Magnetic Induction of $d_{x^2-y^2}$ + i d_{xy} Order in High-T_c Superconductors

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I propose that the phase transition in $Bi_2Sr_2CaCu_2O_8$ recently observed by by Krishana et al [Science **277**, 83 (1997)] is the development of a small d_{xy} superconducting order parameter phased by $\pi/2$ with respect to the principal $d_{x^2-y^2}$ one to produce a minimum energy gap Δ. The violation of both parity and time-reversal symmetry allows the development of a magnetic moment, the key to explaining the experiment. The origin of this moment is a quantized boundary current of $I_B = 2e\Delta/h$ at zero temperature.

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In a recent paper Krishana et al[1] have reported a phase transition in $Bi_2Sr_2CaCu_2O_8$ induced by a magnetic field and characterized by a kink in the thermal conductivity as a function of field strength, followed by a flat plateau. The high-field state is also superconducting. They argued from the existence of this plateau that heat transport by quasiparticles was zero in the new state and that this probably indicated the development of an energy gap. The transition has the peculiarity of being easily induced by small fields. Krishana et al report the empirical relation $T_c \propto \sqrt{B}$, although over the limit field range of $0.6T < B < 5T$, and also that the transition sharpens as T_c is reduced.

I propose that the new high-field state is the parity and time-reversal symmetry violating $d_{x^2-y^2} + id_{xy}$ superconducting state proposed long ago by me[2], which has many properties in common with quantum hall states, including particularly chiral edge modes and exactly quantized boundary currents. The essential point of my argument is that the state must have a magnetic moment in order to account for the experiment, and this is possible only if it violates both parity and time-reversal symmetry. The development of $s + id$ order, for example, or high-momentum Cooper pairing[3] are both ruled out for this reason, as is a restructuring of the vortex lattice.

My hypothesis leads, through reasoning described below, to the model free-energy functional

$$\frac{F}{L^2} = \frac{1}{6\pi}\frac{\Delta^3}{(\hbar v)^2} - \frac{1}{\pi}\frac{eB}{\hbar c}\Delta\tanh^2(\frac{\beta\Delta}{2}) - \frac{4}{\pi}\frac{(k_BT)^3}{(\hbar v)^2}$$

$$\times\left\{\frac{(\beta\Delta)^2}{2}\ln[1+e^{-\beta\Delta}] + \int_{\beta\Delta}^{\infty}\ln[1+e^{-x}]xdx\right\} \quad , \quad (1)$$

where Δ is the induced energy gap and $v = \sqrt{v_2 v_2}$ is the root-mean-square velocity of the d-wave node. There are three key steps leading to this functional:

1. The adoption of conventional quasiparticles at four nodes as the low-energy exitation spectrum of the parent $d_{x^2-y^2}$ state.
2. The derivation of a relation between the minimum energy to inject a quasiparticle in the bulk interior and a quantum-mechanical boundary current.
3. A guess as to the temperature dependence of this boundary current based on legitimate but model-dependent calculations.

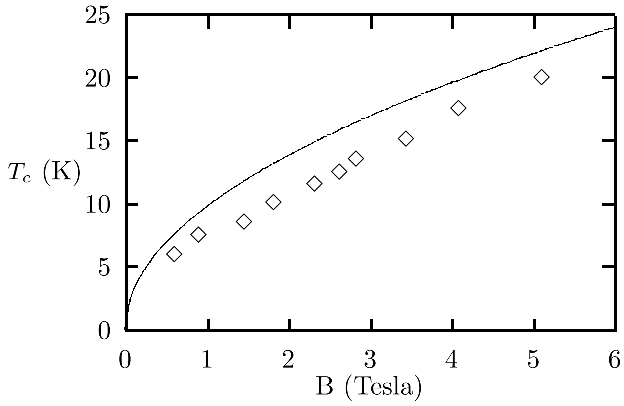

FIG. 1: Comparison of measured transition temperature versus magnetic field (diamonds) with Eq. (5).

