Mechanisms of Spontaneous Current Generation in an Inhomogeneous $d$-Wave Superconductor

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A boundary between two $d$-wave superconductors or an $s$-wave and a $d$-wave superconductor generally breaks time-reversal symmetry and can generate spontaneous currents due to proximity effect. On the other hand, surfaces and interfaces in $d$-wave superconductors can produce localized current-carrying states by supporting the $T$-breaking combination of dominant and subdominant order parameters. We investigate spontaneous currents in the presence of both mechanisms and show that at low temperature, counter-intuitively, the subdominant coupling decreases the amplitude of the spontaneous current due to proximity effect. Superscreening of spontaneous currents is demonstrated to be present in any $d$-$d$ (but not $s$-$d$) junction and surface with $d + id'$ order parameter symmetry. We show that this superscreening is the result of contributions from the local magnetic moment of the condensate to the spontaneous current.

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The time-reversal symmetry ($T$) breaking on surfaces and interfaces of superconductors with $d$-wave orbital pairing has been intensively investigated in the last years both in theory and experiment \cite{1-8}. Several mechanisms of $T$-breaking have been proposed, which fall in two categories: appearance of subdominant order parameter and proximity effect \cite{1-3}.

In the first case the surface or interface suppresses the dominant order parameter ($d_{x^2-y^2}$ in YBCO \cite{4}). If the pairing interaction in other channels is nonzero, the subdominant order parameter will be formed below the corresponding, smaller critical temperature $T_{c2}$ \cite{4}. The combination of the two order parameters with complex coefficients breaks the $T$-symmetry \cite{4} and leads to spontaneous surface currents and magnetic fluxes. Usually $d_{x^2-y^2}$ and $d_{x^2-y^2} \pm id_{xy}$ predictions are combined. Recent observations of zero bias peak splitting in surface tunneling experiments \cite{4} and spontaneous fractional flux (0.1-0.2 Φ$^0$) near the “green phase” inclusions in YBCO films \cite{4} agree with this picture.

The other possibility arises in a junction between two $d$-wave superconductors with different orientations of the order parameter \cite{4}. In this case the two order parameters necessary to form a $T$-breaking state, $d_{1,2}$, are supplied by the bulk superconductors. The equilibrium phase difference across the boundary, $\delta_0$, is generally neither 0 nor $\pi$, and therefore the states with $d_{1,2} \pm e^{\pm i \delta_0} d_{2,1}$ orderings are degenerate and may support spontaneous currents. The same mechanism applies in case of a boundary between an $s$- and a $d$-wave superconductor \cite{4}.

In order to investigate the interplay of both mechanisms, in this letter we consider $d$-$d$ and $s$-$d$ interfaces as well as (110)-surface of a $d$-wave superconductor. We will see that generally the spontaneous currents due to proximity effect are suppressed by the existence of subdominant order parameter. There is also an important distinction between the $d$-$d$ and $s$-$d$ cases: In the former case the superconductor may have local orbital and magnetic moments, contributing to the non-dissipative current. In the latter case such a contribution is absent. Our results indicate that in a clean $d$-$d$ junction all of the spontaneous current can be attributed to this “molecular currents” mechanism. We also show that this effect leads to “superscreening” of spontaneous currents in $d$-$d$ junctions (i.e. to the existence of counter-currents independent of the Meissner effect).

We use the standard approach based on quasiclassical Eilenberger equations for Green’s functions integrated over energy \cite{10}

$$v_F \cdot \nabla \hat{G}_\omega + [\omega \tau_3 + \hat{\Delta}, \hat{G}_\omega] = 0,$$  \hspace{1cm} (1)

where $\omega$ is the Matsubara frequency and

$$\hat{G}_\omega(v_F, r) = \begin{pmatrix} g_\omega f_\omega & f_\omega^* \omega \\ f_\omega^* & -g_\omega \end{pmatrix}, \quad \hat{\Delta}(v_F, r) = \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix}.$$  

Here $\hat{G}_\omega$ is the matrix Green’s function and $\Delta$ is the superconducting order parameter. They both are functions of Fermi velocity $v_F$ and position $r$. We also need to satisfy the normalization condition $g_\omega = \sqrt{1 - f_\omega^* f_\omega}$. In general case $\Delta$ depends on the direction of the vector $v_F$ and is determined by the self-consistency equation

$$\Delta(v_F, r) = 2\pi N(0) T \sum_{\omega > 0} \langle V_{v_F, v_F'} f_\omega(v_F', r) \rangle \theta, \hspace{1cm} (2)$$

where $V_{v_F, v_F'}$ is the interaction potential. In our calculations we will consider two-dimensional case; $N(0) = \frac{\mu}{2\pi}$ is 2D density of states and $\langle ... \rangle_\theta = \int_{0}^{2\pi} \frac{d\theta}{2\pi}$ is the averaging over directions of 2D vector $v_F = (v_F \cos \theta, v_F \sin \theta)$. 





