Temperature-induced 0-π coexistence in clean superconductor-ferromagnet-superconductor Josephson junctions

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A clean ballistic superconductor-ferromagnet metal-superconductor (SFS) junction is studied within the quasiclassical theory of superconductivity. We show that the temperature-induced coexistence of the 0 and π states and the transition 0-π results from the temperature-induced transition between stable and metastable states of the junction. The π shift occurs in small but finite critical intervals $\{Z_c\}$ of the magnetic barrier influence parameter $Z=2dh/\hbar v_0$, where h is the exchange energy and d the barrier thickness. The width of $\{Z_c\}$ and the coexistence temperature $T_{0\pi}$ depend also on the reduced barrier thickness $\bar{d}=d/\xi_0$, where ξ_0 is the zero-temperature superconducting coherence length. The interval $\{Z_c\}$ increases with $\bar{d}$. For $T\neq T_{0\pi}$ the junction is in the 0 or π state. In contrast to the dirty case, the critical current I_c depends monotonously on temperature, changing the sign but not the magnitude at the transition point. The nonvanishing critical current $I_c(T_{0\pi})$ is related to the existence of the second harmonic in the current-phase relation, which could be observed experimentally.

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I. INTRODUCTION

The macroscopic phase difference $\phi=\pi$ in the ground state of a superconductor/ferromagnet/superconductor (SFS) Josephson junction was discovered[1] almost twenty years after its theoretical prediction.[2] The first experimental evidence of the transition from the 0 state to π state was found using a weak ferromagnet barrier. Ryazanov and co-workers[1,3] and Sellier *et al.*[4] used a Cu/Ni alloy, whereas Kontos *et al.*[5] worked with a Pd/Ni alloy barrier. In the former case,[3,4] for some critical values of the barrier thickness d, a nonmonotonous dependence of the critical current on temperature $I_c(T)$ was observed, corresponding to the change of sign of the supercurrent at the minimum of the $I_c(T)$ curve. The nonmonotonous barrier thickness dependence $I_c(d)$ was found by Ryazanov *et al.*[3] and by Kontos *et al.*[5]

The temperature-induced π state in the diffusive junctions[3] was explained as due to the weak ferromagnetism of the barrier alloys, with the exchange energy h in the barrier comparable to k_bT. However, in a theoretical treatment of short SFS junctions with a strong ferromagnet barrier, Konschelle *et al.*[6] demonstrated the possibility of the 0-π transition in the clean limit as well.

Recently, thin film SFS junctions with a strong ferromagnet barrier (Fe, Co, Ni, Py) were fabricated and studied by Robinson *et al.*[7] They observed oscillatory behavior of $I_c(d)$, with multiple transitions between 0 and π states. Depending on the barrier properties, the junctions were in the dirty or in the clean limit regimes. The clean limit, which we are interested in here, was achieved in the Fe and Co cases, where a monotonous temperature dependence of I_cR_N was observed.

Motivated by the recent progress in fabrication of clean SFS junctions[7] and by the proposal of construction of two-dimensional SFS weak links in graphene,[8] we consider in the present paper clean two-dimensional (2D) SFS junctions with a transparent barrier, with the exchange energy h larger or comparable to the superconducting order parameter at $T=0$ Δ_0, $\bar{h}=h/\Delta_0\gtrsim 1$, and with the barrier thickness smaller or comparable to the superconducting coherence length ξ_0, $\bar{d}=d/\xi_0\lesssim 1$. The latter condition could be experimentally achieved using superconductors with smaller coherence length.[9]

In such structures we predict a temperature-induced 0-π transition and coexistence of 0 and π states. The transition temperature, in contrast to the case of short junctions with strong barrier ferromagnets,[6] is found to depend not only on the barrier influence parameter $Z=2\overline{dh}/\pi$, but on both Z and $\bar{d}$. We find also that the shape of the current-phase relation (CPR) near the transition is close to the second harmonics $I\sim\sin 2\phi$,[10,11] and we discuss the possibilities for its experimental evidence.

In the three-dimensional (3D) case, we also found temperature-induced 0-π coexistence, transition, and dependence on reduced barrier thickness. All results are qualitatively the same as the 2D case and thus are not presented within this paper.

