Theory of the Josephson effect in *d*-wave superconductors

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A general formula for the Josephson current in a *d*-wave/insulator/*d*-wave-superconductor junction is presented by taking account of the zero-energy states formed around the interfaces. For a fixed phase difference between the two superconductors, the current component becomes either positive or negative depending on the injection angle of the quasiparticle. Anomalous temperature dependences are predicted in the maximum Josephson current and in the free-energy minima.

The Josephson effect for *d*-wave superconductors has recently emerged as one of the important issues in high-T_c superconductor physics. Sigrist and Rice predicted that the macroscopic phase difference (φ) between the two superconductors which gives the free-energy minimum is located either at $\varphi=0$ or at $\varphi=\pi$ (π junctions) when a Josephson junction involves *d*-wave superconductors.[1] Their phenomenological theory explained the anomalous magnetization experiment in terms of the spontaneous current in the superconducting loop.[2] Stimulated by the theoretical work, several experiments were performed in an attempt to observe the π junction and half flux quanta in high-T_c superconductors. The results strongly suggest *d*-wave symmetry in the pair potential in this material.[3–5] On the other hand, it has been clarified that zero-energy bound states are formed around the surface of the *d*-wave superconductor because the quasiparticle experiences different signs of pair potential depending on the direction of its motion.[6–9] The zero-energy states (ZES's) are detectable in conductance spectra of a normal-metal/insulator/*d*-wave-superconductor junction, and are actually observed in experiments.[9,10] Recently, several theories for Josephson junctions comprising *d*-wave superconductors were presented.[11–17] However, all these theories do not consider the effect of ZES's formed at the interfaces, seriously. It is necessary to include this effect, since the Josephson current is carried by the bound states as shown in the study of the *s*-wave/insulator/*s*-wave-superconductor ($s/I/s$) junctions.[18–20]

In this paper, based on a Green's function method,[21] the Josephson current in a *d*-wave/insulator/*d*-wave-superconductor ($d/I/d$) junction is calculated by taking into account the anisotropy of the pair potentials explicitly. This formula naturally includes the effect of ZES's and is consistent with existing theories of Josephson junctions. For some range of orientational angles with a fixed φ, the current component becomes either positive or negative depending on the injection angle of the quasiparticle. Each component has a different temperature dependence. This results in an anomalous temperature dependence of the maximum Josephson current and free-energy minima especially at low temperatures.

For the calculation, we assume a two-dimensional $d/I/d$ Josephson junction in the clean limit. The material parameters of the two superconductors are chosen to be equal. The flat interfaces are perpendicular to the x axis, and are located at $x=0$ and $x=d_i$, respectively. The insulator is assumed to have a square barrier potential with a height U_0 and a thickness d_i. We introduce two parameters $\lambda_0=\sqrt{2mU_0/\hbar^2}$ and $\kappa=\kappa_F/\lambda_0$, where k_F is the Fermi wave number in the superconductor. The wave function of the quasiparticles in inhomogeneous anisotropic singlet superconductors is given by the solution of the Bogoliubov equation. This equation includes a nonlocal pair potential with two position coordinates for the Cooper pairs. Under the semiclassical approximation and in the weak-coupling limit, the effective pair potential reduces to $\Delta(\gamma,\boldsymbol{r})$, where $\boldsymbol{r}$ is the position and γ is the direction of motion of the quasiparticles.[22,23] The quantity γ satisfies $\exp(i\gamma)\equiv\boldsymbol{k}_x/k_F+i\boldsymbol{k}_y/k_F$ where $\boldsymbol{k}$ is the wave vector of the quasiparticle ($|\boldsymbol{k}|=k_F$). Although the pair breaking effect is expected at the interface,[13,23] we assume, for simplicity, that the effective pair potential $\Delta(\gamma,\boldsymbol{r})$ is given by $\Delta(T)\cos[2(\gamma-\alpha)]\exp(i\varphi_L)$ for $x<0$ and $\Delta(T)\cos[2\gamma$

