Quantized Thermal Hall Effect in the Mixed State of d-Wave Superconductors

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We consider quasiparticles of a clean d-wave superconductor in the vortex lattice state. For vortex lattices that are inversion symmetric, the quasiparticle bands are found to have a Dirac cone dispersion at zero energy, within the linearized approximation. Upon going beyond the linearized approximation by including the effect of the smaller curvature terms, the Dirac cone dispersions acquire a small gap that scales linearly with the applied magnetic field (≈ 0.5 K T^{-1} in YBa$_2$Cu$_3$O$_{6.9}$). When the "chemical potential" for quasiparticles lies within the gap, quantization of the thermal Hall conductivity, $\kappa_{xy}/T = n(\pi^2 k_B^2/3h)$, with $n = \pm 2, 0$, is predicted at low temperatures.

Since the experimental verification of the $d_{x^2-y^2}$ nature of superconductivity in the cuprate materials [1], there has been much activity in studying the physics of quasiparticles in a d-wave superconductor. In contrast to the s-wave case, the d-wave superconducting gap vanishes at points on the Fermi surface leading to low energy quasiparticles that behave like massless Dirac fermions. One question that is of great interest is the behavior of these quasiparticles in the mixed state—a problem that is both theoretically rich and of relevance to explaining several different experiments. This problem has been considered by several authors. Gor'kov and Schriffer, and Anderson [2] proposed a Landau-level–like spectrum, while Franz and Tesanovic computed the quasiparticle band structure for a perfect lattice of vortices [3] in the linearized approximation, which was followed by the detailed studies in [4], while topological issues were highlighted in [5].

Here too we consider d-wave superconductors in the mixed state, assuming the presence of a vortex lattice and ignoring disorder. We use a combination of symmetry arguments and analytical calculations to derive the nature of the low energy quasiparticle spectrum, as well as consequences for thermal Hall transport (which are well defined even in a clean system) in the low temperature limit. Our main result is the following: under appropriate conditions, d-wave superconductors in the mixed state will display a quantized thermal Hall conductance ($\kappa_{xy}/T = \pm 2$, 0 in appropriate units) that sets in at temperatures below a certain characteristic energy scale. This energy scale and its dependence on various physical parameters are derived.

In the following we assume that there are well-defined quasiparticle excitations in the superconducting phase of the cuprates, and these are described by a Bogoliubov–deGennes (BdG) equation with a d-wave gap. We are interested in the effect of relatively weak magnetic fields (~ 1 T $\ll H_{c2}$), for which the separation between vortices is much larger than the vortex core size. Hence we neglect the effect of the cores, i.e., the amplitude modulation of the order parameter. Finally, we assume that the vortices are arranged in a perfect vortex lattice and ignore the effects

of disorder. Then, the BdG equations for d-wave quasiparticles in the mixed state are

$$H_{\text{BdG}}\psi = E\psi, \tag{1}$$

$$H_{\text{BdG}} = \begin{bmatrix} \epsilon(\vec{p} - e\vec{A}(\vec{r})) & e^{i(\phi/2)}\Delta(\vec{p})e^{i(\phi/2)} \\ e^{-i(\phi/2)}\Delta(\vec{p})e^{-i(\phi/2)} & -\epsilon(-\vec{p} - e\vec{A}(\vec{r})) \end{bmatrix},$$

where $\vec{p} = -i\vec{\nabla}$, $\vec{A}$ is the vector potential, and $\phi(\vec{r})$ is the phase of the order parameter. We assume for simplicity a quadratic dispersion $\epsilon(p) = \frac{1}{2m}p^2 - E_F$ and a d-wave gap function with the nodes along the coordinate axes $\Delta(p) = \frac{\Delta_0}{p_F^2}p_x p_y$. The two-component quasiparticle wave function $\psi(r) = [u(r)v(r)]^T$ is a linear superposition of particle and hole states. We now consider a gauge transformation to eliminate the phase variation of the order parameter, i.e., transform to the London gauge, which can be accomplished by the unitary operator $U = e^{-(i/2)\phi(\vec{r})}\sigma_z$. The transformed Hamiltonian $UH_{\text{BdG}}U^{-1}$ takes the simple form

