Low-Temperature Anomaly in the Josephson Critical Current of Junctions in d-Wave Superconductors

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We show that the Josephson critical current increases rapidly with decreasing temperature near $T = 0$ for tunnel junctions between anisotropic superconductors. The enhancement of the critical current has its physical origin in the midgap states bound to the tunnel barrier. The magnitude of the zero-temperature peak in a realistic junction is shown to be sensitive to the barrier transparency and barrier roughness. For some crystal orientations we find a transition from a traditional 0 junction to the unconventional π junction with decreasing temperature. [S0031-9007(96)01570-0]

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Measurements of the dc Josephson effect give valuable information on the symmetry of the order parameter. The most important experimental tests for this symmetry are quantum phase interference experiments [1–5] which probe, in special junction arrangements, directly the unconventional symmetries of the order parameter. Here, we discuss another class of anomalies in Josephson junctions. These anomalies should be observable in single Josephson junctions, and reflect sign changes of the order parameter on the Fermi surface. Such sign changes are typical for anisotropic superconductors with unconventional pairing.

A distinctive feature of anisotropic superconductors is their sensitivity to inhomogeneities and interfaces [4,6–9]. Quasiparticle scattering at interfaces distorts the order parameter and influences the Josephson effect as well as the quasiparticle tunneling current. Of particular importance are zero-energy bound states (midgap states) at surfaces and interfaces [7–13]. These states are a robust phenomenon of quite general origin [14]. In this paper we study anomalies in the Josephson critical current [15], in particular, their dependence on the barrier roughness. The anomalies are a direct consequence of the zero-energy bound states, and include a rapid increase of the critical current with decreasing temperature near $T = 0$, a crossover from a traditional Josephson junction (0 junction) to a π junction at a critical temperature $T_{0\pi}$, and a critical current that vanishes at $T_{0\pi}$.

To derive these results we start from Eilenberger's equations for the quasiclassical propagator $\hat{g}$ [16], which describes the physical properties of quasiparticle excitations in thermal equilibrium. Eilenberger's equations have the 2×2 matrix form [17],

$$[i\varepsilon_n \hat{\tau}_3 - \hat{\Delta}(\boldsymbol{p}_f, \boldsymbol{R}), \hat{g}(\boldsymbol{p}_f, \boldsymbol{R}; \varepsilon_n)] + i\boldsymbol{v} \cdot \boldsymbol{\nabla}_{\boldsymbol{R}} \hat{g}(\boldsymbol{p}_f, \boldsymbol{R}; \varepsilon_n) = 0\,, \quad (1)$$

$$\hat{g}^2(\boldsymbol{p}_f, \boldsymbol{R}; \varepsilon_n) = -\pi^2 \hat{1}\,, \quad (2)$$

where $\varepsilon_n = (2n + 1)\pi T$ are the Matsubara energies, $\boldsymbol{p}_f$ is the momentum on the Fermi surface, $\boldsymbol{v}$ the Fermi velocity, and $\hat{\Delta}$ the order parameter matrix. Following standard notations we use a "hat" to indicate matrices in Nambu space. A convenient basis set of Nambu matrices is the unit matrix $\hat{1}$ and the three Pauli matrices $\hat{\tau}_1$, $\hat{\tau}_2$, $\hat{\tau}_3$. The propagator $\hat{g}$ and the order parameter matrix $\hat{\Delta}$ have the form $\hat{g} = g\hat{\tau}_3 + if_1\hat{\tau}_2 + f_2\hat{\tau}_1$, and $\hat{\Delta} = i\,\mathrm{Re}[\Delta(\boldsymbol{p}_f, \boldsymbol{R})]\hat{\tau}_2 + i\,\mathrm{Im}[\Delta(\boldsymbol{p}_f, \boldsymbol{R})]\hat{\tau}_1$, where $\Delta(\boldsymbol{p}_f, \boldsymbol{R})$ is the order parameter for singlet pairing.

Interfaces are barriers that reflect and transmit quasiparticles and, in general, change their momentum, energy, and spin. An interface enters the quasiclassical theory as a boundary condition [18,19] that relates the quasiclassical propagators $\hat{g}$ on either side of the barrier. The boundary conditions depend on the type and quality of the barrier. An ideal interface (no roughness) will conserve the parallel momentum of an incoming quasiparticle in a reflection [probability $R(\boldsymbol{p}_f)$] and a transmission process [probability $D(\boldsymbol{p}_f) = 1 - R(\boldsymbol{p}_f)$]. The reflection and transmission probabilities depend, in general, on the momentum $\boldsymbol{p}_f$ of the incoming quasiparticle. The boundary conditions at an ideal interface are given by Zaitsev's relations (see Refs. [18,19]), which reduce in the limit of zero transparency to [20]

$$\hat{g}(\boldsymbol{p}_f) = \hat{g}(\underline{\boldsymbol{p}}_f)\,, \quad (3)$$

where the propagators are taken at the metal-insulator boundary, and $\boldsymbol{p}_f, \underline{\boldsymbol{p}}_f$ are the pair of incoming and outgoing momenta.

