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## Chiral optical resonance of vortex core states in type-II superconductors

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The dynamic conductivity of vortex cores in type-II superconductors is calculated. We show that there is a chiral optical resonance well below the superconducting gap, corresponding to creating a pair of quasiparticles inside the vortex core. The chirality is the same as cyclotron resonance. The frequency and intensity of the resonance are estimated by numerically solving the Bogoliubov-de Gennes equations self-consistently.

There has been considerable interest in electronic properties of the vortex lines in type-II superconductors. It was predicted a few decades  $ago^{1-3}$  that a spectrum of quantized low-energy excitations exists in vortex lines. Recent scanning-tunneling-microscopy experiments<sup>4</sup> have given a new insight into the detailed structure of vortex cores. Motivated by these experiments, several groups<sup>5-8</sup> have advanced theoretical techniques to study the electronic structure of a vortex line, which agrees well with the experiments.

In this paper, we study the optical response of the vortex cores in an s-wave superconductor. We calculate the dynamic conductivity of the pinned vortices and show that there is an optical resonance well below the superconducting gap  $\Delta_0$ , corresponding to the quasiparticle pair creation process inside the vortex core. The resonance has right-handed chirality for electron carriers, and left-handed chirality for hole carriers. This chiral resonance may be used to probe the charge of carriers in superconducting states, similar to the Hall effect in the metallic state. The frequency and intensity of the resonance and the depolarization effect are estimated by numerically solving the Bogoliubov-de Gennes (BdG) equations self-consistently.<sup>6</sup> Some experimental relevance and consequences will be discussed.<sup>9</sup>

Let us consider a pinned single vortex line along the zaxis in a pure type-II superconductor. We assume that the background superconductor is described by a simple s-wave BCS theory, and that the system is in the clean limit and has a cylindrical symmetry about the vortex line. Before we go to detailed formalism, we would like to first provide a qualitative explanation of our results. At zero field, a conventional superconductor has a gap  $\Delta_0$ , so that the optical transition occurs only at frequency  $\hbar\omega \ge 2\Delta_0$ . In the presence of vortices, there exist bound states with energies of order of  $\Delta_0^2/E_F \ll \Delta_0$  ( $E_F$  is the Fermi energy), due to the "normal state" core of the vortex. Each of these bound states can be described by a half-integer angular momentum quantum number  $\mu$ . For electron-type carriers, the bound states with  $\mu < 0$  have negative energies relative to  $E_F$ , and are occupied at low temperatures. The bound states with  $\mu > 0$  have positive energies, and are unoccupied. These are quasiparticle states of mainly hole  $(\mu < 0)$  or electron  $(\mu > 0)$  character. Now let us consider a photon with right-handed chirality,  $\alpha = +1$  (counterclockwise), propagating along the z direction. As a consequence of the angular momentum conservation, the only allowed optical process within the gap is the transition from  $\mu = -\frac{1}{2}$  to  $\mu = +\frac{1}{2}$  bound state. If the incident photon has left-handed chirality,  $\alpha = -1$ (clockwise), then no transition between the bound states is allowed. The chirality of the optical transition is a result of the time-reversal symmetry breaking of the vortex states. If the carriers are hole type, then the resonance is only active for photons with left-handed chirality. This is because the system is CT invariant (reverse the charge and time simultaneously). In what follows, we shall consider electron systems (e < 0), and make the above discussions more concrete and quantitative.

