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Anisotropic thermodynamics of *d*-wave superconductors in the vortex state

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We show that the density of states and the thermodynamic properties of a two-dimensional d-wave superconductor in the vortex state with applied magnetic field **H** in the plane depend on the angle between **H** and the order-parameter nodes. Within a semiclassical treatment of the extended quasiparticle states, we obtain fourfold oscillations of the specific heat, measurement of which provides a simple probe of gap symmetry. The frequency dependence of the density of states and the temperature dependence of thermodynamic properties obey different power laws for field in the nodal and antinodal direction. The fourfold pattern is changed to twofold when orthorhombicity is considered. [S0163-1829(99)50514-6]

The experimental data accumulated over the last few years have established a consensus that the superconducting state of the hole-doped high-T_c cuprates has a predominantly d-wave order parameter.[1] Such an order parameter possesses lines of nodes, which results in a gapless excitation spectrum along certain directions in momentum space. An important consequence is that the low temperature dependence of thermal and transport properties of the superconducting cuprates is given by power laws, rather than exponential functions with an activation energy.[2]

The properties of the vortex state of d-wave superconductors also differ significantly from those of s-wave materials: while for the s-wave case the density of states (DOS) and the entropy are determined at low magnetic fields $H \ll H_{c2}$ by the localized states in the vortex cores, in superconductors with lines of nodes they are dominated by the extended quasiparticle states, which exist in the bulk along the nodal directions in momentum space.[3] On the basis of this observation Kübert and Hirschfeld[4] suggested a method of calculating thermal and transport coefficients in the vortex state microscopically by considering only the contribution of the extended states and accounting for the effect of the magnetic field on these states semiclassically, via a Doppler shift of the quasiparticle energy due to the circulating supercurrents. For the field applied perpendicular to the superconducting layers, the supercurrents can be approximated by the circular velocity field around a single vortex, $\mathbf{v}_s=\hat{\beta}/2mr$, where r is the distance from the center of the vortex, and we have set $\hbar=1$. Here $\hat{\beta}$ is a unit vector along the current and we use β as the vortex winding angle. This expression is valid outside the vortex core and up to a cutoff of order $\min\{R,\lambda\}$, where $2R=2a^{-1}\sqrt{\Phi_0/\pi H}$ is the intervortex spacing, Φ_0 is the flux quantum, a is a geometric constant, and λ is the penetration depth. Under these assumptions the energy of a quasiparticle with momentum $\mathbf{k}$ is shifted by $\delta\omega_{\mathbf{k}}(\mathbf{r})=\mathbf{v}_s\cdot\mathbf{k}$, and the calculated physical quantities depend on position and have to be averaged over a unit cell of the vortex lattice. The results obtained within this framework[4–7] describe recent experiments well,[8–13] suggesting that, while the effects left outside of this approach are important for a quantitative analysis, the method proposed in Ref. 4 is qualitatively correct and can be used to analyze the properties of the vortex state of unconventional superconductors.

In this paper we generalize the approach of Ref. 4 to consider the experimental arrangement with the magnetic field H in the CuO_2 plane, and calculate the density of states. We find that it exhibits fourfold oscillations as a function of the direction of the applied field, and that its energy dependence is drastically different for the field directed along the node and antinode.

Since the c-axis coherence length ξ_c is shorter than the interlayer distance s, the structure of the vortex state for **H** in the plane differs from that with $\mathbf{H}\parallel\mathbf{c}$, and is commonly modeled by treating the incoherent c-axis transport as Josephson tunneling between the layers.[14–16] The conclusion of Ref. 3 that the extended states dominate the thermodynamic properties of the vortex state with lines of nodes in the gap remains valid for any orientation of the magnetic field. The superfluid velocity $\mathbf{v}_s$ away from the core is governed solely by the 2π winding of the phase of the order parameter around each vortex, and, at distances large compared to the size of the core, is virtually identical to that of an Abrikosov vortex.[14,15] Since the core size is larger than ξ_c, the velocity field can be approximated by the superflow around a single vortex only for fields $H\ll H_0=\Phi_0/\gamma s^2$, where γ is the anisotropy ratio; above that field the cores begin to overlap.[15] While for extremely anisotropic cuprates, such as the