We first consider a weakly transparent, ideal barrier. This model can be solved analytically by using results derived recently in Ref. [4], which we now summarize. As in Ref. [4], we assume that for a zero-transparency barrier [$D(\boldsymbol{p}_f) = 0$] the order parameter Δ has a fixed, spatially constant phase on each side of the junction. This leads, in first order in the transparency D, to a sinusoidal current phase relation, $j_S = j_c \sin\varphi$, and to the following expression for the critical current in terms of the off-diagonal propagators f_1 and f_2,

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$$j_c = \frac{eN_f^l T}{\pi} \sum_n \langle D(\boldsymbol{p}_f^l) v_x^l(\boldsymbol{p}_f^l) [f_1^l(\boldsymbol{p}_f^l) f_1^r(\boldsymbol{p}_f^r) - f_2^l(\boldsymbol{p}_f^l) f_2^r(\boldsymbol{p}_f^r)] \rangle_{p_{f,x}>0} , \quad (4)$$

where the superscript l (r) labels the left (right) superconducting electrode, $\boldsymbol{p}_f^l$ is the incident and $\boldsymbol{p}_f^r$ the transmitted momentum, N_f^l is the normal density of states at the Fermi energy, and $\langle \cdots \rangle_{p_{f,x}>0}$ means averaging over quasiparticle states at the Fermi surface with $p_{f,x} > 0$.

We now analyze the situation that zero-energy bound states exist on both sides of the barrier for a given trajectory with incident momentum $\boldsymbol{p}_f$. The corresponding singular part of the propagator has a pole term (denoted by an index s), $g_s(\boldsymbol{p}_f, \varepsilon_n) = -iB(\boldsymbol{p}_f)/\varepsilon_n$. The coefficient $B(\boldsymbol{p}_f)$ has been discussed recently in [13], where it is shown that the zero-energy singularity appears in the diagonal components $g(\boldsymbol{p}_f, \varepsilon_n)$ of the Nambu matrix propagator, in its off-diagonal component $f_2(\boldsymbol{p}_f, \varepsilon_n)$, but not in $f_1(\boldsymbol{p}_f, \varepsilon_n)$. The normalization condition (2) then leads to the relation $g_s^2(\boldsymbol{p}_f, \varepsilon_n) = -f_{2,s}^2(\boldsymbol{p}_f, \varepsilon_n) = -B^2(\boldsymbol{p}_f)/\varepsilon_n^2$.