The last of these, which I shall defend below, is pure phenomenology, so this is a theory of energy scales and *not* a theory of the transition. The value of the node velocity is fixed by experiment, in particular photoemission bandwidth[4] and the temperature dependence of the penetration depth in YBCO[5,6]. Following Lee and Wen[7] I shall use the values $v_1 = 1.18 \times 10^7$ cm/sec and $v_1/v_2 = 6.8$, or $\hbar v = 0.30$ eV Å. The uncertainty in this number is about 10%. At zero temperature the free energy is minimized by

$$\Delta_0 = \hbar v\sqrt{2\frac{eB}{\hbar c}} \quad , \quad (2)$$

and has the value

$$\frac{F_0}{L^2} = -\frac{1}{3\pi}\frac{\Delta_0^3}{(\hbar v)^2} \quad . \quad (3)$$

A finite temperature I find a weakly first-order transition to a state with $\Delta = 0$ at

$$k_B T_c = 0.52 \; \Delta_0 \quad . \tag{4}$$

This is plotted against the experiment in Fig. 1. It will be seen to account for both the functional form of the transition temperature and its absolute magnitude with no adjustable parameters.

The assumption of conventional quasiparticles at d-wave nodes leads to the repulsive Δ^3 and free-quasiparticle entropy terms in Eq. (1). The model here is not critical, since only the node matters, so let us use the BCS Hamiltonian

$$\mathcal{H} = \sum_{ks} \varepsilon_k \; c_{ks}^\dagger c_{ks} + \sum_{kk'} V_{kk'} \; c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow} \quad . \tag{5}$$

As usual we consider variational ground states of the form

$$|\Psi> = \prod_k \left\{ u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \right\} |0>$$

$$|u_k|^2 + |v_k|^2 = 1 \quad , \tag{6}$$

and minimize the expected energy

$$<\Psi|\mathcal{H}|\Psi>$$

$$= 2 \sum_k \varepsilon_k |v_k|^2 + \sum_{kk'} V_{kk'} (u_k v_k^*)(u_{k'}^* v_{k'}) \tag{7}$$

to obtain

$$u_k = \sqrt{\frac{1}{2}\left[1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + |\Delta_k^2|}} \right]}$$

$$v_k = \sqrt{\frac{1}{2}\left[1 - \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + |\Delta_k^2|}} \right]} \frac{\Delta_k}{|\Delta_k|} \quad , \tag{8}$$

where

$$\Delta_k = \sum_{k'} V_{kk'} (u_{k'}^* v_{k'}) \quad , \tag{9}$$

or

$$\Delta_k = - \frac{1}{2} \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + |\Delta_{k'}|^2}} \quad . \tag{10}$$

Equivalently we may take Eqs. (8) to define $|\Psi>$ in terms of Δ_k and minimize the expected energy

$$<\Psi|\mathcal{H}|\Psi> = \sum_k \varepsilon_k \left[1 - \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + |\Delta_k|^2}} \right]$$

$$+ \frac{1}{4} \sum_{kk'} V_{kk'} \left[\frac{\Delta_k^*}{\sqrt{\varepsilon_k^2 + |\Delta_k|^2}} \right] \left[\frac{\Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + |\Delta_{k'}|^2}} \right] \quad , \tag{11}$$

to obtain Eq. (10). Regardless of whether the extremal condition is met the expected energy of the quasiparticle

$$|\Psi_{k\uparrow}> = (u_k^* c_{k\uparrow}^\dagger + v_k^* c_{-k\downarrow}) |\Psi> \tag{12}$$

is

$$<\Psi_{k\uparrow}|\mathcal{H}|\Psi_{k\uparrow}> = <\Psi|\mathcal{H}|\Psi> + \sqrt{\varepsilon_k^2 + |\Delta_k|^2} \quad . \tag{13}$$