$Bi_2Sr_2CaCu_2O_{8+\delta}$ family, the crossover field is of order of a few Tesla, for less anisotropic materials, such as $YBa_2Cu_3O_{7-\delta}$, $H_0 \geqslant 50\,\mathrm{T}$, and for all experimentally relevant fields the individual vortices can be treated as Abrikosov vortices in the calculation of bulk properties. Furthermore, in the regime $H \ll H_0$ the intervortex distance and the structure of the vortex state are asymptotically close to those of an Abrikosov vortex lattice,[16] suggesting that the approach of Ref. 4 can be directly applied to the geometry with the field in the plane. Finally, the c-axis transport remains incoherent at low temperatures,[17] and therefore only the energies of the quasiparticles with momenta in the plane are relevant to the thermodynamic properties and should be Doppler shifted.

We now follow the approach of Ref. 4 in neglecting the contribution of the core states and assuming a spatially uniform order parameter $\Delta_{\mathbf{k}}$ over a cylindrical Fermi surface. In most of this work we consider a pure d-wave angular dependence of the gap, $\Delta_{\mathbf{k}} \equiv \Delta_0 f(\phi) = \Delta_0 \cos 2\phi$. We consider a magnetic field $\mathbf{H}$ applied in the a-b plane, at an angle α to the x axis, and account for its effect on the extended quasiparticle states by the Doppler energy shift $\delta\omega_{\mathbf{k}}(\mathbf{r}) = \mathbf{v}_s \cdot \mathbf{k}$. The superfluid velocity is approximated by the flow field of an isolated vortex, which is elliptical due to the anisotropy of the penetration depth. We can however rescale the c axis to make both $\mathbf{v}_s$ and the intervortex spacing $2R$ isotropic–in the London theory this rescaling is $z' = z(\lambda_{ab}/\lambda_c)$–and since the Fermi surface is two-dimensional there is no associated rescaling of momentum. Then, approximating the unit cell of the vortex lattice by a circle of radius R, we obtain

$$\delta\omega_{\mathbf{k}}(\mathbf{r}) = \frac{E_H}{\rho} \sin\beta \sin(\phi - \alpha), \tag{1}$$

where $\rho = r/R$ and E_H is the energy scale associated with the Doppler shift

$$E_H = \frac{a}{2} v^* \sqrt{\frac{\pi H}{\Phi_0}}. \tag{2}$$

Here a is a geometric constant of order unity, and in the London theory the rescaled Fermi velocity $v^* = v_f \sqrt{\lambda_{ab}/\lambda_c}$, where v_f is the Fermi velocity in the plane. In a more general approach v^* should be treated as a parameter related both to v_f and the anisotropy of the vortex lattice.

The main difference between geometric arrangements with the field applied in the plane and that applied along the c axis is clearly seen from Eq. (1). For the field applied perpendicular to the layers the momentum and real-space degrees of freedom decouple,[4] and the average Doppler shift is the same at all points on the Fermi surface. In contrast, for the field in the plane the average Doppler shift becomes dependent on the position at the Fermi surface, and is given by $E_H \sin(\phi - \alpha)$. Since quasiparticles contribute to the density of states when their Doppler-shifted energy exceeds the local energy gap, an immediate conclusion is that the density of states depends sensitively on the angle between the applied field and the direction of nodes of the order parameter.