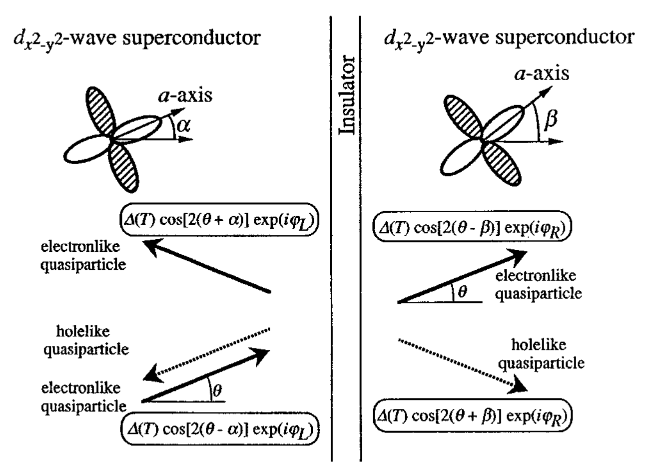

FIG. 1. Schematic illustration of reflection and transmission of quasiparticles at the interface. ELQ and HLQ stand for electronlike quasiparticle and holelike quasiparticle, respectively. The ELQ's are injected from the left hand side.

$-\alpha)]\exp(i\varphi_R)$, for $x>d_i$, where $\alpha(\beta)$ is the angle between the normal to the interface and the α axis of the left (right) superconductor. The macroscopic phase φ_L (φ_R) of the left (right) superconductor is measured from the normal to the interface of the left superconductor. The temperature dependence of the magnitude of the pair potential $\Delta(T)$ is assumed to obey the BCS relation.

When a quasiparticle is injected from the left superconductor at an angle θ to the interface normal, four different effective pair potentials participate in this elementary process (Fig. 1). This idea is the most essential part of our calculation. The four potentials are $\bar{\Delta}_L(\theta_\pm)=\Delta(T)\cos[2(\theta_\pm-\alpha)]$ and $\bar{\Delta}_R(\theta_\pm)=\Delta(T)\cos[2(\theta_\pm-\beta)]$ with $\theta_+=\theta$ and $\theta_-=\pi-\theta$, where the momentum component parallel to the interfaces is conserved. By extending the previous theory[19] to include the anisotropy of the pair potentials, the Josephson current $I(\varphi)$ is given by

$$R_N I(\varphi)=\frac{\pi\bar{R}_N k_B T}{e}\left\{\sum_{\omega_n}\int_{-\pi/2}^{\pi/2}\left[\frac{a_1(\theta,i\omega_n,\varphi)}{\Omega_{L,+}}|\bar{\Delta}_L(\theta_+)|-\frac{\tilde{a}_1(\theta,i\omega_n,\varphi)}{\Omega_{L,-}}|\bar{\Delta}_L(\theta_-)|\right]\cos\theta\, d\theta\right\}, \tag{1}$$

where $\Omega_{n,L,\pm}=\sqrt{\bar{\Delta}_L^2(\theta_\pm)+\omega_n^2}$ and $\varphi=\varphi_L-\varphi_R$. The quantity R_N denotes the normal resistance and $\bar{R}_N$ is expressed as

$$\bar{R}_N^{-1}=\int_{-\pi/2}^{\pi/2}\sigma_N\cos\theta\, d\theta,\quad \sigma_N=\frac{4Z_\theta^2}{(1-Z_\theta^2)^2\sinh^2(\lambda d_i)+4Z_\theta^2\cosh^2(\lambda d_i)}$$

$$\lambda=(1-\kappa^2\cos^2\theta)^{1/2}\lambda_0,\quad Z_\theta=\frac{\kappa\cos\theta}{\sqrt{1-\kappa^2\cos^2\theta}}. \tag{2}$$

Here, σ_N denotes the tunneling conductance for the injected quasiparticle when the junction is in the normal state. The quantity $\omega_n=2\pi k_B T(n+1/2)$ denotes the Matsubara frequency, where analytic continuation is employed for the quasiparticle energy, E, measured relative to the Fermi energy. The Andreev reflection coefficient $a_1(\theta,i\omega_n,\varphi)$ is obtained by solving the Bogoliubov equation, and $\tilde{a}_1(\theta,i\omega_n,\varphi)$ is obtained by substituting $\pi-\theta,-\varphi_L$, and $-\varphi_R$ for θ, φ_L, and φ_R into $a_1(\theta,i\omega_n,\varphi)$, respectively. Straightforward calculation gives

$$R_N I(\varphi)=\frac{\pi\bar{R}_N k_B T}{e}\left\{\sum_{\omega_n}\int_{-\pi/2}^{\pi/2}F(\theta,i\omega_n,\varphi)\sin\varphi\,\sigma_N\cos\theta\, d\theta\right\}, \tag{3}$$