Our starting point is to use the Kubo formula to evaluate the dynamic conductivity of the vortices whose states are described by the BdG equations.<sup>1,2</sup> The conductivity transverse to the z axis of  $N_v$  vortices can be written as, in the dilute density limit,  $\sigma_v = N_v \sigma^{(0)}$ , with  $\sigma^{(0)}$  the conductivity of a single vortex.  $\sigma^{(0)}$  is related to the retarded current-current correlation function  $\pi^{\text{ret}}$ ,  $\sigma^{(0)}_{\alpha,\alpha'}(\mathbf{q},\omega)$  $=(i/\omega)\pi^{\text{ret}}_{\alpha,\alpha'}(\mathbf{q},\omega)$ ,  $\pi^{\text{ret}}$  can be obtained from the corresponding Matsubara function by changing  $i\omega \rightarrow \omega + i\delta$ .

$$\pi_{\alpha,\alpha'}(\mathbf{q},i\omega) = -V^{-1} \int_0^\beta d\tau e^{i\omega\tau} \langle T_\tau j_\alpha^\dagger(\mathbf{q},\tau) j_{\alpha'}(\mathbf{q},0) \rangle ,$$

where **q** is the wave vector along the z axis,  $\mathbf{j}(\mathbf{q}, \tau)$  is the current operator in **q** space, and  $j_{\pm} = (j_x \pm i j_y)/\sqrt{2}$ . The correlation function will be evaluated in terms of quasiparticle amplitudes  $\hat{\psi}^T(\mathbf{r}) = (u(\mathbf{r}), v(\mathbf{r}))$ , in the presence of a single vortex.  $\hat{\psi}(\mathbf{r})$  are the solutions of the BdG equations. We work in the cylindrical coordinate, and choose a gauge<sup>1</sup> where the order parameter  $\Delta(\mathbf{r}) = e^{-i\theta}\Delta(r)$ , with  $\Delta(r)$  real. We can write

$$\hat{\psi}_{n}(\mathbf{r}) = (2\pi L_{z})^{-1/2} e^{ik_{z}z} e^{i(\mu - \tau_{z}/2)\theta} \hat{g}(\mathbf{r}) , \qquad (1)$$

where  $\hat{g}(r)$  is a normalized two-component spinor. The BdG equations then take the form

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$$\tau_{z} \frac{\hbar^{2}}{2m_{t}} \left\{ -\partial_{r}^{2} - \frac{1}{r} \partial_{r} + \frac{1}{r^{2}} \left[ \mu - \tau_{z} \left[ \frac{1}{2} + \frac{eA_{\theta}r}{\hbar c} \right] \right]^{2} - k_{\rho}^{2} \right\} \\ \times \hat{g}(r) + \tau_{x} \Delta(r) \hat{g}(r) = \epsilon \hat{g}(r) , \quad (2)$$

where  $\tau$ 's are Pauli matrices,  $A_{\theta}$  is the vector potential in  $\theta$  direction,  $m_t$  and  $m_z$  are the effective mass in the x-y plane and along the z direction, respectively, and  $k_{\rho}$  is the radial wave number, given by  $k_{\rho}^2 = 2m_t E_F / \hbar^2 - k_z^2 m_t / m_z$ . The  $\Delta(\mathbf{r})$  and  $\mathbf{A}(\mathbf{r})$  are to be determined self-consistently.<sup>6</sup> Using (1) and (2), we find at low T,

$$\pi_{\alpha,\alpha'}(\mathbf{q},i\omega) = V^{-1} \delta_{\alpha,\alpha'} \sum_{n,n'} \frac{|\mathcal{Q}_{n,n',\alpha}|^2}{i\omega - \varepsilon_n - \varepsilon_{n'}} , \qquad (3)$$

where the sum runs over all the states with positive  $\varepsilon_n$ and  $\varepsilon_{n'}$  and Q is the matrix element given by

$$Q_{n,n'\alpha} = \delta_{\mu'+\mu,\alpha} \delta_{k_{z'}+k_{z},q} (e\hbar k_F / im_t \sqrt{8}) C_{n,n'} , \qquad (4)$$

where  $k_F$  is the Fermi wave vector, and  $C_{n,n'} = \int dr F(r)$ is a dimensionless numerical factor, whose integrand

$$F(r) = k_F^{-1}(g_n^{\dagger}M_{n',n}\hat{g}_n^* + \hat{g}_n^{\dagger}M_{n,n}\hat{g}_{n'}^*),$$
  

$$M_{n',n} = i\tau_v(r\partial_r + \alpha\mu) = [(erA_{\theta}/\hbar c) + \alpha/2]\tau_x.$$
(5)

The function  $\delta_{\mu'+\mu,\alpha}$  in (4) describes the angular momentum conservation whose consequence will be discussed below.