The prototypical $d_{x^2-y^2} + i d_{xy}$ state is

$$\varepsilon_k = -2t \Big[\cos(k_x b) + \cos(k_y b) \Big] \tag{14}$$

$$\Delta_k = \Delta_{x^2-y^2} \Big[\cos(k_x b) - \cos(k_y b) \Big]$$

$$+ i \Delta_{xy} \sin(k_x b) \sin(k_y b) \quad . \tag{15}$$

The velocity in Eq. (1) is related to the model parameters by

$$\hbar v_1 = \sqrt{8} t b \qquad \hbar v_2 = \sqrt{2} \Delta_{x^2-y^2} b \qquad v = \sqrt{v_1 v_2} \quad . \tag{16}$$

Assuming now that the extremal condition requires Δ_{xy} to be zero, so that the native ground state has only $d_{x^2-y^2}$ order, and then forcing the minimum quasiparticle energy to be Δ, one finds that the energy is minimized when

$$\Delta_{xy}^2 = \left[\begin{array}{cc} \Delta^2 - (q/\hbar v)^2 & ; \; q \leq \Delta/\hbar v \\ 0 & ; \; q > \Delta/\hbar v \end{array} \right] \quad , \tag{17}$$

where q is the distance to the node in symmetrized units, and equals

$$\delta <\Psi|\mathcal{H}|\Psi> = - \sum_k (\varepsilon_k^2 + |\Delta_k|^2) \delta \left[\frac{1}{\sqrt{\varepsilon_k^2 + |\Delta_k|^2}} \right]$$

$$= \frac{2}{\pi} \hbar v L^2 \int_0^{\Delta/\hbar v} \left[\frac{1}{q} - \frac{\hbar v}{\Delta} \right] q^3 dq = \frac{L^2}{6\pi} \frac{\Delta^3}{(\hbar v)^2} \quad . \tag{18}$$

The quasiparticle contribution to the finite-temperature free energy under these circumstances is

$$\frac{F_{\rm quasi}}{L^2} = - \frac{4}{\pi} \; k_B T$$

$$\times \int_0^\infty \ln[1+\exp(-\beta\sqrt{(\hbar q)^2+\Delta_{xy}^2})]qdq \quad . \tag{19}$$

Let us next consider the zero-temperature magnetic moment, which is due to a circulating boundary current of

$$I_B = 2\frac{e}{h}\Delta_0 \quad . \tag{20}$$

This works out to 0.13 μA for a gap of 1.64 meV induced by a field 1 Tesla. Boundary currents of this magnitude are known to result from the development of a T-violating order parameter of this size[8], so the issue is not the existence of these currents or their disappearance when the second order parameter vanishes but rather their specific functional dependence on Δ and sense of circulation. T and P must both be violated for the boundary currents to generate a moment. The $s+id$ state, for example, will not work because its reflection symmetry about the x-axis forces the currents at the +y and -y edges to flow in the same direction, whereas flow in opposite directions is required to generate a moment.

The $d_{x^2-y^2}+id_{xy}$ state differs fundamentally from $s+id$ conventional s-wave states in *not* being continuously deformable to a fermi sea on a sample with edges, although it can be so deformed on a torus. This is the property underlying Wiegmann's concept of a "topological superconductor"[9]. On a torus we may write

$$|\Phi> = \prod_k \exp\Big[i\Psi_k^\dagger\theta_k\cdot\tau_k\Psi_k\Big]|\Phi_0> \quad , \tag{21}$$

where

$$\Psi_k = \begin{bmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{bmatrix}$$

$$\tau_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \tau_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \tau_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad , \tag{22}$$

as usual, and thus continuously deform the fermi sea $|\Phi_0>$ into any BCS superconducting state $|\Phi>$ we like by appropriate choice of the function θ_k. On a sample with edges, however, this makes no sense because k is not a good quantum number. The best we can do is substitute the time-reversed orbital pairs $\exp(\pm ikx)\ \sin(n\pi y/L)$, where L is the sample width and n is an integer, for the plane waves $\exp(\pm i\mathbf{k}\cdot\mathbf{r})$ in the above expression, in which case we find the order parameter Δ_k to be *even* under parity in the y-direction, a property fundamentally incompatible with $d+id$ pairing. Thus we confront a problem similar to the one encountered in the vortex lattice - the solution of which was the invention of the Bogoliubov-DeGennes equations - namely that excitation of Cooper pairs into time-reversed orbital pairs makes no sense in a magnetic field. In this case, of course, the violation of parity and time-reversal invariance comes not from an external magnetic field but from the vacuum itself.