$$H'_{\text{BdG}} = \epsilon(-i\vec{\nabla} + \vec{P}_s(\vec{r})\sigma_z)\sigma_z + \Delta(-i\vec{\nabla})\sigma_x, \tag{2}$$

where the σ's are in the usual representation, and $\vec{P}_s = \frac{1}{2}\vec{\nabla}\phi - e\vec{A}$, a gauge invariant quantity, is the mechanical momentum carried by each member of the Cooper pair at point $\vec{r}$. We will sometimes refer to this quantity as the superflow, though this terminology is not quite accurate. In the presence of elementary $hc/2e$ vortices, it must be noted that the unitary transformation U, and hence ψ', are not single valued, but change sign on circling an odd number of such vortices. This is a consequence of the Berry phase factor of (-1) acquired by quasiparticles on circling an elementary vortex.

In the interest of clarity we first consider a vortex lattice of hc/e vortices for which the transformed wave function ψ' is single valued, and so only the effect of the superflow $\vec{P}_s$ needs to be taken into account. Armed with an understanding of this simpler situation, we then discuss the more involved but physically important case of $hc/2e$ vortices in a lattice. Nevertheless, in both cases we obtain the same results. As discussed in [6], we can restrict our attention to the quasiparticle excitations near the four

gap nodes. Thus, expanding the wave function of the low energy excitations about the nodal points, for example, for excitations near the nodal point at $\vec{p} = (p_F, 0)$ we write $\psi(\vec{r}) = e^{ik_{Fx}X}\psi_1(\vec{r})$, where the function ψ_1 varies slowly on the scale of the Fermi wavelength. Ignoring internode scattering, we obtain the linearized problem for this node, $H_1\psi_1 = E\psi_1$, with

$$H_1 = v_F\{p_x\boldsymbol{\sigma}_z + \alpha^{-1}p_y\boldsymbol{\sigma}_x + \hat{x} \cdot \vec{P}_s(\vec{r})\mathbf{1}\}, \quad (3)$$

where $\alpha = E_F/\Delta_0$ is the anisotropy. The linearized part above dominates over the remaining terms (curvature terms) of the Hamiltonian in (3), for sufficiently low temperatures and weak fields. In YBa$_2$Cu$_3$O$_{6.9}$ (YBCO) this parameter window corresponds to $T \ll 200$ K and magnetic fields less than a few tesla. The curvature terms, ΔH,

$$\Delta H = \frac{1}{2m}[p^2 + \vec{P}_s^2(\vec{r})]\boldsymbol{\sigma}_z + \frac{1}{2m}\{\vec{p}, \vec{P}_s(\vec{r})\}\mathbf{1}$$
$$+ \frac{\Delta_0}{p_F^2}p_x p_y\boldsymbol{\sigma}_x,$$

though small, are crucial to providing a nonzero thermal Hall response [6], and we will include their effects subsequently. To summarize briefly the results of the forthcoming discussion, the linearized Hamiltonian is found to possess an additional symmetry, $\mathcal{T}_{\text{Dirac}}$, that leads to Dirac nodes (band touchings) at certain special points in the Brillouin zone. For inversion symmetric vortex lattices, there is a Dirac node centered at *zero energy*. Finally, upon including the effect of the smaller curvature terms, a gap is opened at these nodes which can lead to a quantized thermal Hall conductivity.

The linearized problem for a lattice of hc/e vortices.— We analyze the linearized Hamiltonian for node 1, [Eq. (4)] for an arbitrary lattice of hc/e vortices. Since the superflow $\vec{P}_s(\vec{r})$ generated by this vortex lattice is a gauge invariant physical quantity, it is a periodic function with the same periodicity as the lattice. This gives rise to a band structure for the quasiparticles, and the eigenstates are labeled by the band index and the crystal momentum ($\vec{k}$), which takes values within the Brillouin zone.