II. THEORY

The physical cause of the π shift in both dirty and clean SFS Josephson junctions is the oscillatory behavior of induced pairing amplitude f_F in the ferromagnetic barrier. In the clean case, with transparent barrier interfaces, the solution of the Eilenberger's equations[12] for f_F is[13]

$$f_F\sim e^{-x/\xi_F}, \tag{1}$$

with the complex coherence length in F given by $1/\xi_F=1/\xi_{F1}+i/\xi_{F2}$, with $\xi_{F1}=v_0/(2\omega_n)$ and $\xi_{F2}=v_0/(2h)$, where v_0 is the Fermi velocity (assumed the same in both S and F) and $\omega_n=\pi T(2n+1)$ are the Matsubara frequencies. Here and in the following we take $\hbar=k_b=1$. Taking both pairs with $Q=1/\xi_{F2}$ and $-Q$, we get[3]

$$f_F \sim e^{-x/\xi_{F_1}} \cos(x/\xi_{F_2}). \tag{2}$$

The phase difference $\phi=\pi$ is obtained for barrier thicknesses such that the sign of f_F is different on left-hand side and right-hand side electrodes, i.e., when $d/\xi_{F2} \sim (2n+1)\pi/2$, $n=0,1,2\ldots$.

However, this explains only the π shift induced by the variation of d or h, but not by the temperature T. In contrast to the dirty case,[3] where both ξ_{F_1} and ξ_{F_2} depend on h and T, in the clean case only ξ_{F_1} depends on temperature, influencing the temperature decay of f_F. On the other hand, in the quasiclassical theory, the role of the proximity effect is also seen calculating the supercurrent and the junction free energy with the help of the normal Green's functions g in the barrier.[11] The supercurrent density is given by[11]

$$\mathbf{j}(\phi,h,t) = -2i\pi e N_0 T \sum_{\omega_n} \left\langle \mathbf{v}_0 \frac{g(h)+g(-h)}{2} \right\rangle, \tag{3}$$

where $g_{\downarrow}=g(h)$, $g_{\uparrow}=g(-h)$, and $\langle\cdots\rangle$ means averaging over the Fermi surface. The supercurrent through the barrier of the area S, $I=j_x S$ can be expressed as[14]

$$I(\phi,h,T)/I_0 = \frac{T}{\Delta(T)} \lim_{m\to\infty} \sum_{n=-m}^{m} 2\pi D_{\varphi_c} \times \int_{-\varphi_c}^{\varphi_c} \frac{\Im g(h) + \Im g(-h)}{2} \cos\varphi d\varphi. \tag{4}$$

where $2\varphi_c$ is the angle about the interface normal of the acceptance cone for the propagation of quasiparticles.[14]

The temperature-dependent normalizing current is $I_0=2\Delta_0(T)/eR_N$, where the normal resistance is given by $R_N^{-1}=e^2 v_0 N_0 S$ and $2D_{\varphi_c}=1/\varphi_c$. Here

$$g = g_{\downarrow} = g(h) = \frac{\omega_n \cos\gamma_n + i\Omega_n \sin\gamma_n}{\Omega_n \cos\gamma_n + i\omega_n \sin\gamma_n}, \tag{5}$$

where $\Omega_n=\sqrt{\omega_n^2+\Delta^2}$, $\Delta=\Delta_0 \tanh(1.74\sqrt{1/t-1})$, and $t=T/T_c$. We have introduced the notation[11]

$$\gamma_n = \frac{1}{2}\left(\phi + \frac{2hd}{v_o \cos\varphi} - i\frac{2\omega_n d}{v_o \cos\varphi}\right) = \frac{1}{2}\left(\phi + \frac{d/\xi_{F2}}{\cos\varphi} - i\frac{d/\xi_{F1}}{\cos\varphi}\right), \tag{6}$$

where ϕ is the phase difference at the electrodes and φ the angle of the direction of the quasiparticle propagation with respect to the x axis perpendicular to the barrier.

Via γ_n, both proximity-effect parameters ξ_{F1} and ξ_{F2} enter the calculation. In reduced units, $Z=d/\xi_{F2}=2\bar{d}\bar{h}/\pi$ and $d/\xi_{F1}=2\bar{d}\bar{\omega}_n/\pi$, where $\bar{d}=d/\xi_0$, $\bar{h}=h/\Delta$, and $\bar{\omega}_n=\omega_n/\Delta$. For $\varphi=0$, the "magnetic phase" Z is added to the phase difference, $\phi\to\phi+Z$. Note that consequently the supercurrent does depend not only on the magnetic phase Z, but also separately on the barrier thickness $\bar{d}$, via the product $2\bar{d}\bar{\omega}_n/\pi$.

