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Time-reversal symmetry breaking at Josephson tunnel junctions of purely *d*-wave superconductors

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We study spontaneous time-reversal symmetry breaking at Josephson tunnel junctions of *d*-wave superconductors in the absence of subdominant components of the order parameter. For tunnel junctions, when the orientation is close to 0/45 (for which a gap lobe points towards the junction on one side and a gap node on the other), the mechanism of the symmetry breaking is the splitting of midgap states (MGS) by spontaneous establishment of a phase difference $\phi=\pm\pi/2$ across the junction. This occurs for transparencies $D\gg\xi_0/\lambda$ and temperatures $k_BT\ll D\Delta_0$, where ξ_0 is the coherence length, λ is the penetration depth, and Δ_0 is the maximum energy gap. On the other hand, tunnel junctions with $D\ll\xi_0/\lambda$ effectively behave as surfaces, for which the mechanism of symmetry breaking is self-induced Doppler shifts of MGS. For this instability, we calculate the phase-transition temperature $k_BT_{TRSB}=(1/6)(\xi_0/\lambda)\Delta_0$ and show that the spatial shape of the gap is unimportant.

The possibility of spontaneous time-reversal symmetry breaking (TRSB) states at various surfaces and interfaces of *d*-wave superconductors has been intensively studied during the last few years.[1] Some experimental findings, such as fractional flux quanta at certain grain boundaries[2,3] and splitting of the zero-bias conductance peak in zero magnetic field,[4,5] have been interpreted as realizations of this state. Theoretically, several different systems have been under consideration: surfaces,[6,7] twin boundaries,[8] and Josephson junctions[9–16] with special orientations.

In this paper we will study TRSB at Josephson tunnel junctions with orientation close to $\alpha_L=0,\alpha_R=\pi/4$ (Fig. 1) for arbitrary transparency D of the tunnel barrier. We emphasize that we are considering purely *d*-wave superconductors, meaning that a subdominant component of the order parameter is assumed to be *absent*. As will be shown, the TRSB effect is due to the specific properties of the midgap states formed in these structures.

In 1994 Hu[17] showed that surface states with zero energy, so-called midgap states (MGS), are formed at surfaces and interfaces of *d*-wave superconductors if the orientation angle α is nonzero. The largest spectral weight of the MGS appears when a *d*-wave gap node points directly towards the surface/interface ($\alpha=\pi/4$).

It has been pointed out (see, e.g., Refs. 1 and 15) that the large density of states exactly at the Fermi level associated with the MGS is energetically unfavorable: if there exist mechanisms able to shift the MGS and produce a gap in the spectrum, the energy will be lowered and a phase transition into a state with broken time-reversal symmetry will take place. Splitting of MGS due to a complex $d+is$ order parameter, with a subdominant surface/interface *s*-wave component, has been considered both at free surfaces[6,7] and at Josephson junctions.[14,15] The possibility of instabilities at Josephson junctions of purely *d*-wave superconductors was pointed out by Yip[9] for the weak link case (transparency $D=1$, no backscattering in the junction, see also Refs. 11,12). The TRSB state was later shown to be favorable also for finite but rather high transmissivity of the junction,[13–15] $0.3\lesssim D\leqslant 1$. According to the symmetry arguments presented in Refs. 9,13–15, the effect of TRSB in pure *d*-wave junctions heavily relies upon the nonsinusoidal current-phase relation in transparent weak links. Since the higher harmonics in the current-phase relation disappear in the tunnel limit, TRSB in tunnel junctions of pure *d*-wave superconductors is also expected to disappear and it was supposed that TRSB can only occur under such circumstances when a complex order parameter is formed.[14,15] However, it turns out that the symmetry argument holds only for continuum states and for finite-energy bound states, but not for the MGS which contribute to the Josephson current with a term proportional to the first power in D at low temperature.[20,21] In the low-transparency limit it is not the nonsinusoidal current-phase relation itself that is important, but rather the uneven occupation of split MGS. Here we will show that this leads to TRSB also in tunnel junctions of purely *d*-wave superconductors. The driving mechanism of the instability is the displacement of MGS induced by spontaneous establishment of a finite phase difference $\phi=\pm\pi/2$ across the junction, similar to what happens in transparent junctions.[9,13–15] In the extreme tunnel

