Gapless time-reversal-symmetry-breaking superconductivity

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We consider a layered superconductor with a complex order parameter whose phase switches sign from one layer to the next. This system is shown to exhibit gapless superconductivity for sufficiently large interlayer pairing or interlayer hopping. In addition, this description is consistent with experiments finding signals of time-reversal symmetry breaking in high-temperature superconductors only at the surface and not in the sample bulk.

It has been proposed that the many-particle ground state of the high-temperature superconductors breaks time-reversal symmetry $\mathcal{T}$.[1,2] As yet, no clear experimental signatures of $\mathcal{T}$ violation in the superconducting bulk have been found.[3,4] Studies of $\mathcal{T}$-violating ground states for model magnetic Hamiltonians predict the nontrivially complex order parameter $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y + i\epsilon \sin k_x \sin k_y)$ which is known as a $d_{x^2-y^2} + i\epsilon d_{xy}$ $(d+id)$ order parameter.[5] This order parameter does not vanish anywhere on the Fermi surface and therefore appears to be ruled out by experimental studies of high-temperature superconductors which indicate the presence of isolated nodes on the Fermi surface.[6–8] A different set of experiments finds signs of a nodeless $\mathcal{T}$-violating order parameter at the surface of the sample. Evidence of a superconducting gap has been found at isolated point on the sample surface in scanning tunneling microscopy (STM) studies.[9] A gap feature of approximately 5 meV is always observed in c-axis tunneling between Y-Ba-Cu-O and a conventional superconductor.[6] Anomalous distributions of magnetic flux have been observed at crystal grain boundaries in $YBa_2Cu_3O_7$ (YBCO).[10] This experiment is interpreted as evidence for $\mathcal{T}$ violation.[11] In this paper, we study the properties of a complex order parameter with a two-layer unit cell. The phase of the order parameter changes sign from layer to layer. We show that interlayer pairing and tunneling render this superconductor gapless at isolated nodes. Our calculation only describes bulk properties because it relies on the symmetries of the unit cell. Because these symmetries need not be satisfied at sample boundaries, our model is consistent not only with gapless superconductivity in the bulk, but also with $\mathcal{T}$-violating gapped superconductivity at the boundaries.

Let us now investigate the behavior of multilayer $\mathcal{T}$-violating superconductivity. Studies of coupled $\mathcal{T}$-violating systems have found that it is energetically favorable for the sign of the $\mathcal{T}$ violation to be opposite in the two systems.[12] We therefore choose the order parameter to be $\Delta_{\mathbf{k}}$ in the first layer and $\Delta^*_{\mathbf{k}}$ in the second layer. We also assume an in-plane spectrum for the noninteracting electrons of $\epsilon_{\mathbf{k}}$, a hopping matrix element between layers of $t_{\perp\mathbf{k}}$, and a bilayer order parameter of $\Delta_{\perp\mathbf{k}}$. The standard approach is to define quasiparticle creation and annihilation operators $a^\dagger_{\mathbf{k}\sigma i}$ ($i = 1,2$ for the first and second planes, respectively, $\sigma = \uparrow, \downarrow$).[13] The Hamiltonian is then

$$\begin{aligned}\mathcal{H} = &\sum_{\mathbf{k}\sigma i} \epsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma i} a_{\mathbf{k}\sigma i} \\ &+ \sum_{\mathbf{k}\sigma} \left[t_{\perp\mathbf{k}} a^\dagger_{\mathbf{k}\sigma 1} a_{\mathbf{k}\sigma 2} + t^*_{\perp\mathbf{k}} a^\dagger_{\mathbf{k}\sigma 2} a_{\mathbf{k}\sigma 1}\right] \\ &- \sum_{\mathbf{k}} \Big[\Delta_{\perp\mathbf{k}} (a^\dagger_{\mathbf{k}\uparrow 1} a^\dagger_{-\mathbf{k}\downarrow 2} + a_{-\mathbf{k}\downarrow 2} a_{\mathbf{k}\uparrow 1}) + \text{c.c.} \\ &+ \Delta_{\mathbf{k}} (a^\dagger_{\mathbf{k}\uparrow 1} a^\dagger_{-\mathbf{k}\downarrow 1} + a_{-\mathbf{k}\downarrow 2} a_{\mathbf{k}\uparrow 2}) + \text{c.c.}\Big] . \end{aligned} \tag{1}$$

This expression can be rewritten using Nambu notation as

$$\mathcal{K} = \mathcal{H} - \mu\mathcal{N} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \mathbf{Q}_{\mathbf{k}} \; \Psi_{\mathbf{k}}, \tag{2}$$

where

$$\mathbf{Q}_{\mathbf{k}} = \begin{bmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} & t_{\perp\mathbf{k}} & -\Delta_{\perp\mathbf{k}} \\ -\Delta^*_{\mathbf{k}} & -\xi_{\mathbf{k}} & -\Delta^*_{\perp\mathbf{k}} & -t_{\perp\mathbf{k}} \\ t^*_{\perp\mathbf{k}} & -\Delta_{\perp\mathbf{k}} & \xi_{\mathbf{k}} & -\Delta^*_{\mathbf{k}} \\ -\Delta^*_{\perp\mathbf{k}} & -t^*_{\perp\mathbf{k}} & -\Delta_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{bmatrix} ,$$

$$\Psi_{\mathbf{k}} = \begin{bmatrix} a_{\mathbf{k}\uparrow 1} \\ a^\dagger_{-\mathbf{k}\downarrow 1} \\ a_{\mathbf{k}\uparrow 2} \\ a^\dagger_{-\mathbf{k}\downarrow 2} \end{bmatrix}, \tag{3}$$