The junction free energy $W(\phi)$ in reduced units is given by

$$\bar{W}(\phi) = \frac{1}{I_c}\int_0^{\phi} I(\phi')d\phi', \tag{7}$$

where $\bar{W}=W/(\Phi_0 I_c/2\pi)$, Φ_0 is the flux quantum, and I_c the temperature-dependent critical current. The equilibrium phase of the junction at given temperature is obtained from the minimum of W.

Before presenting the numerical results, we note that the physical origin of the superconducting correlations' propagation through a mesoscopic F contact is due to the Andreev reflection of quasiparticles at two interfaces.[4,9] This results in the formation of Andreev bound states (ABSs) which can carry the supercurrent. The spectrum of Andreev correlated electon-hole states follows from the retarded Green's function, obtained in the present case by analytical continuation[11] of $g(h)$ [and $g(-h)$] [Eq. (5)]. The ABS energies $\bar{E}_\sigma=E_\sigma/\Delta<1$ are the solutions of

$$\cos\gamma_\sigma = \pm\bar{E}_\sigma, \tag{8}$$

where $\sigma=\downarrow,\uparrow$ and

$$\gamma_\sigma = \left(\frac{\phi}{2} \pm \frac{\bar{h}\bar{d}}{v_0\cos\varphi} - \frac{\bar{E}_\sigma\bar{d}}{v_0\cos\varphi}\right). \tag{9}$$

The supercurrent at finite temperature (the generalization of the zero-temperature result of Ref. 11), obtained by the summation over ω_n in Eq. (5), can be cast in the form

$$I(\phi)/I_0 = \sum_{j,\sigma} 2\pi D_{\varphi_c} \int_{-\varphi_c}^{\varphi_c} \frac{d\bar{E}_{j,\sigma}}{d\phi} f(E_{j,\sigma}) \cos\varphi d\varphi, \tag{10}$$

where $E_{j,\sigma}$ are the energy levels obtained from Eq. (8) and $f(x)=1/(e^{\beta x}+1)$ is the Fermi function. In this (equivalent) "spectral approach" the temperature dependence is more explicit and one can expect, similarly to the 0-π crossover in diffusive SFS junctions,[4] that a π shift can be temperature induced in the clean case as well. This is confirmed by the numerical calculations in the Matsubara technique, as we show in the next paragraph.

The above Eqs. (4) and (10) are for the 2D case. For 3D the only difference is that the integration over φ is performed from 0 to φ_c and that under the integrals $\cos\varphi \to \cos\varphi \sin\varphi$. Note also the difference in the densities of states $N(0)^{2D}$ and $N(0)^{3D}$ entering, respectively, normalizing the current I_0. Also, in 3D $2D_{\varphi_c}=1/2\pi(1-\cos\varphi_c)$.

III. MANIFESTATIONS OF THE TEMPERATURE π SHIFT IN THE CLEAN BALLISTIC CASE

Temperature-induced 0-π coexistence and π shift for all thicknesses was found from the $\phi_{\mathrm{eq}}(Z)$ dependence. An example, for $\bar{d}=1.5$, with two first π shifts, at $Z\sim 0.4\pi$ and at $Z\sim 1.3\pi$ is shown in Fig. 1. Note that these values correspond roughly to those estimated from the proximity effect, Eq. (2), $Z\sim 0.5\pi$ and at $Z\sim 1.5\pi$. For the second transition at $T=0$, the transition value of $Z=Z_{0\text{-}\pi}$ at which the equilibrium phase becomes $\phi_{\mathrm{eq}}=\pi$ is a little smaller than 1.32π. However, it increases with temperature and at $T=0.8T_c$, $Z_{0\text{-}\pi}$

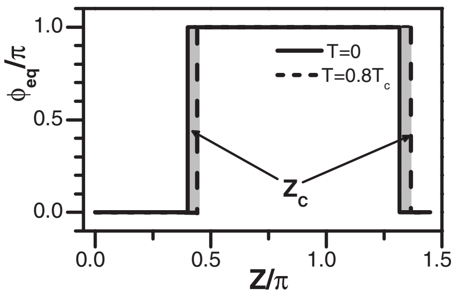

FIG. 1. Equilibrium phase ϕ_{eq} as a function of the magnetic barrier influence Z for the $\bar{d}=1.5$: $T=0$ (solid line) and $T=0.8T_c$ (dashed line). First two Z_c intervals (gray) with temperature-induced 0-π shift are located around 0.4π (0 to π transition) and 1.3π (π to 0 transition).