In general it is possible to obtain a mixture of different symmetries of the order parameter, \( \Delta(\theta) = \Delta_{x^2-y^2}(\theta) + \Delta_{xy}(\theta) + \Delta_s \), where \( \Delta_{x^2-y^2}(\theta) = \Delta_1 \cos 2\theta \), \( \Delta_{xy}(\theta) = \Delta_2 \sin 2\theta \) and \( \Delta_s \) are the \( d_{x^2-y^2} \), \( d_{xy} \), and the \( s \)-wave components of the order parameter respectively. The corresponding interaction potential, \( V_{\theta^d} = V_{\theta^1} \cos 2\theta \cos 2\theta' + V_{\theta^2} \sin 2\theta \sin 2\theta' + V_{\theta} \), must be substituted in the self-consistency equation \( \Box \) for the order parameter in each channel. The current density \( j(r) \) is found from the solution of the matrix equation \( \Box \) as

\[
j(r) = -\frac{4\pi e N(0)T}{\sin \phi} \sum_{\omega > 0} <v_F g_\omega (v_F, r) >_\theta. \quad (3)
\]

Here we consider three cases, (i) boundary between two semi-infinite \( d \)-wave superconductors with crystallographic orientations with respect to the boundary given by angles \( \chi_l \) and \( \chi_r \) ("\( d-d \) interface"), (ii) boundary between an \( s \)-wave and a \( d \)-wave superconductor with 45° orientation ("45° \( s-d \) interface"), and (iii) (110)-surface of a \( d \)-wave superconductor. In all three cases it is possible to have time reversal symmetry breaking ground state. The direction and magnitude of the spontaneous current depends on the relative phases of the order parameters.

Assuming constant order parameters on both sides of an interface, one can obtain an analytical (non-selfconsistent) expression for the current density

\[
j(x) = 4\pi e N(0)T \sin \phi \sum_{\omega > 0} \left\{ \frac{v_F \Delta_l \Omega_l \Omega_r}{\Omega_l \Omega_r + \omega^2 + \Delta_l \Omega_r \cos \phi} \right\} e^{-2|x|\Omega_l / |v_F \cos \theta|} \theta, \quad (4)
\]

where \( l \) (r) labels left (right) side of the interface, and \( \Omega_{l,r} = \sqrt{\omega^2 + |\Delta_{l,r}|^2} \). This expression is valid for arbitrary symmetry of the order parameters \( \Delta_{l,r} \). For a \( d-d \) interface we have \( \Delta_l = \Delta_0(T) \cos 2(\theta - \chi_l) \) and \( \Delta_r = \Delta_0(T) \cos 2(\theta - \chi_r) \), where \( \Delta_0(T) \) depends on the superconducting coupling and temperature.

Our numerical calculations were based on Schopohl-Maki parameterization of Green’s functions \( \Box \),

\[
\begin{align*}
g &= 1 - a \omega + \frac{1}{1 + a \omega}, \\
f &= \frac{2a}{1 + a \omega}, \\
f^\dagger &= \frac{2a^\dagger}{1 + a^\dagger \omega},
\end{align*}
\]

which transforms Eq. \( \Box \) into

\[
\begin{align*}
v_F \cdot \nabla a &= 2\omega a - \Delta^* a^2 + \Delta \quad (5) \\
-v_F \cdot \nabla a^\dagger &= 2\omega a^\dagger - \Delta a^\dagger 2 + \Delta^*. \quad (6)
\end{align*}
\]

For positive \( v_x \), Eq. \( \Box \) (Eq. \( \Box \)) is stable if the boundary condition at \( x \to -\infty \) (+\( \infty \)) is chosen. The opposite is true for negative \( v_x \). We use the solutions in a homogeneous system, \( a = \Delta / (\omega + \Omega) \) and \( a^\dagger = \Delta^* / (\omega + \Omega) \) as boundary conditions at \( \pm \infty \). The values of \( a (a^\dagger) \) at all other points on the trajectory are then easily found. The self-consistency is introduced through iterations, assuming a constant order parameter in either half of the junction for the first iteration.

FIG. 1. (a) Spontaneous current for \( d-d \) and \( s-d \) junctions. The boundary is located at \( x = 0 \). Calculations are done at \( t = T/T_c = 0.05 \), with \( T_{c2} = 0.05T_c \) for the \( d-d \) case and \( T_{cs} = 0.1T_c \) and \( T_{c2} = 0.05T_c \) for the \( s-d \) junction. (b) Spontaneous current at the (110)- surface of a \( d \)-wave superconductor at \( t = 0.05 \) with \( T_{cs} = T_{c2} = 0.1 T_c \) for both \( s \) or \( d \) \( s-d \) subdominant order parameters.

FIG. 2. (a) Spontaneous currents for \( (0^\circ-\delta\chi) \) junctions with different misorientation angles. (b) Spontaneous current at imperfect \( (0^\circ-45^\circ) \) junctions. Solid line: junction with transparency \( D_0 = 0.3 \). Dashed line: junction with roughness \( \rho = 0.3 \). All calculations are done at \( t = 0.1 \).

\[
g = \frac{1 - a a^\dagger}{1 + a a^\dagger}, \quad f = \frac{2a}{1 + a a^\dagger}, \quad f^\dagger = \frac{2a^\dagger}{1 + a^\dagger a},
\]

The same situation takes place near the surface, if the subdominant pairing is present. Fig. \( \Box \) shows the cur-
recent distribution at the (110)-surface of a d-wave superconductor. If \( d_{xy} \) is the leading subdominant order parameter, the form of the current distribution is similar to the one in the d-d boundary. The superscreening is absent if the subdominant order parameter is s-wave.