A symmetry of the linearized problem.— We now point out a crucial symmetry of the linearized Hamiltonian. Consider an eigenstate $\psi_{\vec{k}}$ of the linearized Hamiltonian H_1 with eigenvalue E and crystal momentum $\vec{k}$: $H_1\psi_k = E\psi_k$. Then the transformed wave function

$$\phi_{-\vec{k}} = \boldsymbol{\tau}\psi_{\vec{k}}^* \quad (4)$$

is easily shown to also be an eigenstate with energy E but crystal momentum $-\vec{k}$. Here $\boldsymbol{\tau}$ is the dimension-two antisymmetric matrix $\boldsymbol{\tau} = i\boldsymbol{\sigma}_y$. Since the transformation (5) is formally equivalent to the time reversal operation for *Dirac* particles, we will call it $\mathcal{T}_{\text{Dirac}}$, although, as explained below, it is distinct from the physical time reversal transformation for this problem. This symmetry ensures that states with crystal momentum $\vec{k}$ and $-\vec{k}$ have the same

energy. At those points in the Brillouin zone which are taken to themselves (modulo a reciprocal lattice vector) under time reversal, there is a degenerate pair of states $\psi_{\vec{k}}$ and $\boldsymbol{\tau}\psi_{\vec{k}}^*$. These states are orthogonal, from the antisymmetry of $\boldsymbol{\tau}$. Hence at these special points in the Brillouin zone, which are at the zone center ($\vec{k} = 0$; Γ point), the zone corners (M point), and the center of the zone edges (A and B points), the spectrum is composed entirely of degenerate pairs.

The symmetry operation $\mathcal{T}_{\text{Dirac}}$ that operates on the quasiparticle excitations at a single node is *distinct* from the physical time reversal operation, which transforms states at one node into states at the opposite node. Rather, invariance under $\mathcal{T}_{\text{Dirac}}$ is obtained as a consequence of linearizing the electron dispersion; it is easily seen that the subdominant curvature terms, such as, for example, $\frac{1}{2m}p^2\boldsymbol{\sigma}_z$, violate this symmetry.

Dirac cones from degenerate doublets.— As we move away from the special points in the Brillouin zone at which degenerate doublets are found, the crystal momentum splits these states and gives rise to a Dirac cone, i.e., the energy dispersion of a massless Dirac particle. To see this, consider a pair of degenerate states $[\psi(\vec{r}), \boldsymbol{\tau}\psi^*(\vec{r})]$ at one of these special points in the Brillouin zone. The effect of moving away from this point by crystal momentum $\delta\vec{k}$ can be accounted for by adding the piece $\delta H_{\delta k} = v_F\delta k_x\boldsymbol{\sigma}_z + v_\Delta\delta k_y\boldsymbol{\sigma}_x$ to the Hamiltonian and leaving unchanged the boundary condition for the wave function. If the deviation in crystal momentum is small (compared to the reciprocal lattice vectors), this additional piece can be treated in degenerate perturbation theory within this two-dimensional subspace. Although an explicit calculation requires a knowledge of the wave functions, a few observations can be made right away. The perturbation above splits the previously degenerate pairs of states — they now have energy $+\delta E_{\delta k}$ and $-\delta E_{\delta k}$ relative to the degenerate doublet. Also, given that we consider the first order perturbation in $\delta H_{\delta k}$, the strength of the splitting varies linearly with $|\delta\vec{k}|$. Hence we can write $\delta E_{\delta k} = v_F A(\theta_{\delta k})|\delta\vec{k}|$, where $A(\theta_{\delta k})$ is the velocity an isotropy factor, which depends on the angle $\theta_{\delta k}$ that the vector $\delta\vec{k}$ makes with the k_x axis. Calculating $A(\theta_{\delta k})$, however, requires explicit knowledge of the wave functions. We recognize this as the dispersion of an anisotropic massless Dirac particle, i.e., a Dirac one.