is 1.36π. Therefore for each Z within this critical interval, $Z \in \{Z_c\}$, there would be a 0-π coexistence at a temperature $T_{0\pi}$ (see the phase diagram in the Z-T plane, Fig. 2). The width of the interval $\{Z_c\}$ increases with barrier thickness $\bar{d}$. The physical origin of these π shifts is in the competition between stable and metastable states,[15] as can be seen from the example presented in Fig. 3(a) for the plot of the junction free energy $W(\phi)$ at various temperatures, with coexistence of equally stable 0 and π states at a given temperature $T_{0\pi}$. The corresponding form of CPR changes with T and has an $I \sim \sin 2\phi$-like shape (Fig. 3). At low temperatures $\sin 2\phi$ is deformed. Near the coexistence temperature the critical current (maximal amplitude of the current-phase characteristic CPR) changes its sign, from positive for $T < T_{0\pi}$ (0 phase) to negative for $T > T_{0\pi}$ (π phase), without changing its magnitude. The $I_c(T)$ curves are concave and monotonous, without the jump at the transition (see Fig. 4). The monotonous temperature variation, also with concave curves, is found far from the transition (for Z outside $\{Z_c\}$) as well (not presented). In addition, we want to emphasize that the above results are obtained taking realistic acceptance angle $\varphi_c = 80°$, but also that the temperature-induced transition vanishes for small angles. As mentioned in Sec. I, the temperature-dependent π shift is found in the 3D case as well and all results are qualitatively similar.

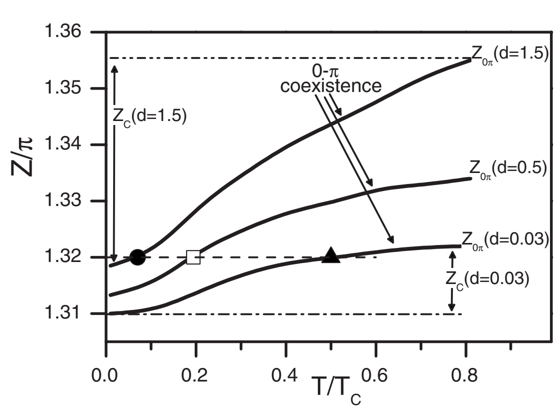

FIG. 2. Phase diagram in the Z-T plane. Solid lines represent the 0-π coexistence for various thicknesses. For each line the zero phase is above and π phase is below the line. Also note the broadening of the critical interval Z_c with increasing barrier thickness.

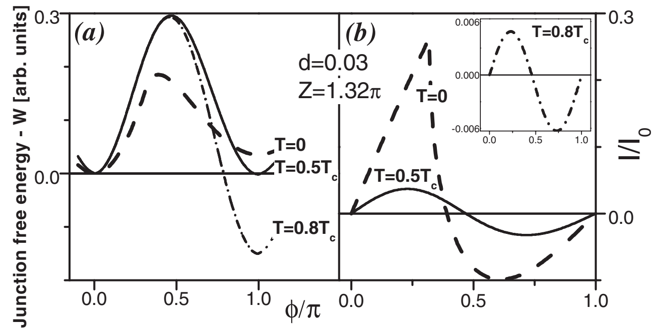

FIG. 3. An example of temperature-induced 0-π shift for $Z = 1.32\pi$ and thin barrier (reduced barrier thickness) $\bar{d}=0.03$. (a) Junction free energy and (b) the supercurrent as a function of the phase ϕ. At $T=0$ (dashed line) the equilibrium phase is $\phi_{\mathrm{eq}}=0$, at $T=T_{0\pi}=0.5T_c$ (full line) there is the coexistence of zero and π phases, and at $T=0.8T_c$ (dotted-dashed line) $\phi_{\mathrm{eq}}=\pi$. Inset in (b): CPR at $T=0.8T_c$.

IV. SUMMARY AND CONCLUSION

Recently, Konschelle *et al.*[6] studied clean SFS junctions assuming $d \ll \xi_0$ and $h \gg T$. In the ballistic regime and using the quasiclassical theory, they found that the temperature-induced 0-π transition depends on a single parameter, $Z = d/\xi_{F2} = 2\overline{dh}/\pi$ in our notation. Determining the transition point ($Z_c \approx 3.72$) from the second minimum on the $I_c(Z)$ oscillatory curve for $T \to Tc$, they calculated $T_{0\pi}$ situated on a concave monotonous $I_c(t)$ curve. Far from the transition, for other values of Z, they got nearly linear or slightly convex curves.

