneous equation

$$G_{L\omega k_y}^{-1}\psi_{L\omega k_y}^{\rm bulk}(x)=\mu_k\tau_3\psi_{L\omega k_y}(0). \tag{6}$$

The right hand side of this equation corresponds to Andreev approximation for which the typical energies and the superconducting gap are much smaller than the chemical potential. In order to solve equation (6) we need to find the Green function $G_{L\omega k_y}(xx')$ such that

$$G_{L\omega k_y}^{-1}G_{L\omega k_y}(xx')=\delta(x-x'), \tag{7}$$

subject to the homogeneous boundary condition $G_{L\omega k_y}(0x')=0$. The Green function thereby obtained for d or p wave superconductors turn out to be markedly distinct from that of s wave ones. This is due to sign change of the pair potential as underlined above.

Solving then for the bulk fields in terms of the fields at $x=0$ and substituting it into Eq. (5) we obtain the effective superconductor action in terms of the surface fields

$$S_L=T\sum_{\omega,k_y}\overline{\psi}_{L\omega k_y}(0)\overline{G}_{L\omega k_y}\psi_{L\omega k_y}(0), \tag{8}$$

with

$$\overline{G}_{L\omega k_y}=\frac{\mu_k}{2m}\frac{\partial}{\partial x}\int_{-\infty}^{0}dx'\,\tau_3G_{L\omega k_y}(xx')|_{x=0}\tau_3. \tag{9}$$

For reasons that will be clear later on we prefer to display the function $\overline{G}_{L\omega k_y}$ for p-wave superconductors. Straightforward calculation yields $\overline{G}_{L\omega k_y}=-(k_0/2m)r_L(\omega)$ with

$$r_L(\omega)=\frac{1}{\omega}\begin{pmatrix}-i\sqrt{\omega^2+|\Delta_L|^2} & -\Delta_L\\ \Delta_L^* & -i\sqrt{\omega^2+|\Delta_L|^2}\end{pmatrix}. \tag{10}$$

Note that the dependence on k_y enters only in k_0. The effective action defined via equations (8)–(10) is indeed distinct from the corresponding quantity derived for s-wave superconductors (note in particular the occurrence of ω in the denominator).

Performing the integration over the boundary fields $\overline{\psi}_{L\omega k_y}(0),\psi_{L\omega k_y}(0)$ in the partition function is now straightforward. The remaining integrations over the $c,\overline{c}$ fields is done by decoupling the Hubbard interaction using a Hubbard-Stratonovich transformation. This implies the introduction of auxiliary fields γ_ω. The result is then

$$Z=C\int\prod_{\omega}d\gamma_\omega\exp\left(-\frac{\gamma_\omega^2}{2UT}-\frac{\tilde{\epsilon}}{T}-\frac{F}{T}\right). \tag{11}$$

Here $F=-T\Sigma_\omega\ln[\det R(\omega)]$ and C is a constant. The matrix R which encodes the coupling between the superconducting (half) planes and the impurity is given by

$$R(\omega)=\tilde{\epsilon}\tau_3+\gamma_\omega-i\omega-\pi N(0)\langle|t|^2[r_L(\omega)+r_R(\omega)]\rangle, \tag{12}$$

where $N(0)$ is the density of states at the Fermi level, and $\langle O\rangle \equiv \pi^{-1}\int_{-\pi/2}^{\pi/2} d\alpha O(\alpha)$. The averaging procedure thus defined is related to a possible dispersion of the transmission matrix element t_{ky}. For a point junction with constant t, only the component of the Josephson current perpendicular to the interface is relevant. In this case, for even (d-wave symmetry) superconductors the midgap zero energy bound state does not contribute to the Josephson current. In clear distinction, for a p-wave pair potential this state defines the main contribution at low temperatures[15] (which is the temperature domain of our interest here). Intuitively, occurrence of dispersive tunneling matrix elements t_{ky} correspond to deviation of the impurity from a point-like defect. Such a case can be realized, e.g., by artificially induced defects.[16] The spectroscopy of $Bi_2Sr_2CaCu_2O_8$ surfaces indicates that such defects appear to be more extended in STM imaging. In this case one can expect nonzero contribution from the midgap level in d-waves superconductors as well.