$$F(\theta,i\omega_n,\varphi)=\frac{4\eta_{L,+}\eta_{R,+}[(1-\sigma_N)\Gamma_1(\theta,i\omega_n)\Gamma_2(\theta,i\omega_n)+\sigma_N|\Gamma_3(\theta,i\omega_n,\varphi)|^2]}{|(1-\sigma_N)\Gamma_1(\theta,i\omega_n)\Gamma_2(\theta,i\omega_n)+\sigma_N\Gamma_3(\theta,i\omega_n,\varphi)\Gamma_4(\theta,i\omega_n,\varphi)|^2}, \tag{4}$$

$$\Gamma_1(\theta,i\omega_n)=1+\eta_{L,+}\eta_{L,-},\quad \Gamma_2(\theta,i\omega_n)=1+\eta_{R,+}\eta_{R,-},\ \eta_{L(R),\pm}=\zeta_{L(R),\pm}\frac{\bar{\Delta}_{L,R}(\theta_\pm)}{|\bar{\Delta}_{L,R}(\theta_\pm)|},$$

$$\Gamma_3(\theta,i\omega_n,\varphi)=1+\eta_{L,-}\eta_{R,-}\exp(i\varphi),\quad \Gamma_4(\theta,i\omega_n,\varphi)=1+\eta_{L,+}\eta_{R,+}\exp(-i\varphi), \tag{5}$$

with $\zeta_{L(R),\pm}=|\bar{\Delta}_{L(R)}(\theta_\pm)|/(\omega_n+\Omega_{n,L(R),\pm})$. If we consider the depairing effect of the pair potential at the interface, $\zeta_{L(R)\pm}$ is given by the wave functions at the interfaces. However, other parts of Eq. (4) are not changed. Equation (3) is consistent with the previous formulae for the Josephson current as limiting cases. By substituting a *s*-wave symmetry, it reduces to the formula for the $s/I/s$ junction[19] which includes arbitrary barrier height.[24,25] If we take only the $\theta=0$ component, the magnitude of the Josephson current is proportional to $\cos(2\alpha)\cos(2\beta)$, and the phenomenological theory by Sigrist and Rice[1] is reproduced. When σ_N is set equal to unity, Eq. (3) reproduces recent results for the pinhole geometry by Yip[12] [see Eq. (7) in Ref. 12]. On the other hand, when $\sigma_N\rightarrow 0$ is satisfied, replacing $\eta_{L,-}$ and $\eta_{R,-}$ with $\eta_{L,+}$ and $\eta_{R,+}$ or only taking the $\theta\sim 0$ component in Eq. (3), other previous results are reproduced.[13,22]

Here, we will simply survey the properties of $F(\theta,i\omega_n,\varphi)$. The denominator of $F(\theta,i\omega_n,\varphi)$, which we will refer to as $F_d(\theta,i\omega_n,\varphi)$, implies the formation of bound states at the interface. If we replace $i\omega_n$ with E, the condition $F_d(\theta,E,\varphi)=0$ can be regarded as the linear combination of two types of bound-state conditions. For a high conductance junction ($\sigma_N\rightarrow 1$), the condition $F_d(\theta,E,\varphi)\approx\Gamma_3(\theta,E,\varphi)\Gamma_4(\theta,E,\varphi)=0$ gives the energy levels of bound states formed between the diagonal pair potentials due to the Andreev-reflection process (see Fig. 1). For a low conductance junction ($\varphi_N\rightarrow 0$), the condition $F_d(\theta,E,\varphi)\approx\Gamma_1(\theta,E)\Gamma_2(\theta,E)=0$ gives the energy level of bound states formed around the surfaces of isolated semi-infinite superconductors. The latter bound states become ZES's when $\bar{\Delta}_L(\theta_+)\bar{\Delta}_L(\theta_-)<0$ [$\bar{\Delta}_R(\theta_+)\bar{\Delta}_R(\theta_-)<0$] is satisfied.[6–9] When ZES's exist, the Josephson current rapidly increases with decreasing temperature due to the vanishing of $F_d(\theta,i\omega_n,\varphi)$. On the other hand, the sign of $F(\theta,i\omega_n,\varphi)$ is determined by the numerator, i.e., the sign of