The $d_{x^2-y^2}+id_{xy}$ state is, however, continuously deformable into a doubly-occupied Landau level. This is demonstrated with the following simple lattice example. Let

$$\mathcal{H}_{HF} = 2t\sum_k \Big\{ \Big[\cos(k_x b)+\cos(k_y b)\Big]\Psi_k^\dagger\tau_3\Psi_k$$

$$+\Big[\cos(k_x b)-\cos(k_y b)\Big]\Psi_k^\dagger\tau_1\Psi_k$$

$$+2m\sin(k_x)\sin(k_y)\Psi_k^\dagger\tau_2\Psi_k\Big\} \tag{23}$$

be the Hartree-Fock Hamiltonian for a $d_{x^2-y^2}+id_{xy}$ superconductor on a square lattice, where m is a constant characterizing the size of the energy gap. Then the Hamiltonian $U^\dagger(\theta)\ \mathcal{H}_{HF}\ U(\theta)$, where

$$U(\theta) = \prod_j U_j(\theta) = \prod_j \exp\Big\{\frac{\theta}{2}$$

$$\Big[1-2(-1)^{\ell_j}+(-1)^{\ell_j+m_j}\Big](c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{j\downarrow}c_{j\uparrow})\Big\} \quad , \tag{24}$$

with ℓ_j and m_j denoting the x- and y- coordinates of the j^{th} lattice site, interpolates between $\mathcal{H}_{HF}$ at $\theta=0$ and a lattice Landau level Hamiltonian at $\theta=\pi/4$, all the while having the same eigenvalue spectrum due to the unitarity of $U(\theta)$[10,11]. More specifically, since

$$c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{j\downarrow}c_{j\uparrow} = i\psi_j^\dagger\tau_2\psi_j \quad , \tag{25}$$

the site transformations repeat with the pattern shown in Fig. 2, where

$$U_1(\frac{\pi}{4}) = 1 \qquad U_2(\frac{\pi}{4}) = \frac{1-i\tau_2}{\sqrt{2}}$$

$$U_3(\frac{\pi}{4}) = \frac{1+i\tau_2}{\sqrt{2}} \qquad U_4(\frac{\pi}{4}) = i\tau_2 \quad , \tag{26}$$

so we have for the transformed bond Hamiltonian from site 2 to site 1

$$U_1^\dagger\ (\frac{\tau_3+\tau_1}{\sqrt{2}})\ U_2 = (\frac{\tau_3+\tau_1}{\sqrt{2}})\ (\frac{1-i\tau_2}{\sqrt{2}}) = \tau_3 \quad , \tag{27}$$

and so forth for the other bonds. The transformation on the diagonal bonds give $\pm i\tau_3$, as appropriate for magnetic bands on a lattice.

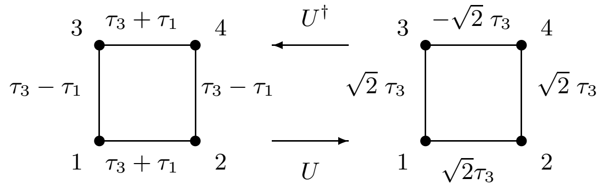

FIG. 2: Illustration of unitary transformation between the $d_{x^2-y^2}+id_{xy}$ superconducting state and a filled Landau level on a lattice.