Inversion symmetry and the Dirac node at zero energy.— If the vortex lattice possesses inversion symmetry, that is, if it is invariant under the transformation $\vec{r} \rightarrow -\vec{r}$ (assuming the origin is the center of inversion), then it is easy to see that the superflow satisfies $\vec{P}_s(-\vec{r}) = -\vec{P}_s(\vec{r})$. This leads to a particle-hole symmetry of the linearized Hamiltonian. If $\psi(x, y)$ is an eigenstate of the Hamiltonian H_1 (4) with energy E, then $\psi(-x, -y)$ is also an eigenstate, but with energy $-E$.

Inversion symmetry ensures there is a degenerate doublet of the linearized Hamiltonian H_1 at *zero energy*

at the Γ ($\vec{k} = 0$) point. The argument is as follows: let us focus on the spectrum at the Γ point, in which case we need to solve for the eigenstates of H_1 on the unit cell with periodic boundary conditions, i.e., on a torus. Consider the case without the Doppler term, that is, a free Dirac particle on a torus, with the Hamiltonian $H_{\text{free}} = v_F p_x \boldsymbol{\sigma}_z + v_\Delta p_y \boldsymbol{\sigma}_x$ which can easily be solved. Clearly, this has a pair of states at zero energy, given by the product of the constant solution times any spinor. The rest of the states also occur in degenerate pairs, and for every pair of states at energy $E \neq 0$ there is a pair of states at energy $-E$; a consequence of the free Dirac Hamiltonian respecting the T_{Dirac} and inversion symmetries. Thus, in the free case, the spectrum consists of an "odd" number of degenerate pairs, due to the existence of the pair at zero energy (this can be made more rigorous by introducing an ultraviolet cutoff, and hence a finite number of states). Now, turning on the Doppler term $\hat{x} \cdot \vec{P}_s$ for inversion symmetric vortex lattices preserves the T_{Dirac} as well as particle-hole symmetry. Therefore the states appear as degenerate doublets, in a particle-hole symmetric spectrum. Since the total number of pairs of states cannot change from the free case, we are forced to have a degenerate doublet at *zero energy*. Then, the total number of pairs of degenerate states remains odd, as it was for the free case. Notice that this argument is also valid perturbatively if the value of the Doppler term is continuously turned up from zero. The doublet of states at zero energy for inversion symmetric lattices will give rise to a Dirac cone centered at zero energy, by our previous arguments. Thus, here we have been able to access the qualitative nature of the low energy physics solely via the use of symmetry arguments. The velocities entering the dispersion, however, can be strongly renormalized from the pure system values.

Lattice of $hc/2e$ vortices.—We now briefly discuss how the preceding arguments for the simpler case of double vortices need to be modified for the physically interesting situation of a lattice of elementary vortices. The new feature that needs to be included is the Berry phase factor of (-1) acquired by quasiparticles on circling a $hc/2e$ vortex. This may be accomplished by the Franz-Tesanovic transformation [3]; a fictitious U(1) gauge field $\vec{a}$ that couples minimally to the quasiparticles is introduced, and delta function solenoids of fictitious flux $\pm\pi$ are attached to the $hc/2e$ vortices. The need for careful regularization when using this transformation with the linearized approximation is discussed elsewhere [7]. The linearized Hamiltonian for this case may be obtained from (4) by the substitution $\vec{p} \rightarrow \vec{p} + \vec{a}$. Now it appears that $\mathcal{T}_{\text{Dirac}}$ is no longer a symmetry of the linearized equations since it transforms $\vec{a} \rightarrow -\vec{a}$. However, since we have the special case of π fluxes, and are only interested in the Aharonov-Bohm phases they generate, this sign change corresponds to a trivial gauge transformation. Thus, the combination of a gauge transformation and $\mathcal{T}_{\text{Dirac}}$ leaves the linearized Hamiltonian invariant. We can use this symmetry to derive precisely the same conclusions, regarding doubly degener-