At low enough temperatures the singularity at zero energy dominates the dc Josephson effect, and the contributions from regular parts can be discarded. The significant increase of the singular terms at low energies leads to two remarkable phenomena: a low-temperature peak in the Josephson critical current (with a maximum at $T = 0$), and a phase transition from a 0-junction state to a π junction at a temperature $T_{0\pi}$. We first discuss two simple physical situations which are expected to show these phenomena. We consider junctions with identical (anisotropic) superconductors. The first is a symmetric tunnel junction (STJ) with superconducting states of the same orientation in both electrodes ($\alpha_l = \alpha_r$). The second is a "mirror" tunnel junction (MTJ) for which the barrier is a reflection-symmetry plane of the superconducting electrodes ($\alpha_l = -\alpha_r$). The angles α_l and α_r describe the orientation of the order parameters on the left and right sides of the junction. For a definition of the angles α_l and α_r see Fig. 1. In both the STJ and MTJ cases the momentum directions of incident $\boldsymbol{p}_f^l$ and transmitted $\boldsymbol{p}_f^r$ quasiparticles are the same. It is essential for further analysis that the singular parts of the propagators $f_{1,s}(\boldsymbol{p}_f)$, $f_{2,s}(\boldsymbol{p}_f)$ at the boundary are odd functions of the momentum direction, while $g_s(\boldsymbol{p}_f)$ and the order parameter are even. Indeed, according to Ref. [13], one has $f_{1,s}(\boldsymbol{p}_f, \varepsilon_n) = 0$ and $f_{2,s}(\boldsymbol{p}_f, \varepsilon_n) = -i\,\mathrm{sgn}[v_x \Delta_\infty(\boldsymbol{p}_f)] g_s(\boldsymbol{p}_f, \varepsilon_n)$, and the change in sign upon reversing $\boldsymbol{p}_f$ follows from the change in sign of v_x. For the STJ one obtains directly $g_s^l(\boldsymbol{p}_f^l, \varepsilon_n) = g_s^r(\boldsymbol{p}_f^r, \varepsilon_n)$, $f_{1,s}^l(\boldsymbol{p}_f^l, \varepsilon_n) = f_{1,s}^r(\boldsymbol{p}_f^r, \varepsilon_n) = 0$, and $f_{2,s}^l(\boldsymbol{p}_f^l, \varepsilon_n) = -f_{2,s}^r(\boldsymbol{p}_f^r, \varepsilon_n)$. The different signs of the f functions on the left and right sides of the interface are a consequence of the trajectory changing from "incoming" to "outgoing" when crossing the interface. The symmetry of an MTJ guarantees the equality of the propagators along trajectories obtained by reflection at the barrier plane. This implies, together with the boundary condition (3), the relations $g_s^l(\boldsymbol{p}_f^l) = g_s^r(\boldsymbol{p}_f^r)$, $f_{1,s}^l(\boldsymbol{p}_f^l) = f_{1,s}^r(\boldsymbol{p}_f^r) = 0$, and $f_{2,s}^l(\boldsymbol{p}_f^l) = f_{2,s}^r(\boldsymbol{p}_f^r)$. Thus, we find at low temperatures, $f_1^l(\boldsymbol{p}_f^l, \varepsilon_n) f_1^r(\boldsymbol{p}_f^r, \varepsilon_n) - f_2^l(\boldsymbol{p}_f^l, \varepsilon_n) f_2^r(\boldsymbol{p}_f^r, \varepsilon_n) \simeq \pm[f_2^l(\boldsymbol{p}_f^l, \varepsilon_n)]^2 \simeq \pm B^2(\boldsymbol{p}_f^l)/\varepsilon_n^2$, and obtain from Eq. (4) the following expression for the Josephson critical current at low temperatures,

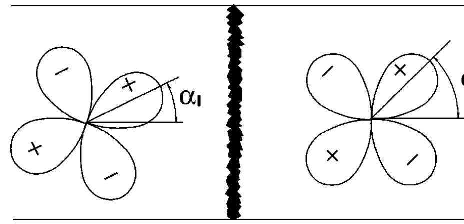

FIG. 1. Schematic geometry of our junction. The clover-shaped d-wave order parameter is fixed to the crystal lattice. The angles α_l and α_r are defined as the angles between the normal of the interface and the crystal lattice on the left and right sides, respectively.

$$j_c = \pm \frac{eN_f^l}{4\pi T} \langle D(\boldsymbol{p}_f^l) v_x^l(\boldsymbol{p}_f^l) B^2(\boldsymbol{p}_f^l) \rangle_{p_{f,x}>0} . \quad (5)$$

The plus (minus) sign corresponds here to the STJ (MTJ). According to this formula, the Josephson critical current is inversely proportional to the temperature and diverges in the limit $T \to 0$. This divergence is obviously the consequence of the presence of the zero-energy delta peak in the quasiparticle density of states on both sides of the junction. A zero-energy bound state only on one side does not lead to singular terms in j_c, because the function f_2 vanishes for the side without zero-energy bound states.

The Josephson critical current of junctions with anisotropic superconductors has been discussed for $T \approx T_c$ in Ref. [4]. The authors obtain in second order in the order parameter Δ the Josephson critical current,

$$j_c = 4\pi e N_f^l T \sum_n \langle D(\boldsymbol{p}_f^l) v_x^l(\boldsymbol{p}_f^l) \times I_l(\boldsymbol{p}_f^l, \varepsilon_n) I_r(\boldsymbol{p}_f^r, \varepsilon_n) \rangle_{p_{f,x}>0} , \quad (6)$$

where

$$I_{l(r)}(\boldsymbol{p}_f^{l(r)}, \varepsilon_n) = \frac{1}{|v_x^{l(r)}|} \int_0^\infty \Delta_{l(r)}(\boldsymbol{p}_f^{l(r)}, x) \times \exp\left(-\left| \frac{2\varepsilon_n}{v_x^{l(r)}} \right| x \right) dx , \quad (7)$$

and x is the distance from the interface. A comparison of Eqs. (5) and (6) for the STJ shows that the Josephson critical currents have near T_c and at low temperatures the same sign. On the other hand, the signs of Eqs. (5) and (6) are different in MTJ's for certain ranges of crystal orientations. This then implies a change in the junction characteristic from a π junction at low temperatures to a 0 junction near T_c. If one rotates a d-wave superconductor on one side of the junction over the angle $\pi/2$, e.g., $\alpha_l \rightarrow \alpha_l + \pi/2$, the junction characteristic is obviously interchanged. All our results obtained so far are valid for any kind of anisotropic singlet superconductors, provided the order parameter changes its sign on the Fermi surface. Hence, the observation of our main results, the low-temperature peak effect in the Josephson critical current and the $0 - \pi$ phase transition, would give evidence of the change of sign of the order parameter on the Fermi surface.