$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu = -2t(\cos k_x + \cos k_y) - \mu$, $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y + i\epsilon \sin k_x \sin k_y)$, and both $\Delta_{\perp\mathbf{k}}$ and $t_{\perp\mathbf{k}}$ are taken to be real. Writing $\Delta_{\mathbf{k}} = \Delta_{R\mathbf{k}} + i\Delta_{I\mathbf{k}}$, we find that $\mathbf{Q}_{\mathbf{k}}$ has energy eigenvalues $E_\pm(\mathbf{k})$ that satisfy

$$\begin{aligned} E^2_\pm(\mathbf{k}) = &\, \xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2 + \Delta^2_{\perp\mathbf{k}} + t^2_{\perp\mathbf{k}} \\ &\pm 2\sqrt{(\xi_{\mathbf{k}} t_{\perp\mathbf{k}} + \Delta_{\perp\mathbf{k}}\Delta_{R\mathbf{k}})^2 + \Delta^2_{I\mathbf{k}}(t^2_{\perp\mathbf{k}} + \Delta^2_{\perp\mathbf{k}})}. \end{aligned} \tag{4}$$

The spectrum for $E_-(\mathbf{k})$ vanishes when

$$\xi_{\mathbf{k}} = t_{\perp\mathbf{k}}\alpha_{\mathbf{k}} \; , \Delta_{R\mathbf{k}} = \Delta_{\perp\mathbf{k}}\alpha_{\mathbf{k}}, \tag{5}$$

and

$$\alpha_{\mathbf{k}}^2 = 1 - \frac{\Delta_{I\mathbf{k}}^2}{t_{\perp\mathbf{k}}^2 + \Delta_{\perp\mathbf{k}}^2} , \tag{6}$$

which is consistent with experiments that find a bulk order parameter with a d-wave-like node.[6–8,14,15] If the phase of the order parameter were the same in neighboring planes, the corresponding energy eigenvalue $E'_{\pm}(\mathbf{k})$ would satisfy

$$E'^2_{\pm}(\mathbf{k}) = (\xi_{\mathbf{k}} \pm t_{\perp\mathbf{k}})^2 + (\Delta_{I\mathbf{k}})^2 + (\Delta_{R\mathbf{k}} \pm \Delta_{\perp\mathbf{k}})^2 \tag{7}$$

instead of Eq. (4) and hence be nodeless except for a special value of $\Delta_{\perp\mathbf{k}}$.

In order to have a nodeless order parameter, we must be able to satisfy Eqs. (5) and (6). The constraint that $\alpha_{\mathbf{k}}$ be real requires

$$t_{\perp\mathbf{k}}^2 + \Delta_{\perp\mathbf{k}}^2 \geq \Delta_{I\mathbf{k}}^2 . \tag{8}$$

This intuitive result tells us that the combined effect of interlayer pairing and interlayer tunneling has to be sufficiently large in order to overcome the gap due to the imaginary component of the order parameter. The existence of a solution to Eq. (5) also requires $|\Delta_{\mathbf{k}}| \geq \Delta_{\perp\mathbf{k}}$.

The zeros of Eq. (4) need not lie on the 45° ($k_x = \pm k_y$) nodal line of the pure $d_{x^2-y^2}$ order parameter. To first order in $t_\perp/t$ and $\Delta_\perp/\Delta_0$ and in the $t >> \epsilon\Delta_0$ limit, the nodal wave vector $\mathbf{k}$ lies at

$$k_x \approx \frac{\pi}{2} + \alpha_{\mathbf{k}} \left(\frac{t_{\perp\mathbf{k}}}{4t} - \frac{\Delta_{\perp\mathbf{k}}}{2\Delta_0} \right) , \tag{9}$$

$$k_y \approx \frac{\pi}{2} + \alpha_{\mathbf{k}} \left(\frac{t_{\perp\mathbf{k}}}{4t} + \frac{\Delta_{\perp\mathbf{k}}}{2\Delta_0} \right) . \tag{10}$$

The node is shifted from the 45° nodal line to an angle

$$\theta = \arctan(k_y/k_x) \approx \pi/4 + \frac{\alpha_{\mathbf{k}}\Delta_{\perp\mathbf{k}}}{\pi\Delta_0}, \tag{11}$$

which is independent of $t_{\perp\mathbf{k}}$ to lowest order. In contrast, the magnitude of $\mathbf{k}$,

$$|\mathbf{k}| \approx \sqrt{2} \left(\frac{\pi}{2} + \frac{\alpha_{\mathbf{k}} t_{\perp\mathbf{k}}}{4t} \right) , \tag{12}$$

is independent of $\Delta_{\perp\mathbf{k}}$ to lowest order. There are now two nodes because $\alpha_{\mathbf{k}}$ may be either positive or negative. These effects (node splitting and angular shift of 10°) have been observed in angular-resolved photoemission studies of $Bi_2Sr_2CaCu_2O_8$.[16] A similar analysis of the momentum shifts has been performed for the case of a purely real order parameter by Lee and co-workers.[17,18] Our expressions are valid in this case with $\alpha_{\mathbf{k}} = \pm 1$ in Eqs. (9)–(12). Therefore, the bulk photoemission experiments cannot distinguish qualitatively between a purely real and an alternating complex order parameter.

