

Magnetic Field Induced id_{xy} Order in a $d_{x^2-y^2}$ Superconductor[†]

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Abstract

The interaction between planar quasiparticles in a $d_{x^2-y^2}$ superconductor and quantized vortices associated with a magnetic field perpendicular to the plane is shown to induce a pair potential with d_{xy} symmetry, out of phase with $d_{x^2-y^2}$ order. A microscopic calculation of a process involving quasiparticle scattering by the supercurrent around a vortex and Andreev reflection from its core is presented. Other processes also leading to an id_{xy} pair potential are discussed. It is argued that such a fully gapped state may be the high field low temperature phase observed by Krishana, Ong et al in magnetothermal conductivity measurements of superconducting single crystal *Bi* – 2212.

I. Introduction

Recent measurements of in-plane thermal conductivity K_T in superconducting single crystal *Bi* – 2212 (1,2) for $T \ll T_c$ and $H \ll H_{c2}$ show a rather sharp change in its magnetic field dependence at a field H_o (of order a Tesla or more) which depends on temperature T_o ($\sim 10K$) nearly quadratically. For $H > H_o$ and $T < T_o$, K_T hardly changes with the magnetic field, in sharp contrast to the decrease exhibited below H_o . This suggests (1,2) a transition from a $d_{x^2-y^2}$ phase to a fully gapped phase at $H_o(T_o)$ with an exponentially small density of heat current carrying quasiparticles. I show here that in a magnetic field, a $d_{x^2-y^2}$ superconductor necessarily develops a pair amplitude of id_{xy} symmetry at low enough temperature, leading to a gapped phase which might be the basis of the observed K_T behaviour.

In the superconducting state, which has vortices due to the external magnetic field, the gap quasiparticles interact with the circulating supercurrent around each vortex, as well as with the order parameter inhomogeneity associated with the vortex core. These interaction terms are obtained explicitly (Section II). The first scatters quasiparticles, eg. it changes their phase. The second causes Andreev reflection. Due to their combined effect, a particle interacting with a vortex comes out as a phase shifted hole, i.e. the vortex is a source of out of phase pair potential. This term is calculated in Section III, and is shown to have id_{xy} symmetry. Thus, at each vortex,

id_{xy} order is necessarily induced. If the vortices are well ordered spatially, there is a homogeneous Δ_{xy} term in the free energy, proportional to the density of vortices or the magnetic field B . I argue (Section IV) that this could be the phase suggested by the observations of Krishana et al (1,2). Related results and questions, such as the temperature and field scale of the transition, effect of vortex lattice periodicity are also discussed (Section IV). Recently, Laughlin has proposed (3) that in a magnetic field, the pair potential is of the form $d_{x^2-y^2} + \alpha id_{xy}$ where α is real, and that there is a (first order) transition to such a phase in the (H, T) plane. The proposal is based on a mapping of a $d_{x^2-y^2} + \alpha id_{xy}$ Hamiltonian to a lattice quantum Hall system, and on exploiting quantum Hall current ideas. Here, I describe a detailed microscopic mechanism for id_{xy} order, and calculate its size.

II. Quasiparticle Vortex Interaction

I show here that the quasiparticle Hamiltonian in the mixed state can be written as a sum of two classes of terms; one is that of the uniform superconductor, and the other describes the effect of vortices on quasiparticles. Since quasiparticles are well defined in the superconducting state, a mean field Hamiltonian is adequate. In the homogeneous superconductor, the otherwise free electrons move in a real, spatially homogeneous pair potential $\tilde{\Delta}$ with $d_{x^2-y^2}$ symmetry, eg. with $\tilde{\Delta}_k = \Delta_o (\cos k_x a - \cos k_y a)$ for nearest neighbour pairing. In the presence of vortices, the pair potential $\Delta(\vec{r}, \vec{r}')$ is inhomogeneous and complex. Its phase changes by 2π on going round a vortex, and the magnitude must vanish at each vortex core \vec{R}_ℓ . Separating out the phase part, we can write $\Delta(\vec{r}, \vec{r}')$ as

$$\Delta(\vec{r}, \vec{r}') = \Delta_m(\vec{r} - \vec{r}', \vec{R} - \vec{R}_\ell) \exp\left[\frac{i}{2} \left\{ \sum_\ell \theta(\vec{r} - \vec{R}_\ell) + \theta(\vec{r}' - \vec{R}_\ell) \right\}\right].$$