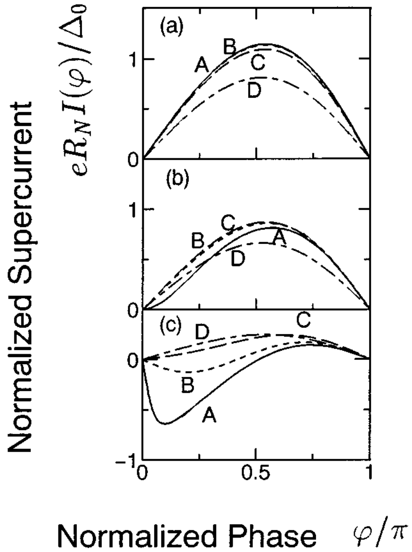

FIG. 2. Josephson current $I(\varphi)$ plotted as a function of φ for $\lambda_0 d_i=1$ and $\kappa=0.5$ with (a) $\alpha=\beta=0$, (b) $\alpha=-\beta=0.05\pi$, and (c) $\alpha=-\beta=0.10\pi$. A: $T/T_d=0.025$, B: $T/T_d=0.15$, C: $T/T_d=0.3$, and D: $T/T_d=0.6$.

$\bar{\Delta}_L(\theta_+)\bar{\Delta}_R(\theta_+)$, independent of temperature. The change of sign of $F(\theta,i\omega_n,\varphi)$ yields a negative current ($-\sin\varphi$) component. This effect results in the shift of the free-energy minimum from $\varphi=0$ which includes the case of the π junction. The total property is determined by the integration of all components weighted by $\sigma_N\cos\theta$.

In the following calculation, the critical temperatures of the two superconductors are tentatively chosen to be $T_d=90$ K$\sim$(7.8 meV/k_B). This particular choice for T_d is not essential. We will denote $\Delta(0)$ by Δ_0. It is sufficient to calculate $I(\varphi)$ for $0<\varphi<\pi$, since $I(\varphi)=-I(-\varphi)$ is satisfied. Figures 2 and 3 show the temperature dependences of the current-phase relation and a maximum Josephson current I_C, respectively, for various $\alpha(=-\beta)$. When $\alpha=0$, $\bar{\Delta}_L(\theta_+)\bar{\Delta}_R(\theta_+)$, $\bar{\Delta}_L(\theta_+)\bar{\Delta}_L(\theta_-)$, and $\bar{\Delta}_R(\theta_+)\bar{\Delta}_R(\theta_-)$ are positive. In this case, $I(\varphi)$ becomes maximum at about $\varphi=\pi/2$ for any temperature, and I_C is a monotonically increasing function with decreasing temperature as shown by Fig. 2(a) and in curve *A* of Fig. 3. Figure 2(b) and curve *B* in Fig. 3 [Fig. 2(c) and curve *C* in Fig. 3] show the results when $\alpha=0.05\pi$ ($\alpha=0.1\pi$). As α and β deviate from zero, $\bar{\Delta}_L(\theta_+)\bar{\Delta}_R(\theta_+)$, $\bar{\Delta}_L(\theta_+)\bar{\Delta}_L(\theta_-)$, and $\bar{\Delta}_R(\theta_+)\bar{\Delta}_R(\theta_-)$ become negative depending on the value of θ. Correspondingly, $I(\varphi)$ deviates from a sinusoidal function, and therefore I_c has a nonmontonous temperature dependence.

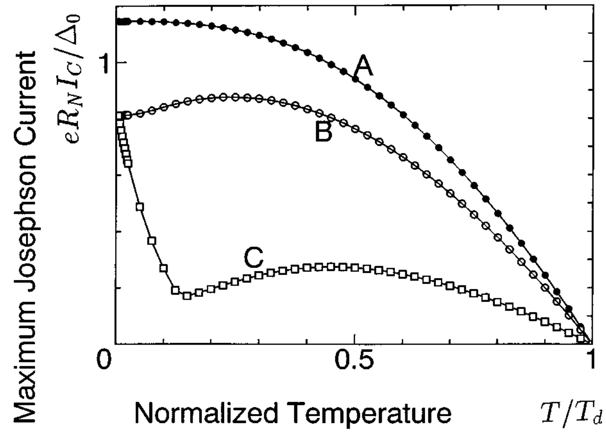

FIG. 3. Maximum Josephson current plotted as a function of temperature for $\lambda_0 d_i=1$ and $\kappa=0.5$. A: $\alpha=\beta=0$, B: $\alpha=-\beta=0.05\pi$, and C: $\alpha=-\beta=0.1\pi$.

