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Electromagnetic response of a static vortex line in a type-II superconductor: A microscopic study

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The electromagnetic response of a pinned Abrikosov fluxoid is examined in the framework of the Bogoliubov–de Gennes formalism. The matrix elements and the selection rules for both the single photon (emission - absorption) and two photon (Raman scattering) processes are obtained. The results reveal striking asymmetries: light absorption by quasiparticle pair creation or single quasiparticle scattering can occur only if the handedness of the incident radiation is opposite to that of the vortex core states. We show how these effects will lead to nonreciprocal circular birefringence, and also predict structure in the frequency dependence of conductivity and in the differential cross section of the Raman scattering.

Recent far infrared transmission experiments on superconducting $YBa_2Cu_3O_7$ thin films[1,2] have revived once again the interest in the quasiparticle excitations of the vortex core. A few decades ago, the microscopic structure of a vortex line in a type-II superconductor was the subject of many theoretical investigations.[3–8] Despite the rich structure in the density of states, predicted by the theory, early experiments on the microwave surface resistance[27] and microwave transmission[10] of the mixed state confirmed only a very simple theoretical prediction: that the vortex core states occupy a fraction $(H/H_{c2})^2$ of the total volume and that the vortex line is roughly equivalent to a normal cylinder of radius $\sim \xi$, the superconducting coherence length. This was largely due to the lack of spatial and frequency resolution: the experimental signal was an average over a large number of vortices. More recently, however, rather spectacular results were obtained, by scanning-tunneling microscopy[11,12] (STM) in which the spatial resolution of the signal was well below the coherence length. These experiments prompted theoretical work by various groups,[13–15] and it turned out that one can understand very well the experimental results within the Bogoliubov–de Gennes (BdG) formalism.[4]

Although the STM experiments reveal many aspects of the electronic structure of the vortex, they do not allow for measurements that probe the discreteness of the quasiparticle spectrum within the vortex, or the handedness imposed by the external magnetic field on the quasiparticle excitations of the vortex core. As we will show later on, this handedness will give rise to magneto-optical effects. It was pointed out to us by Girvin[16] and Kapitulnik[17] that a high-resolution optical gyroscope[18] might be able to detect the optical activity of the vortex core states. In order to probe the quasiparticle spectrum, Karraï *et al.*[1] have recently performed far-infrared transition measurements on $YBa_2Cu_3O_7$ thin films in perpendicular magnetic fields. They observe a broadened edgelike feature at 77 cm^{-1} and attribute this to the quasiparticle pair creation process inside the vortex core. Treating the mixed phase as a heterostructure, they give a phenomenological description of their data and extract the resonant frequency mentioned above, which, however, leads to a somewhat large energy gap: $\Delta = 63$ meV.

In this paper we examine the response of a pinned Abrikosov vortex to an external electromagnetic field within the BdG formalism. We are interested in the case of an isolated, static vortex line carrying a single flux quantum. The external magnetic field is taken in the $+z$ direction, with $H_{c1} < H \ll H_{c2}$. Due to the cylindrical symmetry, one can choose the quasiparticle amplitudes in the following form [$\mathbf{r} = (r, \theta, z)$]:[3]

$$\begin{pmatrix} u_n(r) \\ v_n(r) \end{pmatrix} = \frac{1}{\sqrt{2\pi L_z}} e^{ik_z z} e^{i\mu\theta} e^{-\frac{i}{2}\sigma_z\theta} \begin{pmatrix} g_n^+(r) \\ g_n^-(r) \end{pmatrix} . \quad (1)$$

Here σ_i's are the usual Pauli matrices. The magnetic quantum number μ is half an odd integer. If we measure the energy relative to the Fermi energy, E_F, and the length in units of ξ, in a gauge where the pair potential $\Delta(x)$ is real the BdG equations read

$$C\sigma_z\left\{-\frac{d^2}{dx^2} - \frac{1}{x}\frac{d}{dx} + \frac{1}{x^2}\left[\mu - \frac{1}{2}\sigma_z\right]^2 - k_\rho^2\right\} g_n(r) + \sigma_x\Delta(x)g_n(x) = E_n g_n(x) . \quad (2)$$

In the above equation g is a two-component spinor, $C = \hbar^2/(2m\xi^2)$ and $k_\rho^2 = k_F^2 - k_z^2$. (For simplicity we have assumed an isotropic effective mass.) In general, a self-consistent solution to the above equation can be obtained only numerically.[14,15] The general features of the solution are the following: the bound states, with exponentially decaying quasiparticle amplitudes, have an energy spectrum with $E(\mu) \propto \mu$ at small μ, the spacing between the levels being $\sim \Delta_\infty^2/E_F$, where Δ_∞ is gap in the bulk. The negative-energy states are fully occupied at $T = 0$, whereas the positive-energy states are empty.[6] The scattering states have a continuous spectrum, with energies $|E| > \Delta_\infty$.