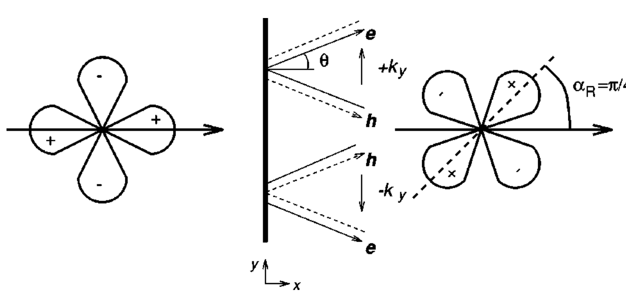

FIG. 1. The specular *d*-wave Josephson junction under consideration: the right superconductor has a gap node pointing towards the junction ($\alpha_R=\pi/4$), while the left superconductor has a gap lobe pointing towards the junction ($\alpha_L=0$). For the surface problem we have a vacuum for $x<0$. Shown are also the scattering events, consecutive normal scattering at the junction and Andreev reflection in the superconductor, leading to the formation of midgap states.

limit, the mechanism crosses over to self-sustained Doppler shifts of MGS, which also produce instabilities at free surfaces.[18,19,25]

Although the MGS contribution does not appear in conventional tunnel model calculations (despite the fact that it is proportional to the first power in transparency D), the quasiclassical Green's function technique, in principle, includes it. However, since the necessary condition for TRSB for low transparency is $k_BT \ll D\Delta_0$ (corresponding to uneven occupation of split MGS, see below), the specific window of transparencies favoring TRSB found in Refs. 13 and 15, $0.3 \lesssim D \leqslant 1$, was actually a result of the choice of temperature, $k_BT = 0.2 k_BT_c \sim 0.1\Delta_0$.

Consider now the Josephson tunnel junction in Fig. 1. We model the junction between the two clean two-dimensional d-wave superconductors by a square specular barrier. In this case, the quasiparticle wave functions can be labeled by the conserved wave vector component parallel to the surface, $k_y = k_F \sin\theta$, where k_F is the Fermi wave vector. The gap functions in the superconductors are $\Delta_{L/R}(x,\theta) = \Delta_0 g_{L/R}(x)\cos[2(\theta-\alpha_{L/R})]$, where all angles are measured relative to the surface normal (Fig. 1). The fact that the gap may be suppressed near surfaces and interfaces of d-wave superconductors is reflected in the x-dependent functions $g_{L/R}(x)$.

For the calculation of the dc Josephson current, one needs to consider contributions both from continuum states and Andreev bound states. If the two superconductors were decoupled (zero transparency), there would be midgap surface states on the right side ($\alpha_R = \pi/4$) and also finite-energy surface states since the gap is suppressed near the surface forming a quantum well. In addition there are gap edge states on the left side ($\alpha_L = 0$). For finite transparency the surface states form states of the entire junction. The energy of these Andreev states are shifted relative to the surface levels, the shift depending on the transparency of the barrier and the phase difference ϕ across the junction. To clearly see the mechanism of the TRSB instability we first consider a step-function dependence of the gap, $g_{L/R}(x) = \Theta(\mp x)$. By solving the quasiclassical Bogoliubov-de Gennes equation for the junction, we find the energy of the midgap state (the θ dependence of the order parameter is not explicitly written out here)

$$E(\phi,k_y) = \frac{-\operatorname{sgn}(k_y)\Delta_L|\Delta_R|D(\theta)\sin\phi}{2|\Delta_L| + D(\theta)[|\Delta_R|-|\Delta_L|]} + O(D^3)$$
$$= -\operatorname{sgn}(k_y)E_0(\theta)\sin\phi + O(D^3), \qquad (1)$$

as plotted in Fig. 2(a). When a phase difference is applied across the junction, the degeneracy of the $\pm k_y$ MGS is lifted, as emphasized by the solid and dashed lines in Fig. 2(a). The contribution to the dc Josephson current from Andreev states is found via the relation $I_x = (2e/\hbar)(dE/d\phi)n_F(E)$, where n_F is the Fermi distribution function. The current carried by the bound states in Eq. (1) is therefore

$$eR_N I_x^{MGS}(\phi) = -\frac{2\pi}{D}\int_0^1 d\eta E_0(\eta)\cos\phi$$
$$\times \tanh\left[\frac{E_0(\eta)\sin\phi}{2k_BT}\right] + O(D^2), \qquad (2)$$