We may also consider other alternating complex order parameters. For instance, our alternating order parameter might be purely complex. Requiring that $\Delta_{R\mathbf{k}} = 0$ is equivalent to imposing an additional constraint upon Eq. (5). This equation will only have a solution in the unlikely case that either $\Delta_{\perp\mathbf{k}} = 0$ or $\alpha_{\mathbf{k}} = 0$. An order parameter with $s + id$ symmetry[19] would only satisfy Eqs. (5) and (6) and if the s component is smaller than $\Delta_{\perp\mathbf{k}}$.

The parameters we choose depend on the material we wish to study. For example, neighboring planes in YBCO may be so strongly coupled that they prefer their order parameters to have the same complex phase. In that case, the bilayer in YBCO may be treated as a single composite $\mathcal{T}$-violating superconducting layer coupled to another composite layer with the opposite sign of $\mathcal{T}$ violation. In order to observe a node, Eq. (8) must be satisfied for the coupling of the composite layers. This description should be consistent with the spin gap calculations for bilayer systems.[20] One may also consider three-layer materials (which arise in the Bi, Tl, and Hg cuprates) or even the effect of intermediate normal layers sandwiched between superconducting layers with alternate signs of $\mathcal{T}$ violation.

It is expected that a $\mathcal{T}$-violating layer will couple to an electron or neutron spin as if it induced a local magnetic field. At long wavelengths, this effect would be suppressed because of the alternating chirality. However, a neutron with momentum $q = (0, 0, \pi/d)$, where d is the distance between planes, will couple to the chirality oscillation. If the coupling is strong enough, a peak at low energies near this momentum should be observable in neutron scattering. The size of this feature will depend on the coupling strength, which has not been accurately calculated. However, muon spin rotation experiments, which probe the local magnetic field, fail to find an effective magnetic field larger than that due to the Cu nuclei.[4] In contrast, similar studies of UPt_3, which is believed to have a $d + id$ order parameter that does not alternate, saw this effect.[21]

Our postulated state can have interesting effects in external magnetic fields if the energy scales allow these effects to occur below H_{c2}. The energy gained aligning the chirality in all of the layers with a c-axis magnetic field may be contrasted with the energy gained alternating the chirality in neighboring layers.[12] If the coupling to the magnetic field is unusually large, there may be an $H^* < H_{c2}$ above which it becomes energetically favorable for the layers to violate $\mathcal{T}$ without alternating phase. Hysteretic effects would also be expected for samples cooled in sufficiently large magnetic fields.

There are three modes made from linear combinations of the phases of the order parameters $\Delta_{\mathbf{k}}$ (the first layer), $\Delta_{\mathbf{k}}^*$ (the second layer), and $\Delta_{\perp\mathbf{k}}$. The mode where the phases are added is the charged Anderson-Bogoliubov mode which is lifted to the plasmon frequency. The other two linear combinations will have interesting dynamics and, as recently pointed out by Kuboki and Lee,[17] should be observable as a Raman signal. However, because of the damping effects that arise when the order parameter is gapless, investigation of these modes will probably not provide a criterion for differentiating between our oscillating $d + id$ order parameter and the purely real one proposed by Kuboki *et al.*[22,23] The effect of a complex order parameter on Josephson tunneling[24–26] should also be studied.

The $\mathcal{T}$-violating component of the alternating order parameter should have a transition temperature $T^* < T_c$ where T_c is the bulk transition temperature. The experimental results that we attribute to $\mathcal{T}$ violation are therefore expected to disappear for temperatures above T^*. In fact, recent experiments in oxygenated samples of YBCO have found a second transition at 30 K in T_2 measurements.[27]

In this paper we propose that a certain class of $\mathcal{T}$-violating superconducting ground states is consistent with numerous experiments. There remain significant inconsistencies. Most notably, several experiments have been interpreted as finding zero Hall conductivity. In contrast, $\mathcal{T}$ violation is consistent with a nonzero value of the Hall conductivity σ_{xy}. It is difficult to compare the limits on the Hall conductivity set by experiment with theoretical predictions because this quantity has not yet been accurately calculated.[2] Gauge field fluctuations are expected to reduce the size of the Hall conductivity.[2,18,28] It is also known that fluctuation effects tend to reduce the quasiparticle gap in single-layer anyon models[29] and hence the size of the $\mathcal{T}$-violating order parameter Δ_I. This effect is expected to be enhanced in a double-layer anyon model.[23]

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