ate states at special points in the Brillouin zone as before, for the case of hc/e vortices. Further, for inversion symmetric vortex lattices, we can argue as before that there is a pair of degenerate states at *zero energy*. Note, however, that here the argument is nonperturbative in nature; the degenerate pairs are obtained only for the special value $\pm\pi$ of fictitious flux. Thus, for the case of an inversion symmetric $hc/2e$ vortex lattice as well, there is a Dirac node centered at zero energy in the linearized approximation.

Beyond the linearized approximation.—We now consider the effect of the subdominant curvature terms (ΔH) on the spectrum obtained from the linearized equations. For simplicity, we consider a vortex lattice of hc/e (double) vortices. The physically relevant case of the $hc/2e$ vortex lattice is very similar. In view of the smallness of these curvature terms, their primary effect will be to lift degeneracies that are present in the spectrum of the linearized problem. Therefore we study the effect of these terms near the Dirac cones (band touchings) of the linearized problem. Since the curvature terms are not invariant under $\mathcal{T}_{\text{Dirac}}$ they split the degenerate pairs of states. This splitting can be calculated within degenerate perturbation theory; the effective Hamiltonian in the vicinity of these points is now that of a massive Dirac particle with mass m_D, with dispersion $\delta E_{\delta k} = \pm\sqrt{[v_F^2 A^2(\theta_{\delta k})|\delta \vec{k}|^2] + m_D^2}$, where the Dirac mass term m_D is induced by the curvature terms ΔH.

Of particular interest is the case of an inversion symmetric vortex lattice, where we have seen that there is a Dirac node at zero energy, which is the position of the quasiparticle chemical potential (ignoring Zeeman splitting). Upon including the effect of the curvature terms, a gap develops, and the low energy spectrum is like that of a massive Dirac particle. It is well known that in two dimensions massive Dirac particles, with the negative energy branch completely filled, exhibit a quantized Hall effect at zero temperature [8,9]; $\sigma_{xy} = \frac{1}{2} \frac{e_D^2}{h} \text{sgn}(m)$, where e_D is the charge associated with the Dirac particle, and m is the mass appearing in the Dirac equation. The quasiparticle problem with the chemical potential in the gap is topologically identical to this system of free Dirac particles with a mass term. In other words, the two systems can be continuously deformed into another *without* closing the gap at the chemical potential. Superconductor quasiparticles of course do not carry a well-defined electrical charge, however, for the case of interest the component of the quasiparticle spin along the applied magnetic field is conserved. Hence a quantized spin Hall effect will result [10,11], and, as a consequence of the Widermann-Franz law that relates thermal and spin conductivity at low temperatures in a superconductor, the thermal Hall coefficient (κ_{xy}) will also be quantized. More precisely the ratio of κ_{xy} from each node, and temperature T, will take on the value $\kappa_{xy}/T \rightarrow \frac{1}{2}(\frac{\pi^2}{3} \frac{k_B^2}{h}) \text{sgn}(m_D)$ in the limit of low temperatures. The total thermal Hall conductivity receives contributions from all four nodes. It is easily seen from the