The perturbing Hamiltonian describing single-photon (emission-absorption) processes can be given as

$$\mathcal{H}_1 = -\frac{e\hbar}{mci}\int d^3r \sum_\alpha \psi_\alpha^\dagger(r)\mathbf{A}(r)\boldsymbol{\nabla}\psi_\alpha(r) , \quad (3)$$

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where the sum is over the spin indices. The power absorbed by the system irradiated with an external electromagnetic field can be given in two different ways: $\mathcal{P} = (2\omega^2/c^2)\sigma_1(\omega) = \hbar\omega W$, where $\sigma_1(\omega)$ is the real part of the conductivity $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$ and W is the transition rate of the system under the influence of the perturbation $\mathcal{H}_1$:

$$W = \frac{2\pi}{\hbar^2}\sum_f |H_{fi}|^2\delta(E_f - E_i - \hbar\omega), \tag{4}$$

where $H_{fi} \equiv \langle f|\mathcal{H}_1|i\rangle$. Depending on the final state $|f\rangle$, the matrix elements will involve different coherence factors. For example, when the photon emission-absorption process scatters a single particle from one state to another the transition rate is given as

$$W_{\text{em-abs}} = \frac{2\pi}{\hbar^2}\left(\frac{e\hbar}{mc}\right)^2 \sum_{n,n'} |M_{n,n'}|^2 f_{n'}(1-f_n) \times\delta(E_n - E_{n'} \pm \hbar\omega)\ , \tag{5}$$

where $f_n \equiv f(E_n)$ is the Fermi function. We consider here the absorption process only, since we are ultimately interested in the low-temperature limit, where there is no spontaneous photon emission. The most interesting case for the present problem is that of the circular polarized light: $\mathbf{A}(r) = A_q\hat{\mathbf{e}}_\pm \exp[i(\mathbf{q}\cdot\mathbf{r} - \omega t)]$, where $\hat{\mathbf{e}}_\pm$ stands for the usual polarization vectors corresponding to the left (right) circular polarized light, $\hat{\mathbf{e}}_\pm = \hat{\mathbf{e}}_x \pm i\hat{\mathbf{e}}_y$ (note that we consider the case of a transverse electromagnetic wave propagating parallel to, and in the same direction as, the external magnetic field). In this particular case the matrix elements are

$$M^{\pm}_{n,n'} = 2A_q\delta(k_z - k_z' - q)\delta_{\mu',\mu\mp1}\left\{\int dr\left[rg_n^+\frac{d}{dr}g_{n'}^+ \mp\left(\mu' - \frac{1}{2}\right)g_n^+g_{n'}^+\right] - \int dr\left[rg_n^-\frac{d}{dr}g_{n'}^- \pm\left(\mu + \frac{1}{2}\right)g_n^-g_{n'}^-\right]\right\}, \tag{6}$$

implying the following selection rules:

$$k_z - k_z' - q = 0, \tag{7}$$

$$\mu' - \mu \pm 1 = 0, \tag{8}$$

$$E_n - E_{n'} - \hbar\omega = 0\ . \tag{9}$$

Further simplification occurs when we take the low temperature limit: then all the states with negative angular momentum $\mu' < 0$ are occupied,[6] and therefore the selection rules can be satisfied only for $\mu = \mu' + 1$ with the final state $\mu = +1/2$ and initial state $\mu' = -1/2$. But this is possible *only when the light is left circularly polarized.* Explicitly inserting these values for the angular momenta, we find

$$M^+_{n,n'} = 2A_q\int drr\left(g_n^+\frac{d}{dr}g_{n'}^+ - g_n^-\frac{d}{dr}g_{n'}^-\right) \tag{10}$$

and

$$M^-_{n,n'} \equiv 0\ . \tag{11}$$

Thus, the chirality of the vortex core states becomes manifest in the above selection rules governing the absorption of circularly polarized electromagnetic radiation.

The pair creation process, where the incoming photon creates a pair of quasiparticle excitations, can be discussed in a similar fashion. At zero temperature only the $\mu > 0$ are available, so that a photon with an energy just above the pair creation threshold will create a pair of quasiparticles with opposite spins but the same angular momentum $\mu = 1/2$. The transition probability corresponding to this process can be obtained by explicit calculation in the same way as that of the single-particle process. It is, however, possible to obtain the selection rules and the matrix elements corresponding to this process directly from the single-particle quantities, via a particle-hole-like symmetry connecting the positive- and negative-energy states.[19] According to this symmetry,[4] if (g_n^+, g_n^-) describes the state with energy and momentum E_n, k_z, μ, then $(g_n^-, -g_n^+)$ corresponds to $-E_n, -k_z, -\mu$. In this way, the single-particle process, where a negative-energy state is destroyed and a positive-energy state is created, can be easily related to the pair creation where two positive-energy states are created. In particular, the selection rule for the angular momentum for this process is that $\mu' + \mu = \pm1$. Since the pair with the lowest possible energy has $\mu' = \mu = 1/2$, the selection rule can again be satisfied only by a light carrying positive helicity, i.e., having left circular polarization.