Schematically shown in Fig. 1 are the solutions of Eq. (2). The scattering states have continuous spectrum, whose energy  $\varepsilon < -\Delta_0$ , or  $>\Delta_0$ . For each set of  $(\mu, k_z)$ , there is one and only one bound state, whose  $\varepsilon$  is within the gap.  $\varepsilon < 0$  if  $\mu < 0$ , and  $\varepsilon > 0$  if  $\mu > 0$ . The relative sign between  $\varepsilon$  and  $\mu$  can be best understood as the following. The occupied bound states ( $\varepsilon < 0$ ) generate a counter-



FIG. 1. Schematic plot of the energy spectra of the vortex states. The states of  $\varepsilon < 0$  are all occupied at T=0. The solid arrows indicate the allowed optical dipole transitions between two bound states, resulting in a resonance below the gap. (a)  $\mu = -\frac{1}{2}$  to  $\mu = +\frac{1}{2}$  for electron carriers and for photon chirality  $\alpha = +1$ ; (b)  $\mu = +\frac{1}{2}$  to  $\mu = -\frac{1}{2}$  for hole carriers and for  $\alpha = -1$ . The dashed arrows represent the transitions (not all shown) inducing an edge in absorption at  $\omega = \Delta_0 + \varepsilon_{1/2}$ .

clockwise paramagnetic current, hence the electrons move clockwise, thus  $\mu < 0$ . Therefore, the transition between the two bound states is only possible for  $\alpha = +1$ , and from a state  $\mu = -\frac{1}{2}$  to  $\mu = +\frac{1}{2}$ . Note that in the superconducting phase the ground state is considered as a vacuum, an operator which destroys a state of  $\varepsilon < 0$  with  $\mu = -\frac{1}{2}$  and spin up (down) should be regarded as a creation operator for an excitation of  $\varepsilon > 0$  with  $\mu = +\frac{1}{2}$ and spin down (up). Hence the transition from  $\mu = -\frac{1}{2}$  to  $\mu = +\frac{1}{2}$  should be regarded as in (4) to create a pair of spin-up and -down quasiparticles both with  $\mu = +\frac{1}{2}$ . This transition corresponds to the frequency of  $2\epsilon_{1/2} < \Delta_0$ , where  $\varepsilon_{1/2}$  is the bound-state energy of  $\mu = \frac{1}{2}$ . The other transitions conserving the angular momentum necessarily involve at least one scattering state. In particular, we predict an edge of absorption at  $\omega = \Delta_0 + \varepsilon_{1/2}$ , instead of  $2\Delta_0$  occurring at B=0 in dirty superconductors. This absorption is not polarized.

The real part of conductivity of vortices with density  $n_v$  is then, in the limit,  $q \rightarrow 0$ , for  $\omega < \Delta_0$  and  $\alpha = +1$ ,

$$\operatorname{Re}\sigma_{v}(\omega)=N(\omega)n_{v}e^{2}\pi C^{2}E_{F}/4m_{t}\omega$$
,

where  $N(\omega) = L_z^{-1} \sum_{k_z} \delta(\omega - 2\epsilon_{1/2})$  is the density of state associated with the z axis degree of freedom. In the limit  $m_z \gg m_t$ , the above expression leads to

$$\operatorname{Re}\sigma_{v}(\omega) = \eta(\omega_{p}^{2}/4)\delta(\omega - 2\varepsilon_{1/2}), \qquad (6)$$