In the following, we consider special orientations of the order parameter, which lead to the anomalies described above. We consider two identical d-wave superconductors with the basis functions of type $p_x^2 - p_y^2$ and cylindrical Fermi surfaces with the cylindrical axes parallel to the barrier plane on both sides of the junction. For the junction with a reflection-symmetry plane (MTJ) the angle α between the normal to the boundary and the crystalline axis is, in fact, the misorientation angle. According to (5), the critical current j_c has negative sign at low temperatures. As a function of α, $|j_c|$ has its maximum for $\alpha = 45°$, diminishes when α moves off from this value, and vanishes for $\alpha = 0, \pi/2$ (in accordance with the fraction of trajectories along which the order parameter changes its sign under the specular reflection from the boundary). The sign of j_c near T_c depends in the case of MTJ's on the misorientation angle and, generally speaking, on the particular type of pairing. Indeed, the order parameters entering Eqs. (6) and (7) are $\Delta_l(\boldsymbol{p}_f^l, x) = \eta_l(|x|)\cos[2(\phi + \alpha)]$, $\Delta_r(\boldsymbol{p}_f^r, x) = \eta_r(|x|)\cos[2(\phi - \alpha)]$. Here, the angle ϕ describes the quasiparticle trajectory (the direction of the incident momentum relative to the normal to the boundary) and $\eta_{l(r)}(x)$ are functions, which may be determined from the Ginzburg-Landau equations including boundary conditions at the interface. One finds a positive critical current near T_c for $\alpha = 0$ and negative one for $\alpha = 45°$. The critical current has its maximum for $\alpha = 0$ and is comparatively small at $\alpha = 45°$ due to the suppression of $\eta_{l(r)}(x)$ at the boundary [4]. For intermediate values of α the actual sign of j_c must be determined by explicit integration over the angle ϕ in (6). We take, for simplicity, a standard reflection law, $D(\boldsymbol{p}_f^l) \propto (v_x^l)^2 \propto \cos^2\phi$, and find near T_c a positive critical current (6) for $|\alpha| < \alpha_0 = 23.7°$ and sign changes for larger $|\alpha|$'s. So, for the MTJ the $0 - \pi$ phase transition has to take place at some temperature $T = T_{0\pi}$ for misorientation angles $|\alpha| < \alpha_0$.

The above considerations lead to quantitative results for the critical Josephson current at low temperatures and near T_c, and to a qualitative understanding at intermediate temperatures. In order to obtain the critical Josephson current in the whole temperature range numerical calculations are indispensable. We solve for this purpose the system of equations (1) and (2), combined with Zaitsev's boundary conditions at the interface, and the self-consistency equation for the order parameter. We use a cylindrical Fermi surface with an isotropic Fermi velocity $\boldsymbol{v}$ and a constant normal state density of states N_f. The calculation of $\hat{\Delta}(\boldsymbol{p}_f, \boldsymbol{R})$ involves the pairing interaction $V(\boldsymbol{p}_f, \boldsymbol{p}_f')$ which we write in the case of a d-wave superconductor as $V(\boldsymbol{p}_f, \boldsymbol{p}_f') = 2V\cos(2\phi)\cos(2\phi')$. In Fig. 2 we present the numerical results for a weakly transparent, ideal MTJ ($R_0 = 0.99$). We find a sign change of the critical current in a region $0° < \alpha \leq 25°$. The critical current seems to diverge for all angles besides $\alpha = 0°$. The inset of Fig. 2 shows results for the STJ for the same misorientation angles α as for the MTJ. No sign change of the critical current is observed in this case. The low-temperature peak actually does not diverge but is limited due to the finite transparency of the interface which is not taken into account by our previous analysis but included in our numerical calculations.