Here \vec{R} is the centre of mass coordinate $(\vec{r} + \vec{r}')/2$. Making a gauge transformation $\tilde{\psi}_\uparrow^+(\vec{r}) \exp\left\{\frac{i}{2} \sum_\ell \theta(\vec{r} - \vec{R}_\ell)\right\} \Rightarrow \psi_\uparrow^+(\vec{r})$, the quasiparticle Hamiltonian becomes

$$H = \frac{1}{2m} \sum_\sigma \int d\vec{r} \psi_\sigma^+(\vec{r}) (\vec{p} + m\vec{v}_s(\vec{r}))^2 \psi_\sigma(\vec{r}) \quad (1)$$

$$+ \int d\vec{r} d\vec{r}' [\Delta_m(\vec{r} - \vec{r}', \{\vec{R} - \vec{R}_\ell\}) \psi_\uparrow^+(\vec{r}) \psi_\downarrow^+(\vec{r}') + h.c.] \quad (1) \quad (2)$$

where

$$\vec{v}_s(\vec{r}) = (2m)^{-1} \sum_\ell \{ \hbar \vec{\nabla} \theta(\vec{r} - \vec{R}_\ell) - 2e\vec{A}(\vec{r} - \vec{R}_\ell)/c \}$$

is the in-plane gauge invariant superfluid velocity. In the London limit, Δ_m can be considered spatially uniform (\vec{R} independent) with $d_{x^2-y^2}$ symmetry, except for

order parameter deficits $\delta\Delta_m$ around each vortex. (These have to be determined self consistently)

The quasiparticle Hamiltonian Eq.(1) can be written as the sum of an unperturbed term H_o , and the remainder describing quasiparticle vortex interaction. In the momentum representation, and the Nambu formalism, one has

$$H = H_o + (H_\theta + H_m + H_{KE}) \quad (4a)$$

where

$$H_o = \sum_k a_k^\dagger (\tilde{\epsilon}_k \tau_3 + \Delta_k \tau_1) a_k \quad (4b)$$

$$H_\theta = \sum_{k,q} a_k^\dagger \hbar \vec{k} \cdot \vec{v}_s(\vec{q}) a_{k-q} \quad (4c)$$

$$H_m = -\Delta_o \sum_{k,q} f_{kq} (a_k^\dagger \tau_1 a_{k-q}) \quad (4d)$$

and H_{KE} is the superfluid kinetic energy. Eq.(4b) describes a $d_{x^2-y^2}$ superconductor. H_θ is the quasiparticle superfluid velocity interaction and H_m is the inhomogeneous pair potential due to the vortex core, with $-\Delta_o f_{\vec{k},\vec{q}}$ being the Fourier transform of the deficit $\delta\Delta_m(\vec{r}-\vec{r}', \{\vec{R}-\vec{R}'\})$. The superfluid velocity $\vec{v}_s(\vec{q})$ is assumed to have the standard Ginzburg Landau form

$$\vec{v}_s(\vec{q}) = \frac{\lambda^2}{2m} \frac{1}{2A} \sum_{\vec{q}\ell} \left(\frac{i\vec{q} \times \hat{e}_z}{1 + \lambda^2 q^2} \right) e^{i\vec{q} \cdot \vec{R}_\ell} \quad (5)$$

away from the vortex cores. For wavevector transfers $q \ll \lambda^{-1}$, this has the unscreened form independent of λ^2 . We now use the mean field Hamiltonian Eq.(4) to show that id_{xy} order is induced in a magnetic field.

III. id_{xy} Order

The form Eq.(4) is natural for looking into the question of the pair potential in the presence of a magnetic field. In its absence, H_θ, H_m and H_{KE} vanish, and Δ_k in Eq.(4b) is just the $d_{x^2-y^2}$ uniform value. We imagine H_o and H_m being turned on, and ask if any out of phase order is induced, i.e., in the notation above, whether $\lambda_k = \langle a_k^\dagger \tau_2 a_k \rangle \neq 0$. We are also interested in the k dependence of λ_k . We shall calculate λ_k with H_θ and H_m as perturbations. This enables us to focus directly on processes leading to a particular order parameter symmetry.

The first nonvanishing contribution to λ_k comes from a term linear in H_θ as well as in H_m ; there are no contributions to second order, either in H_θ or H_m . The process is diagrammatically represented in Fig.1a. It describes the combined effect

of quasiparticle scattering from state \vec{k} to $(\vec{k} - \vec{q})$ by the supercurrent due to the vortex, and Andreev reflection from $(\vec{k} - \vec{q})$ to a hole of momentum $-\vec{k}$ caused by the inhomogeneous order parameter magnitude associated with the vortex core.