where  $\omega_p$  is the plasma frequency, and  $\omega_p^2 = 4\pi n_e e^2/m_t$ , and  $n_e$  is the electron density,  $n_e = k_F^2/(2\pi c_0)$ , with  $c_0$  the interplane distance,  $\eta = n_v \xi^2 \pi^3 C^2/16K$  is dimensionless;  $\xi$  is the coherence length. In the derivation, a BCS relation  $k_F \xi = 2E_F / \pi \Delta_0$  has been used. K is a numerical factor, given by  $\varepsilon_{1/2} = K \Delta_0^2 / E_F$ . We have solved (2) selfconsistently at T=0 in a finite disk geometry following Gygi and Schluter<sup>6</sup> for parameter  $E_F / \Delta_0 = \frac{1}{7}$  and found C = 1.9 and K = 0.75. Results for spatial dependences of  $\psi$ , and F(r) are shown in Fig. 2. The intensity of the resonance can be estimated by integrating out Eq. (6) around the resonant frequency,  $\int_{-\infty}^{+\infty} d\omega \operatorname{Re}\sigma_v(\omega) = \eta \omega_p^2/4$ . Since  $\omega_p^2/4$  is the Drude conductivity weight of the metallic state, we see that  $\eta$  is the ratio of the vortex resonance strength relative to the Drude conductivity. Using  $H_{c2} = \Phi_0 / (2\pi \xi^2)$ ,  $n_v = H / \Phi_0$  with  $\Phi_0 = hc / 2e$ , we have  $\eta = (\pi^2 C^2 / 32K)h$  with  $h = H/H_{c2}$ .  $\eta = 1.6h$  for the parameters suitable for Y-Ba-Cu-O. Note that the above estimate applies only to  $h \ll 1$ . If  $m_r/m_t$  is finite, the resonance will have a dispersion, primarily determined by  $N(\omega)$ . As studied in Ref. 1,  $\varepsilon_{1/2}(k_z) \propto 1/k_{\rho}$ ,  $N(\omega) \propto [\omega - 2\varepsilon_{1/2}(k_z=0)]^{-1/2}$ . A relative sharp resonance is also expected.

In comparison to the cyclotron resonance, the vortex core resonance has the same chirality for electrons (or for holes). However, the underlying physics is very different. The frequency of the cyclotron resonance is proportional to H, while the frequency of the vortex core resonance is determined by the quasiparticle pair energy, and is independent of H.

Very recently, Karrai et al.<sup>9</sup> have reported the

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transmission measurements in the presence of high magnetic field on superconducting Y-Ba-Cu-O thin film and identified a vortex core resonance. The frequency and field-dependent intensity observed are consistent with the theory.<sup>9</sup> The chirality predicted in the present theory needs further experimental test. The preliminary experimental results were inconclusive. Accompanying the vortex core resonance, there is also a cyclotron resonance in the mixed superconducting state,<sup>10</sup> which complicates the detection. We believe that optical absorption experiments should distinguish the two, and would be desirable.

It will also be interesting to study the vortex resonance for unconventional superconductors, such as the *d*-wave state. We notice that the optical transition for a free vortex line has been recently studied by Hsu.<sup>11</sup> Since the resonance frequency is order of  $\Delta_0^2/E_F$ , which is low for the superconductors with lower  $T_c$  and longer coherence length, the microwave technique would be necessary to observe the resonance in these materials. The optical absorption edge at  $\Delta_0 + \varepsilon_{1/2}$ , however, should be relatively easy to observe.

Finally, we estimate the effect of the inhomogeneity in the conductivity. Since the vortices are embedded in the host superconductor, the conductivity is spatially dependent. This effect was qualitatively discussed in Ref. 9. Here we give more quantitative analyses. Similar to the technique applied to semiconductors,<sup>12</sup> we treat the single vortex as a cylinder of radius  $r_{\rm eff} = \gamma \xi$  and of dielectric function  $\epsilon_v$ , embedded in the host superconductor of dielectric function  $\epsilon_s$ .  $\gamma$  is a parameter, and may be estimated from the spatial dependence of the oscillator strength F(r) in (5). We choose to estimate  $\gamma$  from a mean-square value  $r_{\rm eff}^2 = \int F(r)r^2 dr/C$ . Then the single vortex conductivity is defined within the cylinder of a radius of  $\gamma \xi$ , and can be written as, in the limit  $m_z/m_t >> 1$ ,