intrinsic particle-hole symmetry of the BdG equations that the contribution from opposite nodes is always of the same sign. Thus, two situations can arise. First, when all nodes contribute to the thermal Hall coefficient with the same sign, then $\kappa_{xy}/T = \pm 2(\frac{\pi^2}{3}\frac{k_B^2}{h})$. Second, when the pair of nodes 1, $\bar{1}$ contribute with the opposite sign from the pair 2, $\bar{2}$, then $\kappa_{xy}/T = 0$. The first case is topologically equivalent to a homogeneous $d_{x^2-y^2} + id_{xy}$ superconductor, while the second case is equivalent to a thermal insulator. Which of these two situations is realized is a function of the anisotropy (α) and the geometry of the vortex lattice [12]. In both cases the longitudinal thermal conductivity vanishes ($\kappa_{xx}/T \to 0$) at low temperatures. The temperatures below which the quantization is seen is set by the value of the gap, that is, the magnitude of the Dirac mass term. The typical size of the gap may be estimated as follows: ignoring the last term in ΔH (which arises from the gap curvature, and is smaller than the preceding terms by a factor of Δ_0/E_F), the Dirac mass induced by ΔH can be written in the form $m_D = \chi\frac{\hbar eB}{2m}$, where χ is a constant of order unity, whose magnitude and sign depend only on the anisotropy (α) and the geometry of the vortex lattice. The mass term thus scales linearly with magnetic field. For the case of YBCO this scale is roughly of order ~ 0.5 K T^{-1}. An accurate calculation of the induced Dirac mass, following the procedure described in the previous paragraph, requires a numerical computation of the zero energy wave functions of the linearized theory. A concrete calculation in a model system can be found in [7].

When comparing with experiments, the effect of the Zeeman splitting, which plays the role of chemical potential for the quasiparticles, needs to be taken into account. The Zeeman energy has the same linear scaling with applied field and similar magnitude (0.7 K T^{-1}) as the induced gap $|m_D|$. Quantization in the clean system is observed if the gap exceeds the Zeeman energy. Then, the effective gap that sets the temperature scale below which these effects are observed is given by $|m_D| - |E_Z|$. Calculating $|m_D|$ in a real system, to an accuracy that will allow a comparison with E_Z, is a difficult proposition requiring detailed knowledge of the microscopic parameters of the material. Therefore we do not attempt it here, but simply note that obtaining a Dirac mass that exceeds the Zeeman splitting is a distinct possibility in the cuprates. In addition, the presence of weak disorder can make the quantization more robust by localizing the states and increasing the gap between the extended states. With strong disorder, however, a completely different analysis that does not rely on the Bloch nature of the quasiparticle states will be required. We now turn to the relevant experiments in one particular d-wave system.

Currently, low temperature thermal Hall measurements on YBa$_2$Cu$_3$O$_7$ [13] in a field of 14 T, go down to a temperature of about 12 K, which is presumably still too high to observe the quantization, should it exist. Indeed, although the measured κ_{xy}/T at a given temperature is found to saturate for stronger fields, the value at this plateau is not quantized, but scales as T. Even so, it is an intriguing fact that the plateau value of κ_{xy} at the lowest temperature measured is very close to what would be expected from a quantized thermal Hall conductance of $|\kappa_{xy}/T| = 2$ (in appropriate units). While this experiment is not conclusive with regard to the low temperature state of the quasiparticles, specific heat measurements down to 1 K in magnetic fields of 14 T in YBa$_2$Cu$_3$O$_7$ [14] show no evidence of a gap. Further, low temperature $T < 0.1$ K longitudinal thermal conductivity measurements in fields up to 8 T in YBa$_2$Cu$_3$O$_{6.9}$ [15] reveal κ_{xx}/T saturating to a nonzero value that rules out a quantized thermal Hall effect in this material down to these low temperatures. Thus, for the case of YBCO, either the Zeeman splitting causes the chemical potential to lie outside the gap region or else the vortex lattice in this case is so disordered that the perfect lattice assumption we start with requires serious modification. Nevertheless, given the large number of potentially different experimental systems with a d-wave gap that are available, it is not unreasonable to expect that the quantized thermal Hall effect, realized in the manner described, will be observed in the future.

After completion of this work we learned of [16], where a numerical computation of Chern numbers of quasiparticle bands is reported, which, in the region of overlap, agrees with our results.

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