The pair amplitude λ_k can be calculated from Fig.(1a), and Eq.(4). At $T = 0$, it is

$$\langle a_k^\dagger \tau_2 a_k \rangle = \sum_q (\Delta_o f_{kq}) \{ (\hbar^2/2mA) (\vec{k} \times i\vec{q} \cdot \hat{e}_z) q^{-2} \} [(\epsilon_{k-q}/E_k E_{k-q} (E_k + E_{k-q}))]. \quad (6)$$

In Eq.(6), the first bracket is the pair potential due to the vortex core; approximately, $f_{kq} = f_q \{ \cos(k_x + q_x)a - \cos(k_y + q_y)a \}$ where $\sum_q f_q = 1$. The second factor, in curly brackets, is the quasiparticle supercurrent coupling $\vec{k} \cdot \vec{v}_s(\vec{q})$ for $q \gg \lambda^{-1}$ (the regime of interest). The last term arises from the intermediate state sum, with $E_k = |(\epsilon_k^2 + \Delta_k^2)^{1/2}|$. On expanding the integrand as a power series in q , the leading term is

$$\lambda_k = \alpha (n_v/n) (\Delta_o/E_k) (\hat{k}_x \hat{k}_y) \quad (7)$$

Here, α is a constant of order unity, and n_v is the vortex density.

We notice that λ_k has d_{xy} symmetry. It is a result of the coupling between the internal and centre of mass states of the pair near a vortex. In the Fourier representation used, the former is described by the momentum \vec{k} , and the latter by \vec{q} . The quasiparticle supercurrent coupling has a structure $(\vec{k} \times \vec{q}) \cdot \hat{e}_z$ that affects the angular state of a pair, through the constituent single particle dispersion. Algebraically, $(\vec{k} \times \vec{q}) \cdot \hat{e}_z (\epsilon_{\vec{k}-\vec{q}}) \simeq k_x k_y (q_x^2 - q_y^2)$. This term is clearly nonlocal, ie. it arises from higher powers of q or of gradient/derivative terms. Thus, a fully local, semiclassical theory, working in terms of a spatially slowly varying superfluid velocity $\vec{v}_s(\vec{r})$ and a local (diagonal) quasiparticle momentum or Fermi surface (4), will miss this effect, while it may be appropriate for quasiparticle density of states etc.. The id_{xy} order can also be induced by higher order terms involving only H_θ or the quasiparticle-supercurrent interaction. An example is shown in Fig.(1b). Other contributions, involving induced s wave order, are also possible.

We have focussed so far on spatially uniform single site terms. The id_{xy} order induced around each vortex is spatially nonuniform. The leading nonvanishing contribution is of *first order* in H_θ , and is shown in Fig.1c. It describes a $d_{x^2-y^2}$ pair becoming a d_{xy} pair *and* simultaneously acquiring a momentum q , near a vortex. For $q \gg \lambda^{-1}$, the contribution from this diagram is nonvanishing at small q . However, because of London screening, the $q \ll \lambda^{-1}$ limit vanishes. A related process involving d_{xy} order near a spin orbit impurity potential has been recently discussed by Balatsky (5).

The perturbative approach described above raises the obvious question of the expansion parameter. On general coupling constant and phase space grounds this can be argued to be $(1/k_F \xi)$ for both H_θ and H_m , where ξ is the pair coherence length. This is about $(1/5)$ or $(1/6)$. Thus, perturbation theory is expected to converge.

The id_{xy} order λ_k leads to a gap $i\Delta_{xy}$ with xy symmetry, in two ways. A process for λ_k corresponding to Fig.1a has, associated with it, an anomalous self energy Fig.1d, which leads to an xy symmetry gap function. Thus even if there is no interaction in the xy particle particle channel, a Δ_{xy} is induced. Secondly, there may actually be such a potential (attractive or repulsive), say V_{xy} . Then in the mean field approximation, a gap $\Delta_{xy}(k) \simeq \sum_{k'} V_{xy}(kk') \lambda_{k'}$ is induced. The question of self consistency can be fully addressed only if the microscopic mechanism of pairing (say in the $d_{x^2-y^2}$ channel) is known. In a BCS theory, if appropriate pseudopotentials $V_{x^2-y^2}$ and V_{xy} are assumed, the relevant Gor'kov equations (in the presence of vortices) or the quasiparticle problem (described by Bogoliuov-de Gennes equations) need to be solved self consistently. We have not done this; the lack of self consistency does not affect either the existence or the approximate size of the $T = 0$ id_{xy} pair amplitude.

IV. The Gapped Phase

We have shown above that an id_{xy} pair amplitude is inevitable for a $d_{x^2-y^2}$ superconductor in a magnetic field, and that there is a consequent id_{xy} gap. Thus, the ground state of the system in a magnetic field is necessarily a fully gapped superconductor in which the gap parameter $\Delta_k = \sqrt{\Delta_{x^2-y^2}^2(k) + \Delta_{xy}^2(k)}$ is nonzero at all points k on the Fermi surface. This has obvious thermodynamic and transport consequences. In particular, since the number of quasiparticles is exponentially small at very low temperatures, their contribution to thermal conductivity is negligible. We thus expect, at low enough temperature and sufficient vortex density, that there will be a transition to a gapped phase. We do not have a complete theory of this transition, but discuss possibilities below, following a brief analysis of experimental results (1,2).