$$\sigma_{v}^{(0)}(\omega) = i\kappa(2\varepsilon_{1/2}/\omega)(\omega_{p}^{2}/4\pi)/(\omega-2\varepsilon_{1/2}+i\delta),$$

with  $\kappa = \pi^2 C^{2/1} 6K \gamma^2$ , a dimensionless constant. The internal electric field  $E_v$  transverse to the z axis inside the vortex is then related to the external field  $E_{\text{ext}}$  by  $E_v = 2E_{\text{ext}}/(1 + \epsilon_v/\epsilon_s)$ . The effective conductivity in the vortex is  $\sigma_v^{\text{eff}} = 2\sigma_v^{(0)}/(1 + \sigma_v^{(0)}/\sigma_s)$ . The main effect of the depolarization is to redshift the resonant frequency



FIG. 2. Self-consistent numerical solutions of the Bogoliubov-de Gennes equations for (a)  $\mu = \frac{1}{2}$  bound state quasiparticle amptitudes, arbitrary units; (b) the spatial dependence of the integrand of the matrix element F(r) of Eq. (5), in units of  $\xi^{-1}$ ; (c) the gap function  $\Delta(r)$ . The calculations were done in a finite disk with a radius  $R = 370k_F^{-1}$ , and for parameters  $\Delta_0/E_F = \frac{1}{7}$ .

from  $\omega = 2\varepsilon_{1/2}$  to  $\omega = 2(1-\kappa)\varepsilon_{1/2}$ . From the numerical solutions of the BdG equations, we estimate  $\gamma = 2.6$  and  $\kappa = 0.43$ . A more accurate estimate on the resonant frequency requires a more sophisticated treatment of the inhomogeneous medium.

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- <sup>1</sup>C. Caroli, P. G. de Gennes, and J. Matricon, Phys. Lett. 9, 307 (1964).
- <sup>2</sup>J. Bardeen, R. Kummel, A. E. Jacobs, and L. Tewordt, Phys. Rev. **187**, 556 (1969).
- <sup>3</sup>L. Kramer and W. Pesch, Z. Phys. 269, 59 (1974).
- <sup>4</sup>H. F. Hess, R. B. Robinson, R. C. Dynes, J. M. Valles, Jr., and J. V. Waszczak, Phys. Rev. Lett. **62**, 214 (1989).
- <sup>5</sup>J. D. Shore, M. Huang, A. T. Dorsey, and J. P. Sethna, Phys. Rev. Lett. **62**, 3089 (1989).
- <sup>6</sup>F. Gygi and M. Schluter, Phys. Rev. Lett. **65**, 1820 (1990); Phys. Rev. B **43**, 7609 (1991).

- <sup>7</sup>U. Klein, Phys. Rev. B **41**, 4819 (1990).
- <sup>8</sup>S. Ullah, A. T. Dorsey, and L. Buchholtz, Phys. Rev. B 42, 9950 (1990).
- <sup>9</sup>K. Karrai, E. J. Choi, F. Dunmore, S. Liu, H. D. Drew, Q. Li, D. B. Fenner, Y. D. Zhu, and F. C. Zhang, Phys. Rev. Lett. **69**, 152 (1992).
- <sup>10</sup>K. Karrai, E. Choi, F. Dunmore, S. Liu, X. Ying, Q. Li, T. Venkatesan, H. D. Drew, and D. B. Fenner, Phys. Rev. Lett. 69, 355 (1992).
- <sup>11</sup>T. C. Hsu, Phys. Rev. B 46, 3680 (1992).
- <sup>12</sup>S. J. Allen, Jr., et al., Phys. Rev. B 28, 4875 (1983).