To clarify matters, let us decompose $R_N I(\varphi)$ into its negative component $G_n(\varphi)$ and the positive component $G_p(\varphi)$. In the above case, since $\alpha=-\beta$ is satisfied, the quantity $F(\theta,i\omega_n,\varphi)$ becomes negative for $\pm\pi/4-|\alpha|<\theta<\pm\pi/4+|\alpha|$. These conditions happen to coincide with those for the formation of ZES's at the interfaces. The quantity $G_n(\varphi)$ is given by

$$G_n(\varphi)=\frac{\bar{R}_N\pi k_B T}{e}\left\{\sum_{\omega_n}\int_{-\pi/4-\alpha}^{-\pi/4+\alpha}F(\theta,i\omega_n,\varphi)\sigma_N\cos\theta d\theta+\int_{\pi/4-\alpha}^{\pi/4+\alpha}F(\theta,i\omega_n,\varphi)\sigma_N\cos\theta d\theta\right\}\sin\varphi, \tag{6}$$

and $G_p(\varphi)=R_N I(\varphi)-G_n(\varphi)$. We denote the phase difference φ by φ_M, where $I(\varphi)$ gives the maximum Josephson current. For $\sigma_N\to 0$, $G_P(\varphi)$ and $G_n(\varphi)$ can be regarded as the Josephson current in the 0 junction and π junction. In Fig. 4, $|G_n(\varphi_M)|$ and $G_p(\varphi_M)$ are plotted using the same parameters used for curve *C* in Fig. 3. In the inset of Fig. 4, the temperature dependence of φ_M is also plotted. It is clear that $|G_n(\varphi_M)|$ and $G_p(\varphi_M)$ have different temperature dependences. The magnitude of $|G_n(\varphi_M)|$ is drastically enhanced at low temperatures reflecting the divergence of the denominator due to the formation of ZES's. This effect results in the jump of φ_M and the current inversion at T_p($T_p\sim 0.2T_d$), where $|G_n(\varphi_M)|=G_p(\varphi_M)$ is satisfied.

Let us consider the free-energy minima (φ_0), where $I(\varphi)=0$ and the first derivative of $I(\varphi)$ is positive. When $\bar{\Delta}_L(\theta_+)\bar{\Delta}_R(\theta_+)>0$ is satisfied for any θ, φ_0 equals zero for all temperatures (curve *A* in Fig. 5). Conversely, when $\bar{\Delta}_L(\theta_+)\bar{\Delta}_R(\theta_+)<0$ is satisfied for any θ, φ_0 equals π for all temperatures (this corresponds to the π junction, not shown in the figure). When the sign of $\bar{\Delta}_L(\theta_+)\bar{\Delta}_R(\theta_+)$ depends on θ, φ_0 is not constant and can vary between 0 and π. Even in the absence of ZES's, φ_0 can be neither 0 nor π when $\sigma_N\approx 1$ is satisfied as discussed by Yip[12] (curve *B* in Fig. 5). However, the existence of ZES's exaggerates the anomalous temperature dependence of φ_0 (curve *C* in Fig. 5).

In this paper, a generalized formula for the Josephson current in *d/I/d* junctions has been presented fully taking account of the anisotropy of the pair potentials. In the tunneling limit, the Josephson junction can be expressed by the

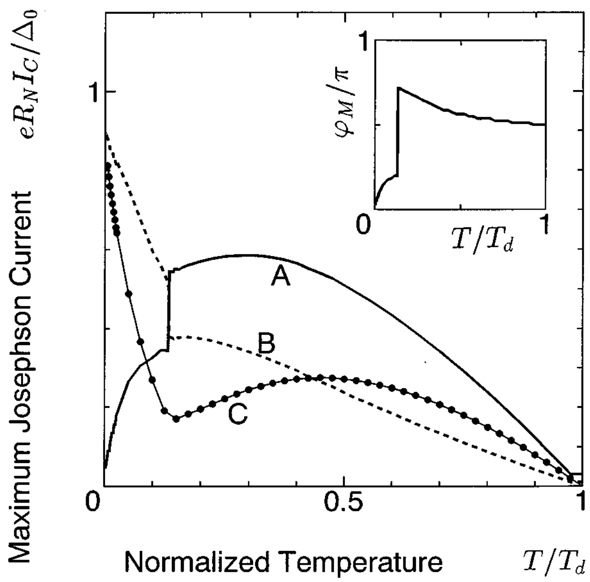

FIG. 4. Positive and negative components of R_NI_C obtained from curve C of Fig. 3 as a function of temperature. A: $G_p(\varphi_M)$, B: $|G_n(\varphi_M)|$, and C: R_NI_C. In the inset φ_M is plotted as a function of temperature.

combination of the 0 junction and π junction. The different temperature dependence of the Josephson current in each junction induces nonmontonous temperature dependence of the Josephson current. The calculated features are completely different from those expected for conventional $s/I/s$ junctions. Similar properties can also be expected for Josephson junctions of other symmetries where the pair potential has the opposite sign for some regions of the Fermi surface.