The superscreening effect can be obtained analytically from the non-selfconsistent expression in case of 0-45\(^\circ\) junction. The nullification of the total current results from integrating the spontaneous current

\[
\int_0^\infty dx j_y(x) \propto \left( \frac{\Delta_1 \Delta_2 \sin \theta \text{sign}(\cos \theta) v_F | \cos \theta |}{\Omega_r \Omega_r + \omega^2 + \Delta_1 \Delta_2 \cos \phi \Omega_r} \right) j_\theta \sin \phi
\]

which is zero after angle averaging. Our numerical calculations however show that in clean boundary junctions the total current is zero (within the numerical accuracy) even after self-consistent calculation and at all other mis-orientation angles (see Fig. 3). To understand the situation, let us recall that in a system with local magnetic moment density \( \mathbf{m}(r) \) the “molecular currents” flow with density \( j(r) = e \nabla \times \mathbf{m}(r) \). In a superconductor with order parameter \( d_x^2 d_y^2 + e^{i\phi_0} d_{xy} \) local orbital/magnetic moment density

\[
\mathbf{m}(r) \approx \frac{1}{i} \frac{\partial}{\partial \theta} \left( \Delta_1(x) \cos 2\theta + \Delta_2(x) e^{-i\phi_0} \sin 2\theta \right)
\]

The contribution to the spontaneous current is thus \( j(r) \propto \nabla \times \mathbf{m}(r) \parallel \mathbf{y} \). Notice that the same expression is obtained from the Ginzburg-Landau equations \( j \propto \nabla \times (\mathbf{z} \text{Im} d_1(r) d_2(r^*) \mathbf{p}) \). The total current in y-direction due to this mechanism is \( I_{total} \propto \int d\Omega \mathbf{S} \cdot \nabla \times \mathbf{m} = \int_{\Omega} d\Omega d \mathbf{m} = 0 \), where \( \Omega \) is a cross section perpendicular to the junction from \( x = -\infty \) to \( \infty \) and \( \partial \Omega \) is its boundary. The latter integral is obviously zero because \( d \mathbf{m} = 0 \) everywhere except where the contour closes \( (x = \pm \infty) \), but there \( \mathbf{m} = 0 \). This is certainly not the case in s-d junctions (cf. Fig. 4). (Of course, since the Meissner currents must be taken into account in this case, the results presented in Fig. 4 are valid only if the system size is much less than the London penetration depth.)

We also calculate the spontaneous current for an imperfect boundary, i.e a boundary with arbitrary transparency \( d_0 \) and also with finite roughness \( \rho \). We use Zaitsev’s condition \( [12, 14] \) to incorporate the finite transparency effect. For surface roughness we assume a thin layer with scattering centers at the junction. We take the mean free path \( l \) and the layer thickness \( d \) to zero while keeping \( \rho \equiv d/l \) finite. The details of calculations will be given in a separate publication. Here we only present the results of our calculation for asymmetric (0°-45°) d-d junction in Fig. 4. As is clearly seen, the spontaneous currents now does not necessarily have a counterflow (at small \( \rho \) or \( D_0 \approx 1 \) there will be some countercurrent), and the exact superscreening no longer takes place. They are now carried merely by Andreev bound states at the interface, the same as in s-d and SND junctions. Although near realistic surfaces/interfaces with d-d ordering the superscreening is not complete, the magnetic fields created by the spontaneous currents are nevertheless suppressed on very short distances. This can be practically important for attempting to build a “quiet” qubit based on such junctions.

Fig. 4 presents the spontaneous current as a function of the subdominant critical temperature \( T_{c2} \) at the (110)-surface of a d-wave superconductor. One notices that the spontaneous current vanishes when \( T_{c2} < T \). In fact, at temperatures below \( T = T_{c2} \) the subdominant order parameter starts to appear at the surface through a second-order phase transition. Spontaneous symmetry breaking and generation of the spontaneous current are the consequences of the emergence of this second order parameter. The symmetry of the subdominant order parameter is dictated by whichever channel (s or \( d_{xy} \)) has stronger interaction potential.

In the d-d and s-d interfaces on the other hand, the subdominant order parameter is induced by the proximity to a different superconductor. One important difference is
In conclusion, we have investigated the spontaneous currents near the surface and d-d and s-d boundaries in d-wave superconductors. We obtained the contributions to the spontaneous currents due to the proximity effect and due to the subdominant order parameter generation, and found that at interfaces the latter generally decreases the magnitude of the effect. In d-d junctions, we separated the contribution from the local orbital/magnetic moment of the condensate; this contribution dominates spontaneous currents in clean d-d junctions, which explains the superscreening of the spontaneous currents in such systems.

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