As mentioned earlier, Krishana et al (1,2) find a transition at T_o from a K_T which decreases with increasing H to a field independent value at H_o ; approximately, $T_o \propto \sqrt{H_o}$. It is argued that this implies a thermodynamic transition to a gapped or coherent phase from an ungapped, incoherent phase. The transition is most likely continuous, since for a discontinuous change one expects a jump in K_T at the transition point.

The physical picture of the transition is that around each vortex an inhomogeneous d_{xy} order develops. If the vortices are not regularly arranged, and if the d_{xy} amplitudes are small as well as patchy or disconnected, quasiparticles see an inhomogeneous medium which scatters them, and a pseudogap develops near the nodes; this pseudogap deepens as the vortex density increases so that the electronic thermal conductivity decreases with increasing vortex density. At some critical vortex density dependent on temperature, the id_{xy} order parameters overlap, or the vortices order spatially, and a nonzero gap develops for the lowest lying quasiparticle

excitations. This is the new phase.

If the d_{xy} pair amplitude, (labelled m_{xy}^k) is the expected order parameter, an order parameter functional can be obtained using the standard auxiliary field method. We have calculated low order terms at $T = 0$ in such an expansion. There is a linear term, due to the fact that averages $\langle a_k^\dagger \tau_2 a_k \rangle$ with $k_x k_y$ symmetry, discussed in Section III, are nonzero. There are quadratic terms arising from both V_{xy} symmetry interactions between electrons (pairs) as well as a nonzero xy pair susceptibility. There is a cubic kinetic energy term (3). Because of the linear term, m_{xy}^k is nonzero; unsurprisingly, it has the value $\langle a_k^\dagger \tau_2 a_k \rangle_{xy}$ for which some terms have been indicated in Section III. We have not carried through the calculation for $T \neq 0$, and so are unable to find the temperature below which m_{xy}^k becomes nonzero. The linear in m term persists however at $T \neq 0$.

The gap in the excitation spectrum at $T = 0$ is due to both anomalous self energy (Fig. 1d) and the mean xy pair potential if there is a V_{xy} interaction. The gap due to the former is approximately $\Delta_o(n_v/n)$ and due to the latter, $4(|V_{xy}|/\epsilon_F) \Delta_o(n_v/n)$. Here Δ_o is the d_{xy} gap magnitude and n is the carrier density. The actual value thus depends on V_{xy} which is not known. Assuming $V_{xy}/\epsilon_F \simeq 1$ (a large value) and $\Delta_o \simeq 300K$, for a field of 5T, the minimum gap Δ_{xy} is about 10K. This comparable to the temperature 20K at which the gapped phase transition occurs for 5T, though smaller. Also, equating T_o to Δ_{xy} , we find that $T_o \propto H$; the experimental points are closer to \sqrt{H} .

This suggests that the identification of the observed transition with the development of a uniform part of d_{xy} pair amplitude may not be correct. One curious feature of this identification is that even when the vortices are distributed randomly the pair amplitude is uniform (there is a diagonal in k term) It is the sum of N_v independent identical single vortex terms irrespective of their arrangement. However, the d_{xy} order developed due to quasiparticle vortex interaction is spatially inhomogeneous, on the scale of the screening length λ , as discussed in Section III. If the vortices order spatially, there are coherent terms linear in H_θ , with wavevectors \vec{q} equal to Bragg vectors of the reciprocal vortex lattice. (These are $\vec{q} = \vec{G}$ components of the term shown in Fig.1c). They have the right energy scale. The relation between the magnetic field and the related energy scale is $T_c \propto G$ or $T_c \propto \sqrt{H}$, close to that observed. The gapped nature of this vortex lattice phase, the preferred lattice structure, and the nature of the transition to this lattice on cooling, are being investigated (6).

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References

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* Also at Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore-64

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Figure Captions

Diagrams describing processes leading to id_{xy} pair amplitude and related anomalous self energy.

- (a) An interference term for id_{xy} order involving a quasiparticle (straight line) being scattered by supercurrent (wavy line) around a vortex (marked by a cross), and by order parameter inhomogeneity around the vortex core (dotted line).
- (b) A higher order term for id_{xy} order, solely from quasiparticle supercurrent coupling H_o .
- (c) A spatially inhomogeneous id_{xy} pair amplitude term, first order in H_θ .
- (d) Anomalous self energy connected with the process of Fig. (1a).