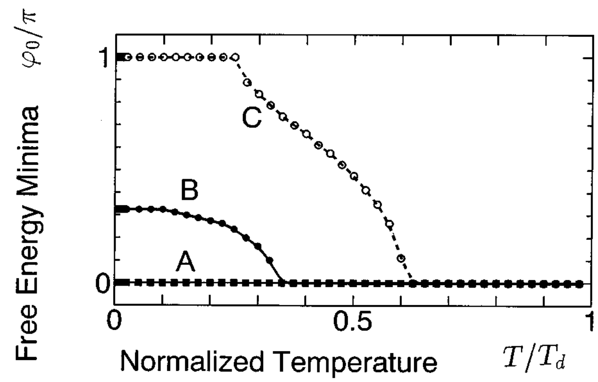

FIG. 5. Position of the free-energy minima φ_0 plotted as a function of temperature. A: $\alpha=\beta=0$, $\lambda_0 d_i=1$, and $\kappa=0.5$, B: $\alpha=-\beta=0.1\pi$, $\lambda_0 d_i=0$, and $\kappa=0.5$, C: $\alpha=-\beta=0.12\pi$, $\lambda_0 d_i=1$, and $\kappa=0.5$.

Throughout this paper, depairing effects in the pair potential around the interface is neglected in the actual numerical calculation. Even if we were to adopt self-consistently obtained pair potentials, the quantitative results would change somewhat, the essence of the present results would not change, since the formation of ZES's would still be expected.[26]

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[1] M. Sigrist and T. M. Rice, J. Phys. Soc. Jpn. **61**, 4283 (1992).
[2] M. Sigrist and T. M. Rice, Rev. Mod. Phys. **67**, 503 (1995).
[3] D. A. Wollman *et al.*, Phys. Rev. Lett. **71**, 2134 (1993).
[4] D. J. Van Harlingen, Rev. Mod. Phys. **67**, 515 (1995).
[5] C. C. Tsuei *et al.*, Phys. Rev. Lett. **73**, 593 (1994).
[6] C. R. Hu, Phys. Rev. Lett. **72**, 1526 (1994).
[7] M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn. **64**, 1703 (1995).
[8] S. Kashiwaya *et al.*, Jpn. J. Appl. Phys. **34**, 4555 (1995); Phys. Rev. B **53**, 2667 (1996).
[9] S. Kashiwaya *et al.*, Phys. Rev. B **51**, 1350 (1995).
[10] Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. **74**, 3451 (1995).
[11] S. Yip, J. Low Temp. Phys. **91**, 203 (1993).
[12] S. Yip, Phys. Rev. B **52**, 3087 (1995).
[13] Yu. S. Barash, A. V. Galaktionov, and A. D. Zaikin, Phys. Rev. B **52**, 665 (1995).
[14] Yu. S. Barash, A. V. Galaktionov, and A. D. Zaikin, Phys. Rev. Lett. **75**, 1676 (1995).
[15] Y. Tanaka, Phys. Rev. Lett. **72**, 3871 (1994); Physica C **235-240**, 3205 (1994).
[16] C. Bruder, A. van Otterlo, and G. T. Zimanyi, Phys. Rev. B **51**, 12 904 (1994).
[17] A. B. Kuklov, Phys. Rev. B **52**, 6729 (1995).
[18] A. Furusaki and M. Tsukada, Phys. Rev. B **43**, 10 164 (1991).
[19] A. Furusaki and M. Tsukada, Solid State Commun. **78**, 299 (1991).
[20] G. Arnold, J. Low Temp. Phys. **59**, 143 (1995).
[21] Y. Tanaka and S. Kashiwaya, Phys. Rev. B (to be published).
[22] A. Millis, D. Rainer, and J. A. Sauls, Phys. Rev. B **38**, 4504 (1988).
[23] C. Bruder, Phys. Rev. B **41**, 4017 (1990).
[24] V. Ambegaokar and A. Baratoff, Phys. Rev. Lett. **10**, 486 (1963).
[25] I. O. Kulik and A. N. Omel'yanchuk, Fiz. Nizk. Temp. **4**, 296 (1978) [Sov. J. Low Temp. Phys. **4**, 142 (1978)].
[26] Y. Nagato and K. Nagai, Phys. Rev. B **51**, 16 254 (1995).