To analyze this dependence quantitatively we employ the single-particle Green's function which is obtained by introducing the Doppler shift into a BCS Green's function[4]

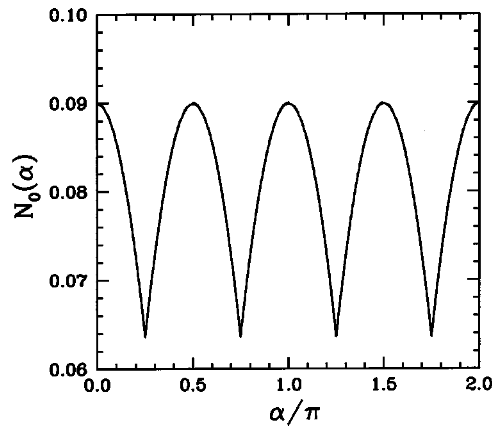

FIG. 1. The density of states at the Fermi level, $N_0(\alpha)$, for $E_H/\Delta_0 = 0.1$. The solid curve is the full numerical evaluation of Eq. (5), and the dashed (almost indistinguishable) is the nodal approximation Eq. (7).

$$G(\mathbf{k}, \omega_n; \mathbf{r}) = -\frac{(i\omega_n - \mathbf{v}_s \mathbf{k})\tau_0 + \Delta_{\mathbf{k}}\tau_1 + \zeta_{\mathbf{k}}\tau_3}{(\omega_n + i\mathbf{v}_s \mathbf{k})^2 + \zeta_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}, \tag{3}$$

where ω_n is the fermionic Matsubara frequency, $\zeta_{\mathbf{k}}$ is the band energy measured with respect to the Fermi level, and τ_i are Pauli matrices. Standard many-body techniques can be used to compute physical quantities $F(\mathbf{r})$ at a fixed position $\mathbf{r}$ in real space, and the measured quantities are obtained by averaging over a unit cell of the vortex lattice according to

$$\langle F \rangle_H = \frac{1}{\pi} \int_0^1 \rho d\rho \int_0^{2\pi} d\beta F(\rho, \beta). \tag{4}$$

We first consider the density of states at the Fermi level which is easily accessible experimentally via specific-heat measurements and is given by

$$N_0(\alpha) \equiv -\frac{1}{2\pi} \mathrm{Im} \sum_{\mathbf{k}} \langle \mathrm{Tr}\, G(\mathbf{k}, \omega = 0; \mathbf{r}) \rangle_H \tag{5}$$

$$= \frac{1}{2\pi^2} \int_0^{2\pi} d\phi \int_0^{2\pi} d\beta \int_0^1 \rho d\rho \times \mathrm{Re}\left[\frac{|\sin\beta \sin(\phi - \alpha)|}{\sqrt{\sin^2\beta \sin^2(\phi - \alpha) - (\Delta_0/E_H)^2 \rho^2 f^2(\phi)}} \right]. \tag{6}$$

The integrals over ρ and β can be done analytically, and the numerical evaluation of Eq. (5) is trivial. It has been shown[4] that the nodal approximation, which takes advantage of the fact that the density of states is dominated by the contribution of the regions of the Fermi surface near the gap nodes to replace $\mathbf{v}_s \cdot \mathbf{k}$ by the Doppler shift at the nodes, $\mathbf{v}_s \cdot \mathbf{k}_n$, provides a remarkably good agreement with the numerical results for $T, E_H \ll \Delta_0$. Here it yields

$$N_0(\alpha) \simeq \frac{E_H}{\Delta_0 \pi} \sum_{nodes} |\sin(\phi_n - \alpha)| = \frac{2\sqrt{2} E_H}{\Delta_0 \pi} \max(|\sin\alpha|, |\cos\alpha|). \tag{7}$$

This result was first obtained by Volovik.[18] In Fig. 1 we

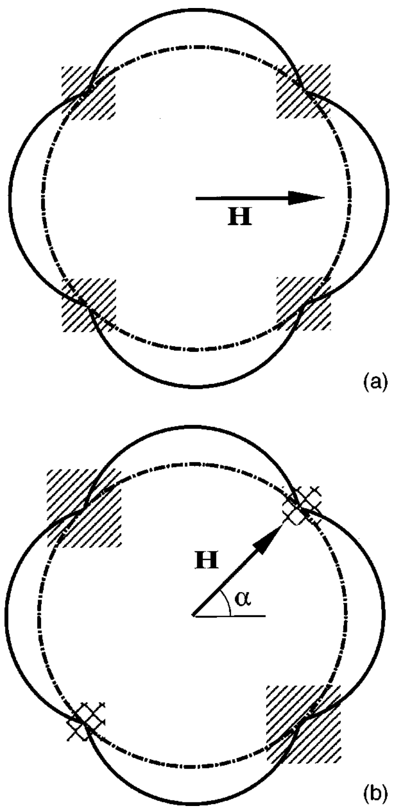

FIG. 2. The regions contributing to the density of states for the antinodal (a), and nodal (b) orientation of the magnetic field.