With this point in mind we now proceed and consider the p-wave case. The functional integral in Eq. (11) is approximated by the saddle point method. The appropriate optimum solution for γ_ω (denoted hereafter by γ) should then minimize the free energy

$$F=-T\sum_{\omega>0}\ln\{A^2(\omega)+4\gamma^2\omega^2[1+a(\omega)]^2\}+\frac{\gamma^2}{2U}+\tilde{\epsilon}. \quad (13)$$

Here we use the notations

$$A(\omega)=\tilde{\epsilon}^2+\omega^2[1+a(\omega)]^2-\gamma^2-b^2(\omega)|\Delta|^2\cos^2\left(\frac{\phi}{2}\right), \quad (14)$$

$$a(\omega)=\Gamma\frac{\sqrt{\omega^2+|\Delta|^2}}{\omega^2}, \quad (15)$$

where $\Gamma=2\pi t^2N(0)$ is the bare impurity level width, $b(\omega)=\Gamma/\omega$, and $\phi\equiv\phi_L-\phi_R$ is the phase difference between the two superconductors. The self-consistent equation for γ is

$$\frac{1}{2U}-2T\sum_{\omega>0}\frac{2\omega^2[1+a(\omega)]^2-A(\omega)}{A^2(\omega)+4\gamma^2\omega^2[1+a(\omega)]^2}=0. \quad (16)$$

Once the solutions are defined we can calculate the current $J=(2e/\hbar)\partial F/\partial\phi$ and the impurity occupancy $n=\partial F/\partial\epsilon_0$,

$$J=-(2e/\hbar)\sin(\phi)T\sum_{\omega>0}\frac{|\Delta|^2b^2(\omega)A(\omega)}{A^2(\omega)+4\gamma^2\omega^2[1+a(\omega)]^2}, \quad (17)$$

$$n=1-4T\sum_{\omega>0}\frac{\tilde{\epsilon}A(\omega)}{A^2(\omega)+4\gamma^2\omega^2[1+a(\omega)]^2}. \quad (18)$$

We now analyze the main results of the present study. All the parameters having the dimension of energy (ϵ,U,Γ,T) are expressed in units of $|\Delta|$ and the current is given in units of $|\Delta|e/\hbar$. In Figs. 2(a),2(b) the current is displayed versus temperature in the low-temperature region and for coupling strengths Γ ranging between 0.001 and 0.0882. At small Hubbard interaction [$U=2.1$, Fig. 2(a)] the junction is in a π state for which the current (within the present geometry of

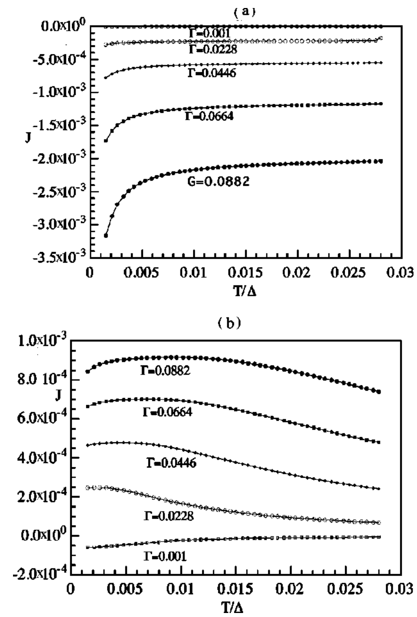

FIG. 2. Dependence of the Josephson current on temperature for $U=2.1$ (a) and $U=3.0$ (b) for different transparencies Γ. Note the sign reversal for strong U. Here $\epsilon_0=-2.0$ and $\phi=\pi/12$ are fixed. The units of all quantities are explained in the text.

the tunneling direction) is negative. At higher values of U [Fig. 2(b)] the pattern is inverted: The current for most coupling strengths is now positive and the π junction is transformed into a 0 junction. The current is strongly dependent on temperature, which is rather distinct from the classical Ambegaokar-Baratoff formula. It is typical for superconducting systems for which the zero energy midgap bound state plays the major role. A similar situation takes place also in s-wave superconductors,[12,14] where it is attributed to the single occupancy of the impurity which then becomes a degenerate magnetic moment. We have thus presented another example for this scenario, though the temperature dependence is quite different.