In realistic systems the zero-energy bound states are broadened due to the roughness of the interface, and as a consequence the (negative) contribution of the zero-energy bound states to the critical current is reduced. In order to study the effects of interface roughness we generalize Ovchinnikov's model for rough surfaces [21] to rough interfaces [22]. We coat both sides of an ideal interface by Ovchinnikov's thin dirty layer. The degree of roughness is measured by the ratio $\rho_0 = d/\ell$ [23], where d is the thickness of the layer, and ℓ the mean free path in the layer. In Fig. 3 we plot the temperature dependence of the critical current for a slightly rough MTJ ($R_0 = 0.99$, $\rho_0 = 0.1$) for the same tilt angles as in Fig. 2. The sign change of the critical current is removed for small misorientation angles and is now limited to the region $15° \leq \alpha \leq 25°$. The inset of Fig. 3 shows the critical current for $\alpha = 25°$ for different degrees of roughness,

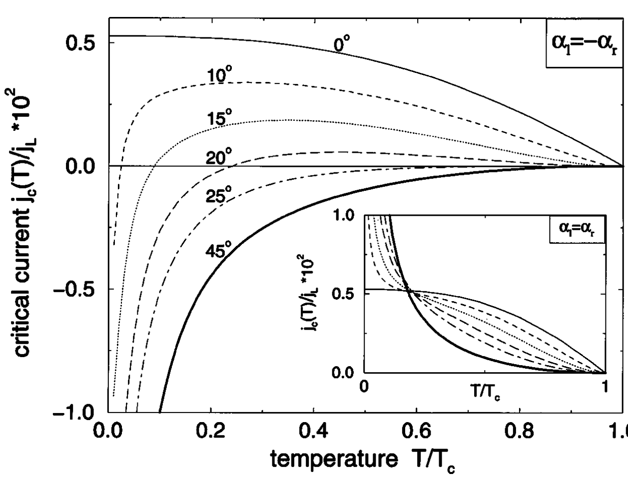

FIG. 2. Temperature dependence of the critical current of an MTJ with a weakly transparent smooth interface ($R_0 = 0.99$, $\rho_0 = 0$) for different misorientation angles ($\alpha_l = 0°$–$45°$). Inset: The same but for an STJ.

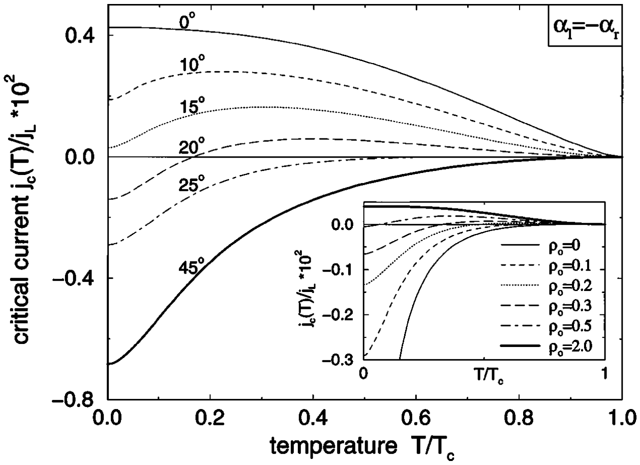

FIG. 3. Critical current as a function of temperature for an MTJ with a weakly transparent slightly rough interface ($R_0 = 0.99$, $\rho_0 = 0.1$) for different orientations of the two superconductors ($\alpha_l = 0°-45°$). Inset: The same but for a fixed misorientation angle ($\alpha_l = -\alpha_r = 25°$) and different degrees of roughness.

i.e., different values of ρ_0. With increasing roughness the anomalous temperature dependence of the critical current is more and more suppressed, and the maximum seen for special geometries flattens out. The critical current is normalized in all figures by $j_L = evN_f\Delta_0$ ($\Delta_0 = 1.76T_c$) which is the Landau critical current at $T = 0$ for an s-wave superconductor with the same critical temperature as our d-wave superconductor.

For $\alpha = 0°$ we find no anomaly because there are no zero-energy bound states at the interface. With increasing misorientation angle α more and more bound states appear. In the case of an MTJ they give a negative contribution to the critical current and become important especially at low temperatures. This leads to a sign change of the critical current with decreasing temperature. This sign change disappears at angles between 20° and 25° for a smooth interface as predicted by our analytical considerations. For 45° the order parameter changes sign along all trajectories of incoming quasiparticles. In this case there are zero-energy bound states for all Fermi momenta $\boldsymbol{p}_f$ and the divergence of the critical current is most pronounced.

In summary, we have discussed the temperature dependence of the Josephson critical current for d-wave superconductors. Analytical calculations show that the zero-energy bound states at the interface are responsible for anomalies of the temperature dependent critical current. These anomalies should be measurable in junctions of high quality, and for properly oriented superconducting electrodes.

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