Similar results were obtained independently, and parallel with our work, by Zhu, Zhang, and Drew.[20] These authors consider the superconducting ground state as a vacuum. In this picture, which is equivalent to ours, the electromagnetic radiation can be absorbed only by pair creation at $T = 0$. They also point out that if the carriers in a type-II superconductor are of the hole type, such as in most of the high-T_c compounds, the situation is reversed, with only right circularly polarized light is absorbed at zero temperature. This is a consequence of the CT invariance (simultaneous charge conjugation and time reversal).

These asymmetries will probably lead to experimentally observable consequences for the following reason. A difference in conductivity will cause a difference in the refractive index of the system with respect to the light waves of different circular polarization, since the complex refractive index is given by $N^2(\omega) = \epsilon_\infty + i4\pi\sigma(\omega)/\omega = (n + i\kappa)^2$, where ϵ_∞ is the dielectric constant at large frequencies, n is the real refractive index, and κ is the absorption coefficient. Different refractive indices for the two circular polarizations $n^\pm$ will result in a nonzero Faraday angle, with which the polarization plane of a linearly polarized light is rotated by a sample with thickness z: $\phi_F = (\omega z/2c)(n_+ - n_-)$.

An attempt was made by Karraï *et al.*[2] to check the angular-momentum selection rule and look for chirality in the vortex response by performing circularly polarized light transmission measurements on superconducting $YBa_2Cu_3O_7$ thin films. They found no evidence for optical activity in the vortex response. Instead, the signal is dominated by magneto-optical effects attributed to the condensate, and it is interpreted as a cyclotron resonance of the superconducting ground state.

A possible explanation for the lack of optical activity has been proposed by Hsu.[21] In this alternative picture, the $\mu = -1/2 \rightarrow +1/2$ dipole transition is hidden by the resonance of the circular motion performed by an *unpinned* vortex, which occurs at the same frequency as the dipole transition $\sim \Delta_\infty^2/E_F$. This resonance is clearly not sensitive to the polarization of the external electromagnetic radiation, which drives the motion of the vortex. However, we find it surprising that the resonance of this circular motion would occur at such a high frequency.

Let us now discuss the inelastic light scattering on the vortex core states. The electronic Raman scattering in metals with energy and momentum transfer $\omega = \omega_i - \omega_s$ and $q = k_i - k_s$ can be understood as a scattering on the *effective* density $\tilde{\rho}_q = \sum_{k,\alpha} \gamma_k a^\dagger_{k+q,\alpha} a_{k,\alpha}$,[22,23] where the scattering strength γ_k is strongly polarization dependent and satisifies $\gamma_k = \gamma_{-k}$ by time-reversal symmetry. Note that the continuity equation is *not* necessarily valid for $\tilde{\rho}_q$.[24] In direct space this is equivalent to the following effective density:

$$\rho_{\text{eff}}(r) = \int d^3R \sum_\alpha \psi^\dagger_\alpha(r)\psi_\alpha(r+R)\gamma(R) \ . \tag{12}$$

For an isotropic system γ_k = const, and consequently $\gamma(R) = \delta(R)$. The photon cross section per unit area and time is given by[25]

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{1}{2\pi}\left(\frac{\omega_2}{\omega_1}\right)^2 \frac{1}{|A_{k_i}|^2|A_{k_s}|^2\cos\theta} \times \sum_f |\langle f|\mathcal{H}_{\text{eff}}|i\rangle|^2 \delta(E_f - E_i - \hbar\omega) \ , \tag{13}$$

where θ is the angle of incidence and the effective interaction Hamiltonian is defined as

$$\mathcal{H}_{\text{eff}} = \frac{r_0}{2} A_{k_i} A_{k_s} \int d^3r d^3r' \times \sum_\alpha e^{i\mathbf{q}\cdot\mathbf{r}} \gamma(r' - r)\psi^\dagger_\alpha(r)\psi_\alpha(r') \ . \tag{14}$$