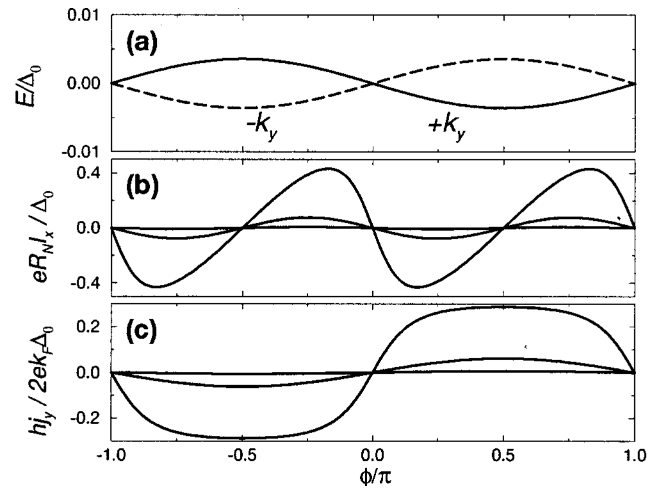

FIG. 2. (a) Dispersion of the Andreev bound state with the phase difference across the junction. Solid and dashed lines are bound states at angles $\theta = \pi/9$ and $\theta = -\pi/9$, respectively, $D(\theta = \pm\pi/9) \approx 0.01$. (b) The current-phase relation at three different temperatures: $T = 0.1T_c$, $T = 0.01T_c$, and $T = 0.001T_c$, for $D \approx 0.009$ ($k_Fd = 5, U = 1.2E_F$, where U and d are the height and width of the barrier and E_F is the Fermi energy). For decreasing temperature, the current crosses over from being of order D^2 to D and becomes increasingly nonsinusoidal. (c) Phase dependence of the surface current density calculated to the right of the barrier.

where T is the temperature, $R_N = \pi h/e^2 k_F L_y D$ is the normal-state resistance of the junction, L_y is the junction width, $\eta = \sin\theta$, and $D = \int d\eta D(\eta)/2$. From Eq. (2) we find that the MGS contribution to the Josephson current at low temperature, $k_BT \ll |E_0| \sim D\Delta_0$, is of *first order in the transparency* D. In what concerns the continuum, $\pm k_y$ states are degenerate and carry current in opposite directions, which results in a cancellation of the main (of order D) current. The residual continuum contribution is small, of order D^2. This cancellation is due to the sign change of Δ_R when we let $k_y \to -k_y$, see Fig. 1. Both k_y and $-k_y$ contributions have $\sin\phi$ dependences, but they are π shifted relative to each other (the sign of Δ_R is equivalent to a phase π) and carry current in opposite directions. This is the symmetry argument[9,14,15] referred to above. Also the $\pm k_y$ bound states near the gap edges carry current in opposite directions. Although they are not degenerate (like the MGS they split under phase bias) they are equally populated for $k_BT \ll \Delta_0$ and the sum of $\pm k_y$ currents is of order D^2. We would like to emphasize that the MGS do not obey the $\pm k_y$ symmetry at low temperature because MGS with opposite signs of k_y disperse on opposite sides of the Fermi level and are unequally populated. In Fig. 2(b) we plot the total current including the dominant MGS contribution and the small contributions from the gap edge states and the continuum states. In agreement with previous work,[9–12,14–16,13,20,21] the current-phase relation is π periodic. For increasing temperature, the MGS contribution is reduced, and when $k_BT \gg D\Delta_0$ [the $T = 0.1\ T_c$ curve in Fig. 2(b)] the current is small, of order D^2. In the intermediate region, the current in Eq. (2) scales as D^2/T.[20–22] The above arguments leading to the dominating, of order D, MGS currents and small, of order D^2, non-MGS currents hold also for general spatial dependences of the gap functions. However, as shown in Ref. 23, the numerical prefactor of the current calculated for step-function gaps is overestimated by a factor of about 2, due to an overestimation of the shift of the MGS with phase difference. However, this will not influence the instability we discuss in the following.

By a phenomenological argument Yip[9] showed (see also the paper by Östlund[16]) that when the $\pm k_y$ symmetry cancels the first harmonic of the current in purely d-wave junctions with orientation $\alpha_L=0,\alpha_R=\pi/4$, time-reversal symmetry is broken if the parameters of the theory are chosen in such a way that the coefficient in front of the second harmonic is negative. The current due to MGS has indeed this negative sign. As a consequence, the equilibrium phase difference across the junction is $\phi_{eq}=\pm\pi/2$, since the Josephson energy minimum appears where the current through the junction is zero and the slope of the current-phase relation is positive. That these phase differences really correspond to Josephson energy minima can be understood by noting that the energy of the midgap state is the lowest for $\phi_{eq}=\pm\pi/2$, see Fig. 2(a) and also Eq. (6). Considering low temperature, when only the negative-energy states are occupied, we see that the degenerate $\phi_{eq}=\pm\pi/2$ junction states correspond to occupation of $\pm k_y$ time-reversed MGS, see the illustration in Fig. 1. Assuming that the system chooses one minimum ($\phi_{eq}=\pi/2$) or the other ($-\pi/2$), surface currents in the positive or negative y direction will appear and time-reversal symmetry is broken. The spontaneous surface current, calculated via