Now let us discuss the behavior of the current $J(\phi)$ as function of the phase difference as displayed in Figs. 3(a),3(b) for fixed $U=2.6$ and $T=0.01$ and for numerous transparencies Γ. First we fix the transparency to be relatively low ($\Gamma=0.0446$) and plot both the current and the dot occupancy. Remarkably, the corresponding curves are not continuous with jumps at certain values of ϕ [Fig. 3(a)]. These jumps are in one to one correspondence with points at which the dot occupation changes abruptly. Between these points the occupation is nearly constant and the impurity is virtually incompressible. This remarkable behavior in which a Josephson current undergoes a discontinuous sign change was noticed also for s-wave superconductors albeit for large transparency $\Gamma=1$ [see Fig. 2(b) in Ref. 14]. In contrast, for p-wave superconductors the effect is pronounced at smaller Γ, being strongly influenced by the zero-energy state.

Next we consider in Fig. 3(b) the case of slightly higher transparencies $\Gamma=0.1-0.5$. In this case the curves are continuous but deviate significantly from the classical $\sin\phi$ behavior. In particular there is a sign change [Fig. 3(b)], of the current as a function of phase difference $0<\phi<\pi$. This feature is more pronounced at low transparencies $\Gamma<0.3$. Such deviation is not expected in superconductors with s-wave

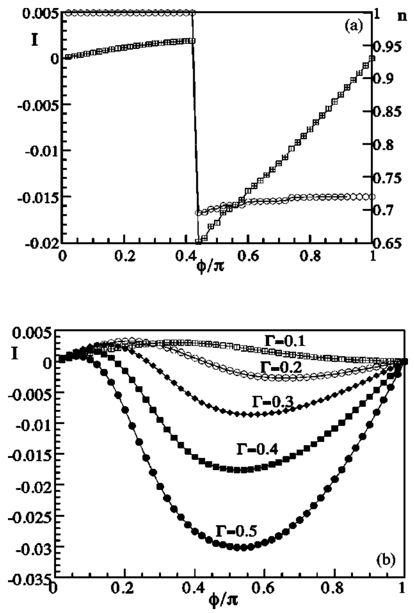

FIG. 3. (a) Dependence of the Josephson current (squares, left scale) and occupancy (circles, right scale) on the phase difference for $\Gamma=0.0446$. The other parameters are $\epsilon_0=-2.0$, $T=0.01$, and $U=2.6$. (b) Dependence of the Josephson current for larger transparencies $\Gamma=0.1-0.5$. The other parameters are as in (a).

symmetry and is again related to the midgap state which is the hallmark of unconventional superconductors in contact with an interacting quantum dot.

Evidently, a deviation from $\sin\phi$ behavior should manifest itself also in current-voltage characteristics, when the flowing current I satisfies the inequality $I>J_c\equiv\max|J(\phi)|$. Within the framework of the resistivity shunted junction model the averaged voltage $\overline{V}$ across the junction is related to the current I and the resistance R as

$$R=\overline{V}\int_0^{2\pi}\frac{d\phi}{2\pi[I-J(\phi)]}. \tag{19}$$

We then expect a deviation of the $\overline{V}(I)$ characteristics from its classical expression $I=\sqrt{J_c^2+(\overline{V}/R)^2}$. It can indeed be seen in Fig. 4 where the difference is mainly exhibited at low voltage.