Here $r_0 = e^2/mc^2$ is the Thomson radius. We are now able to examine the matrix elements corresponding to different processes. For example, a photon can be absorbed and reemitted by a particle, or a pair can be created, which will finally recombine into the condensate and provide the outgoing photon by emission. The fermion subspace of the initial and final state is practically the same as for the single-photon processes we have discussed. In the case of an isotropic system, with $\gamma(r) = \delta(r)$ the matrix elements can be easily calculated. Here, for the sake of simplicity, we choose a special experimental geometry in which the direction of the momentum transfer q is along the z axis. The generalization for other geometries is quite straightforward. The single-particle processes are described by

$$M_{n,n'} = \int drr\{g^+_n g^+_{n'} - g^-_n g^-_{n'}\} \ , \tag{15}$$

along with the selection rules

$$k_z = k_z' + q, \tag{16}$$

$$\mu' = \mu, \tag{17}$$

$$E_n = E_{n'} + \hbar\omega \ . \tag{18}$$

The corresponding relations for the pair creation process can be obtained with the particle-hole symmetry mentioned before.

The anisotropic case can also be discussed if we assume that the function $\gamma(r)$ obeys cylindrical symmetry. This is approximately the case in a layered superconductor, when the axis of the vortices and the incident and the scattered light waves are perpendicular to the layers. Then one can choose the following trial form: $\gamma(\mathbf{r}) = \gamma_{m,\Gamma}(r)e^{im\theta}e^{i\Gamma z}$. The evaluation of the matrix elements in this case is somewhat lengthy but still straightforward. As a result we obtain that the selection rules are still the same as in the isotropic case: this is a consequence of the cylindrically symmetric scattering strength $\gamma(r)$.

The more interesting feature is the dependence of the scattering cross section on the transfer energy. This will be investigated by evaluating the matrix elements explicitly, using the numerical solutions[14,15] of the Bogoliubov–de Gennes equations. The detailed numerical results will be reported elsewhere. Nevertheless, it is possible to discuss intuitively the most important features of the frequency dependence. In a bulk superconducting phase the dynamic structure factor is zero until the energy transfer reaches the $\hbar\omega = 2\Delta$ threshold: the superconducting ground-state cannot absorb energy unless the photon has enough energy to break a Cooper pair. Above the threshold, the dynamic structure factor is divergent: the states excluded from the gap pile up above 2Δ giving rise to a square root singularity in the density of states and consequently in the dynamic structure factor. This divergency is in practice removed by gap anisotropy[23] or final-state interaction.[26] In a type-II superconductor in the mixed phase, the situation is quite different: the quasiparticle excitations of the vortex core are capable of absorbing the energy of the incoming photon. As mentioned before, these states occupy a fraction $(H/H_{c2})^2$ of the total volume and provide a quasinormal region where the dissipation is possible *unless* the energy of the incoming photon is less then twice the minigap: $\hbar\omega < 2\Delta^2/E_F$. Although this minigap is often very small in conventional superconductors, it is larger in a few materials. For example, in Nb_3Sn, $2\Delta^2/E_F \sim 0.9$ K, which is not necessarily unattainable experimentally.[27,28] For high-T_c superconductors, this value is even higher.

It is also interesting to ask whether the interaction between the quasiparticles would have significant effect on the Raman spectrum. If the final-state interaction is included in the description of Raman scattering on superfluid He II (Ref. 29) or superconductors (Ref. 26), the quasiparticles can form a bound state below the threshold. Similar effects may occur in the mixed state of superconductors.

In conclusion, we have investigated the electromagnetic response of the superconducting vortex states. Due to the handedness of the vortex states, strong asymmetries are discovered for the low-temperature absorption of circularly polarized light: the $\mu = -1/2 \rightarrow \mu = 1/2$ dipole transition and quasiparticle pair creation are possible *only* with left circular polarization, a striking consequence of the handedness of the vortex core states. We related the matrix elements to experimentally accessible quantities such as the dissipative part of the conductivity and the Faraday angle, and argued that the asymmetry in the absorption of circularly polarized light in a superconducting vortex and a finite rotation of the plane of polarization of a linearly polarized light at low temperatures might be experimentally observable.

We proposed that inelastic light (Raman) scattering could be used to investigate the vortex core states and developed the theory of Raman scattering on a superconducting vortex for isotropic and two-dimensional, layered superconductors. We argued that the presence of the vortex core states will lead to finite Raman intensity below the usual 2Δ threshold and that the minigap in the discrete spectrum of the vortex core states may be observable using low-frequency Raman spectroscopy. This is even more likely in high-T_c superconductors, where such a measurement, if successful, can reveal the magnitude of the energy gap. The results of conventional measurements for the energy gap in the cuprates, such as tunneling, infrared, and high-frequency Raman spectroscopy are not yet consistent, mainly due to the fact that at high frequencies the spectrum is convolved with the phonon and other excitation spectra.[30]

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