On the other hand, Cayssol and Montambaux[16] studied the Josephson effect in a clean SFS junction by solving Bogoliubov–de Gennes equations for arbitrary spin polarization. They found that for strong ferromagnets the oscillations of the critical current depend separately on h and d and not on a single parameter $Z = 2\overline{dh}/\pi$ (in our notation), as predicted by the quasiclassical theory.[6] The temperature $I_c(t)$ curves for values of h_c (for given d) corresponding to 0-π

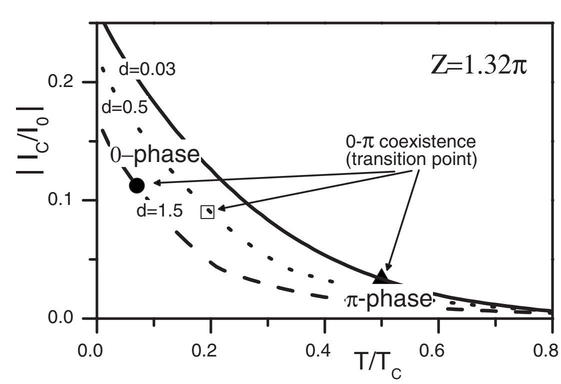

FIG. 4. Temperature variation of the critical current for $Z = 1.32\pi$ and three barrier thicknesses: $\bar{d}=0.03$ (full line), $\bar{d}=0.5$ (dotted line), and $\bar{d}=1.5$ (dashed line). The bullets represent the zero and π-state coexistence at corresponding transition temperature $T_{0\pi}$ (see Fig. 3). For each line, the zero-phase appears at $T < T_{0\pi}$ and the π phase at $T > T_{0\pi}$.

transitions decay exponentially, whereas for h corresponding to the maxima of $I_c(h)$ the decay is much slower.[16] The comparison between these works and our results, as well as the comparison with experiments, is presented in the following summary.

In the present article, we have shown by numerical calculation within the quasiclassical theory that:

(1) The temperature-induced π shift and 0-π coexistence in clean ballistic SFS junctions appear for the finite interval of $Z \in \{Z_c\}$, as consequence of temperature-induced competition between stable and metastable states.

(2) In the critical region $\{Z_c\}$, the CPR consists of the second harmonic, $I(\phi) \sim \sin 2\phi$. This gives the nonzero value of critical current at transition point $I_c(T_{0\pi})$, where the first harmonic component cancels.[10]

(3) The transition temperature $T_{0\pi}$ occurring for $Z \in \{Z_c\}$ does depend on $\bar{d}$ going toward lower temperatures with increasing $\bar{d}$.

(4) The interval $\{Z_c\}$ is broadening with $\bar{d}$.

(5) The temperature variation of $I_c(t)$ curves is concave and monotonous, without cusps characteristic for the dirty case,[3] and the critical current changing the sign but not the magnitude at the 0-π shift. The concave shape of the curves persists even further from the transition, becoming nearly linear for small Z.

For comparison with experiments by Robinson *et al.*,[7] we may consider only Co and Fe junctions, exhibiting the clean limit behavior for ferromagnetic film thicknesses from 1 to 5 nm. Assuming that the second minima on the $I_c(d)$ curves correspond to the second π shift, $Z \sim 1.3\pi$, we estimate the exchange energy h in the barrier. Taking for Nb $\xi_0 \sim 38$ nm and $\Delta_0 \sim 1.35$ meV, we get h of the same order of magnitude ($h \sim 200$ meV) as in experiment. For Co, the curves $I_c(T)$ are nearly linear, and for Fe concave or nearly concave, for all devices with different barrier thickness, corresponding not only to the minima of $I_c(d)$.[7] This is in accordance with our result.

In conclusion, we expect that the recent progress in fabrication of clean ballistic SFS junctions should provide the experimental evidence of the temperature-induced 0 and π-state coexistence and 0-π transition. The second-harmonic form of CPR at the transition should lead to the formation of half-integer Shapiro steps[10] on the current-voltage characteristics. In the presence of an external magnetic field I_c should exhibit a Fraunhofer pattern with period of $\phi_0/2$.[14] These manifestations of the 0-π coexistence and the π shift could be observed by varying the temperature in devices with various thicknesses of the same ferromagnetic material in the barrier, similarly as in the dirty case.[3]

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