$$j_y(x)=\frac{e\hbar}{m}\sum_{\mathbf{k}} k_y\hat{\Psi}^{\dagger}_{\mathbf{k}}(x)\hat{\Psi}_{\mathbf{k}}(x)n_F(E_{\mathbf{k}}), \tag{3}$$

where $\hat{\Psi}_{\mathbf{k}}$ are the wave functions satisfying the quasiclassical Bogoliubov-deGennes equation, is dominated by the MGS for the same reasons as the MGS dominate the Josephson current. In Fig. 2(c) we plot $j_y(\phi)$ calculated to the right of the barrier at $x=0$. The surface current approaches its maximum value at the equilibrium phase differences $\phi_{eq}=\pm\pi/2$, but it has opposite signs since MGS with opposite signs of k_y are occupied at these two phase differences.

Since the MGS surface current produces a magnetic field which costs energy, we must include this effect into the discussion of the instability. The spatial dependence of the magnetic field $\mathbf{h}$ is determined by the counterflowing screening currents, and can be calculated via the superfluid momentum $\mathbf{p}_s$, $\mathbf{h}=-(c/e)\nabla\times\mathbf{p}_s$. For type II superconductors, like the high-T_c superconductors, $\mathbf{p}_s$ is found via the London equation $\nabla^2\mathbf{p}_s-\mathbf{p}_s/\lambda^2=(4\pi e/c^2)j_y^{MGS}(x)\hat{y}\equiv f(x)\hat{y}$. Because the MGS surface current remains finite in the limit $D=0$, we are allowed to let $D\rightarrow 0$ and perform the calculation of the source current with the free surface MGS wave function. This allows us to explicitly take into account the spatial dependence of the gap. The surface current then takes the form

$$j_y(x)=\frac{e\hbar}{m}\frac{k_F^2}{2\pi}\int_0^1 d\eta\,\eta\frac{e^{-2\zeta}}{N}\tanh\left(\frac{-E_0(\eta)}{2k_BT}\right), \tag{4}$$

where $\zeta=\int dl|\Delta(l)|/\hbar v_F$, $x=l\sqrt{1-\eta^2}$, and $N=\int_0^\infty dx e^{-2\zeta}$ is the normalization constant of the MGS wave function. The integration over trajectory angles η is effectively cut off at $\eta<1$ because of the tunneling cone described by $D(\eta)$. Since the MGS source only has a y component, the nontrivial component of $\mathbf{p}_s$ is the y component which only depends on x, $\mathbf{p}_s=p_s(x)\hat{y}$. The solution of the differential equation, satisfying the boundary condition $\lim_{x\rightarrow\infty}h_z(x)=0$ is $p_s(x)=b_0e^{-x/\lambda}+\lambda\int^x dx' f(x')\sinh[(x-x')/\lambda]$. The constant b_0 is fixed by the boundary condition $h_z(x=0)=0$ at the junction, $b_0=-\lambda\int_0^\infty dx f(x)\cosh(x/\lambda)$.

An important aspect of the screening problem is the separation of length scales: the surface current due to the MGS flows within a thin layer of width ξ_0 near the surface, while the screening currents flow in a much thicker layer of width λ. For high-T_c superconductors the ratio $\xi_0/\lambda\ll 1$, and all quantities may be expanded in this small parameter. For this reason the convergence of the integrals in the expression for p_s is governed by the function $f(x')$ which decays on the ξ_0 length scale. If one expands the hyperbolic functions, the spatial shape of the gap function is cancelled in the leading term of the expression for p_s: it appears both in the normalization N of the MGS wave function and in the integrals over $f(x')$ which are integrals over the MGS wave function. Thus, the detailed spatial shape of the gap drops out of the calculation and the final form of p_s is

$$p_s(x)=-\frac{\hbar}{\lambda}e^{-x/\lambda}\int_0^{\eta_1}d\eta\,\eta\tanh\left(\frac{-E_0(\eta)}{2k_BT}\right)\left[1+O\left(\frac{\xi_0}{\lambda}\right)\right]. \tag{5}$$

We are now able to quantitatively study the difference in the thermodynamic potential Ω of junctions with and without broken symmetry: it consists of two parts, the energy cost of having a magnetic field and the energy gain due to the shifts of MGS

$$\Delta\Omega=\int_0^\infty dx\frac{h_z^2(x)}{8\pi}-k_BT\frac{k_F}{\pi}\int_0^{\eta_1}d\eta\ln\left[\cosh\frac{E_0(\eta)}{2k_BT}\right]$$
$$=\frac{k_F\Delta_0}{4\pi}\left[\frac{\xi_0}{4\lambda}-\int_0^1 d\eta\,\eta\sqrt{1-\eta^2}D(\eta)\right], \tag{6}$$

where the second line is valid in the low-temperature limit $k_BT\ll|E_0|\sim D\Delta_0$. Clearly, for $D\gg\xi_0/\lambda,\Delta\Omega<0$ and there is an instability.