show the results of full numerical evaluation of the residual density of states from Eq. (5) along with the results of Eq. (7). The density of states exhibits fourfold oscillations as a function of the angle of the applied field. There is a broad maximum for the field applied in the antinodal direction, and a sharp minimum for the field along the node. Both can be understood if we notice that the Doppler shift is given by $E_1 = E_H|\sin(\pi/4-\alpha)|$ at two of the near-nodal regions, and by $E_2 = E_H|\cos(\pi/4-\alpha)|$ at the other two nodes. When a field is applied in the antinodal direction, $E_1 = E_2$ and all four nodes contribute equally to the density of states, as shown in Fig. 2(a). On the other hand, when the field is applied along a nodal direction, quasiparticles at that node, which travel parallel to the field, do not contribute to the DOS; the Doppler shift vanishes at these points. Moreover, since $E_H \ll \Delta_0$, the gap grows faster as a function of the angle ϕ near the node than the Doppler shift over most of the unit cell of the vortex lattice, and therefore the quasiparticle contribution to the density of states is suppressed over the whole near-nodal region, see Fig. 2(b). For a field not exactly in the nodal direction there is always a finite region of the momentum space where the Doppler shift exceeds the local gap, resulting in a contribution to the DOS and sharp minima of $N_0(\alpha)$.

Consequently, for a field in the nodal direction two of the nodes do not contribute to DOS, while the contribution of the other two is a factor of $\sqrt{2}$ larger than it is for the field along an antinode. The density of states is therefore reduced by 30%, in agreement with the numerical results. To check how robust the oscillations are we numerically computed $N_0(\alpha)$ in a three-dimensional superconductor and found that the results remain qualitatively unchanged, although the amplitude of the oscillations is reduced to about 8%, in agreement with an analytic estimate. This reduction results from incomplete suppression of the contribution to the DOS from the nodal lines aligned with the field since for quasiparticles outside the equatorial plane the Doppler shift does not vanish. We suggest that in realistic materials the amplitude of the oscillations is somewhere between the two estimates and within the experimental resolution of the specific-heat measurements; the published results suggest that this amplitude is of order $0.3\,\mathrm{mJ/mol\,K^2}$ at $H = 0.005 H_{c2\parallel}$.[18] So far, one reported measurement performed for two orientations of the applied field in the plane did not find the predicted oscillations.[8] However, an estimate shows that for the samples used in Ref. 8 the energy scale E_H for $H \sim 8$ T is close to the impurity bandwidth, γ, which may have resulted in significant smearing of the fourfold pattern. We also note that in an orthorhombic system the induced s-wave component of the gap would shift the position of the DOS minimum away from the $\pi/4$ direction, and in a heavily twinned crystal, such as used in Ref. 8, this would result in rapid filling of the minima and significant suppression of the amplitude of oscillations.

While for a clean sample $N_0(\alpha) \propto \sqrt{H}$ independently of the angular orientation of **H**, the energy dependence of the density of states depends crucially on the direction of the field. For $\omega, E_H \ll \Delta_0$,

$$N(\omega,\alpha) \simeq [N_1(\omega,\alpha) + N_2(\omega,\alpha)]/2, \tag{8}$$

where[4]

$$N_i(\omega,\alpha) = \begin{cases} \dfrac{\omega}{\Delta_0}\left(1+\dfrac{1}{2x^2}\right), & \text{if } x=\omega/E_i \geq 1; \\ \dfrac{E_i}{\pi\Delta_0 x}[(1+2x^2)\arcsin x + 3x\sqrt{1-x^2}], & \text{if } x \leq 1 \end{cases} \tag{9}$$