To summarize, we have solved the problem of transport between two unconventional superconductors through an impurity and traced the dependence of the current on temperature, Coulomb interaction barrier transparency and phase of condensates. The essentially nonperturbative, self-consistent approach we have used yields a finite value for the current without adding relaxation terms that should be included if perturbation approach is adopted. It is mandatory at this final stage to point out the peculiarities related to the physics of non-s-wave superconductors.

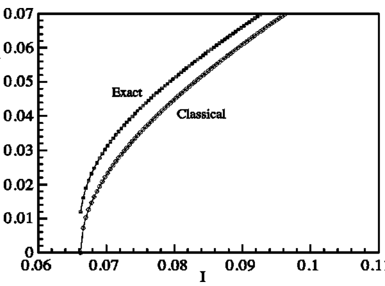

FIG. 4. $V(I)$ characteristics of the p wave junction (upper curve) compared with the classical square root expression (lower curve). The relevant parameters are $\epsilon_0=-2.0$, $U=3.0$, $T=0.01$, and $\Gamma=0.66$.

(1) The contribution to the current in our case originates principally from the surface bound state which is related to the asymmetry of the pair potential, and has no analog for s-wave superconductors. The contribution of this state in low transparency junctions results in a large current, that is, $|J_p/J_s|\sim\sqrt{\Delta/\Gamma}$. It is also marked by a stronger temperature dependence especially at low temperatures.

(2) For unconventional superconductors, the Josephson tunneling through an interacting quantum dot can serve as an indicator to distinguish odd parity superconductors from even parity ones. It might be difficult to fabricate junctions whose superconducting electrodes have the required specific symmetry, but such technical problem might be solved in the near future. Superconductors with both p and d-wave symmetry of the order parameter have surface bound state which contributes to the current (mainly at low temperatures). Yet, as we indicated above, for even-symmetry (d-wave) superconductors, the current vanishes in the limit of pointlike impurity. In sharp distinction, under the same conditions, the current is maximal for odd-symmetry (p-wave) superconductors.

This research is supported by grants from the Israeli Science Foundation (Center of Excellence and Non-Linear Tunneling), The German-Israeli DIP foundation, and the US-Israel BSF foundation.

*Electronic address: yshai@bgumail.bgu.ac.il
†Electronic address: agolub@bgumail.bgu.ac.il
[1] C. R. Hu, Phys. Rev. Lett. **72**, 1526 (1994).
[2] Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. **74**, 3451 (1995).
[3] Yu.S. Barash, H. Burkhardt, and D. Rainer, Phys. Rev. Lett. **77**, 4070 (1996).
[4] Y. Tanaka and S. Kashiwaya, Phys. Rev. B **56**, 892 (1997).
[5] M.P. Samanta and S. Datta, Phys. Rev. B **55**, 8689 (1997).
[6] R.A. Riedel and P.F. Bagwell, Phys. Rev. B **57**, 6084 (1998).
[7] D.J. Van Harlingen, Rev. Mod. Phys. **67**, 515 (1995).
[8] Y. Maeno *et al.*, Nature (London) **372**, 532 (1994).
[9] T.M. Rice and M. Sigrist, J. Phys.: Condens. Matter **7**, L643 (1995).
[10] H. Shiba and T. Soda, Prog. Theor. Phys. **41**, 25 (1969).
[11] L.I. Glazman and K.A. Matveev, Pis'ma Zh. Éksp. Teor. Fiz. **49**, 570 (1989) [JETP Lett. **49**, 659 (1989)].
[12] B. I. Spivak and S.A. Kivelson, Phys. Rev. B **43**, 3740 (1991).
[13] A.A. Golub, Phys. Rev. B **54**, 3640 (1996).
[14] A.V. Rozhkov and D.P. Arovas, Phys. Rev. Lett. **82**, 2788 (1999).
[15] Y. Tanaka, T. Hirari, K. Kusakabe, and S. Kashiwaya, Phys. Rev. B **60**, 6308 (1999).
[16] A. Yazdani *et al.*, Phys. Rev. Lett. **83**, 176 (1999).