If one rotates the superconductors away from the $\alpha_L=0$, $\alpha_R=\pi/4$ orientation, the equilibrium phase difference across the junction is shifted continuously away from $\pm\pi/2$ towards either 0 or $\pm\pi$ depending on the direction of rotation. This happens because the $\pm k_y$ symmetry is lost and non-MGS contributions are able to dominate. However, a numerical calculation shows that in the low-temperature region, $k_BT\ll D\Delta_0$, where the MGS dominate, the TRSB, that is $\phi_{eq}\neq 0$ or $\pm\pi$, is quite robust: it survives rotations up to 10°.

From Eq. (6) it is found that when $D\lesssim\xi_0/\lambda$ the energy of the magnetic field may become larger than the Josephson energy and the instability is lost. However, for such small transparencies it is necessary to take into account the Doppler shift of the MGS due to the finite superfluid momentum, which will assist and uphold the TRSB instability. In the low transparency limit $D\ll\xi_0/\lambda$, for which the Doppler shift is much larger than the shift due to finite-phase difference, the junction behaves like a free surface with the MGS localized on the right side of the junction. Using the above calculation but taking the energy of the MGS to be $E_0(\eta)=\mathbf{p}_s\cdot\mathbf{v}_F=p_s v_F\eta$, one finds from Eq. (6) in the zero-temperature limit $\Delta\Omega=(E_F/16\lambda)(1-4)[1+O(\xi_0/\lambda)]<0$ showing that the TRSB state is favorable. Equation (5) with $E_0(\eta)=p_s v_F\eta$ takes the form of a self-consistency equation for $p_s(T)$. Near the phase transition temperature, p_s is small and the inequality $p_s v_F\ll 2k_BT$ is fulfilled; this allows an expansion of the hyperbolic function, which leads to $|p_s|=2\sqrt{5/3}(\hbar/\lambda)\sqrt{1-T/T_{TRSB}}$, where $k_BT_{TRSB}=(1/6)(\xi_0/\lambda)\Delta_0$ is the temperature where the second-order phase transition into the TRSB state occurs. This surface instability was discovered by Higashitani[18] in connection with a study of the paramagnetic response of the MGS to external magnetic fields. Our present calculation shows that the surface instability is not sensitive to the spatial profile of the gap; since we considered a finite value of the parameter ξ_0/λ we were able to calculate the phase-transition temperature.[24] Within the framework of the quasiclassical Green's function technique analogous results were recently obtained by Barash *et al.*[25]

For orientations of the surface different from $\alpha=\pi/4$, MGS exists only for trajectories satisfying $\mathrm{sgn}(\Delta\bar{\Delta})=-1$. The surface current is then reduced, leading to a continuous reduction of the phase transition temperature, $k_BT_{TRSB}=(1/6)(\xi_0/\lambda)\Delta_0(\cos^3\delta\alpha-\sin^3\delta\alpha)$, with misorientation $\delta\alpha=|\pi/4-\alpha|\in[0,\pi/4]$. For small misorientations, $\delta\alpha\ll 1$, the reduction is quadratic in $\delta\alpha$ and the instability is not dramatically sensitive to the exact orientation of the surface. Note, however, that the instability is quite sensitive to surface roughness.[18,25]

In conclusion, we have studied time-reversal symmetry breaking at Josephson tunnel junctions of *d*-wave superconductors assuming that a subdominant component of the order parameter is absent. For the $D\gg\xi_0/\lambda$ junction case, at temperatures $k_BT\ll D\Delta_0$ for which MGS contribute to the Josephson current with a term proportional to the first power in D, the TRSB is due to spontaneous establishment of a phase difference $\phi=\pm\pi/2$ across the junction which splits the MGS and produces a surface current. In the extreme low transparency limit, $D\ll\xi_0/\lambda$, the mechanism responsible for the instability is instead the same as for the free surface. In this case, below a phase-transition temperature $k_BT_{TRSB}=(1/6)(\xi_0/\lambda)\Delta_0$, it is energetically favorable to have Doppler shifted MGS carrying a surface current and associated screening currents upholding the Doppler shifts. The detailed spatial shape of the gap does not influence this instability.

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