Let us now imagine wrapping a ribbon of $d_{x^2-y^2}+id_{xy}$ superconductor into a loop and adiabatically inserting magnetic flux hc/e through this loop following the procedure used in a quantum hall thought experiment[12]. This insertion commutes with the rotation of the superconductor into the quantum hall state by virtue of the gap and therefore has the same effect in the two cases, i.e. to "pump" one $\uparrow$ and one $\downarrow$ quasiparticle from one edge to the other. The edge currents in either case may be identified by separating this spectral flow into

1. Transfer of a state from the chemical potential at the left edge to the *lowest* available energy in the bulk interior.

2. The mirror image of this at the right edge.

Only the lowest-energy bulk state matters because the anti-crossing rule prevents any higher-energy states from flowing to the chemical potential. The edge current is then given by Eq. (20), where Δ_0 is the difference in energy between this lowest-energy bulk excitation and the chemical potential. This result is exact.

Flux addition also induces bulk supercurrent, formal gauge transformations being not so innocuous in a superconductor, but this is easily removed by causing the ring circumference L to diverge, since the energy in question is

$$\delta E_{\rm bulk} = \frac{\hbar^2}{2m}(\frac{2\pi}{L})^2 \int n_s(\vec{r}) d\vec{r} \quad , \tag{28}$$

where n_s is the superfluid density, which falls off as 1/L. Equivalently one may say that there is is a physical difference between current already present and current induced by the injected flux.

The final matter for consideration is the reduction of this moment by thermal excitation of quasiparticles. This is, unfortunately, sensitive to details and thus difficult to calculate with sufficient accuracy to describe the phase transition. It can be understood simply in terms of the flux Hamiltonian obtained by rotating Eq. (23) by $\theta = \pi/4$. This consists of upper and lower quantum hall bands with opposite quantizations, these being manifested primarily in the states of energy near $\Delta = 4tm$. Evaluating the Hall conductance of this model by the Kubo formula in the limit of small m we find that[11]

$$\sigma_{xy} = \frac{e^2}{h} \int_0^\infty \tanh\left[\frac{\beta\Delta}{2}\sqrt{1+x}\right] \frac{dx}{(1+x)^{3/2}} \quad . \tag{29}$$

The strong quenching effect at $k_B T \geq \Delta$ occurs because free quasiparticles contribute a Hall conductance opposite to that of the ground state. Assuming now that Δ varies slowly in space and equals zero at the sample edge, we may integrate in from the edge to obtain

$$I_B \simeq 2\frac{e}{h} k_B T \int_0^\infty \ln\left[\cosh(\frac{\beta\Delta}{2}\sqrt{1+x})\right] \frac{dx}{(1+x)^2} \quad . \tag{30}$$

The version of this appropriate to Eq. (17) is

$$I_B \simeq 4\frac{e}{h} k_B T \ln\left[\cosh(\frac{\beta\Delta}{2})\right] \quad . \tag{31}$$

This is quite close to the functional form appearing in Eq. (1) in the range of interest, saturates to linearity in Δ at zero temperature, becomes exponentially quenched for temperatures $k_B T >> \Delta$, but gives no phase transition. The phenomenological function I chose is merely an approximation to this one constrained to be analytic in Δ and odd. The proportionality of T_c to Δ_0, however, is expected on general grounds because there is no other energy scale in the problem.

The complete absence of thermal transport above T_c in the experiment is not explained by thermal activation to a gap of order Δ_0, as this is simply too small to freeze out all the quasiparticles. This criticism, however, applies equally well to any theory of the effect one would care to consider, for it is physically unreasonable for a gap much larger than $k_B T_c$ to develop spontaneously. I therefore believe that absence of transport is an effect of enhanced scattering and trapping of quasiparticles in the new state and is a detail to be worked out once the symmetry of the second order parameter is established. There is certainly the potential for violent scattering in the $d_{x^2-y^2}+id_{xy}$ state given the inhomogeneity of the magnetic field due to the vortex lattice and the possibility that the transition is weakly first-order, but it is a mistake to use this as a criterion for deciding whether the symmetry I have identified is the right one.

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