for $i = 1,2$, and E_1 and E_2 were defined above. For the field in the antinodal direction

$$N(\omega,0) \approx \frac{2\sqrt{2}E_H}{\pi\Delta_0}\left(1+\frac{1}{3}\frac{\omega^2}{E_H^2}\right), \tag{10}$$

while for the field along a node

$$N(\omega,\pi/4) \approx \frac{2E_H}{\pi\Delta_0} + \frac{\omega}{2\Delta_0}, \tag{11}$$

see Fig. 3. The frequency dependence of the density of states follows different power laws for the field along a node or an antinode, and in the former case the linear slope of $N(\omega,\pi/4)$ does not depend on the magnetic field. Note that the value of $N(0,0)$ and $N(0,\pi/4)$ differ by a factor of $\sqrt{2}$ as expected and that the slope of the linear term in Eq. (10) is just half the value of the zero-field case as only two nodes contribute.

Since the frequency dependence of the density of states determines the temperature dependence of thermal and trans-

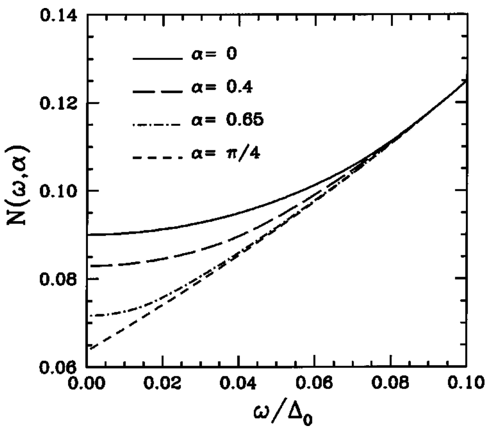

FIG. 3. The energy-dependent density of states for different directions of the applied field and $E_H/\Delta_0=0.1$.

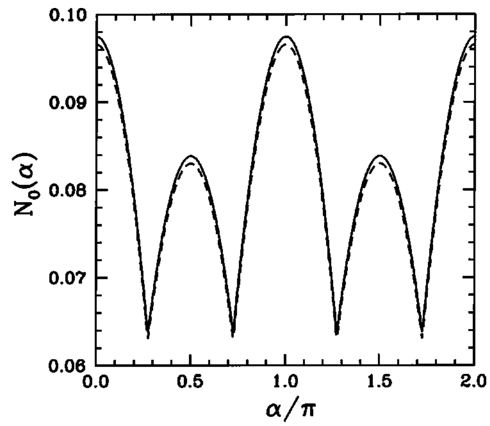

FIG. 4. The effect of orthorhombicity included in the gap $(d+0.15s)$ on $N_0(\alpha)$ for $E_H/\Delta_0=0.1$. The solid curve is the full numerical evaluation and the dashed line is the result of the first equality in Eq. (7).

port coefficients, our results have profound effects on the properties of clean d-wave superconductors. In particular, in addition to the fourfold oscillations of the linear-T term in the specific heat as a function of the direction of **H**, the temperature dependence of $C/T\sqrt{H}$ is linear for the field in a nodal direction, and quadratic for **H** away from the node. The nuclear spin-lattice relaxation time T_1T and superfluid density will also exhibit fourfold oscillations and a linear or quadratic T dependence depending on the direction of the field. However, if the latter quantity is inferred from the penetration depth measurements, nonlocal effects due to a diverging coherence length[19] in the nodal directions may be important.

Any orthorhombic distortion in the system lifts the fourfold degeneracy of the maxima. One possible way to account for such a distortion is to consider a $d+qs$ superconductor, where $q\ll 1$. Then, even though the position of the nodes is shifted insignificantly, the fourfold pattern is replaced by two pairs of peaks with the amplitude ratio $|\sin[\alpha-0.5\arccos(-q)]|/|\sin[\alpha+0.5\arccos(-q)]|$, which differs significantly from unity even for relatively small q, as shown in Fig. 4. The anisotropy in the density of states and the thermodynamic properties however remains robust and is a particularly simple experimental probe of the nodal structure of the order parameter.

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