Absence of dipole transitions in vortices of type-II superconductors

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The response of a single vortex to a time-dependent field is examined microscopically and an equation of motion for vortex motion at nonzero frequencies is derived. Of interest are frequencies near Δ^2/E_F, where Δ is the bulk energy gap and E_F is the Fermi energy. The low-temperature, clean, extreme-type-II limit and maintenance of equilibrium with the lattice are assumed. A simplification occurs for large planar mass anisotropy. Thus the results may be pertinent to materials such as $NbSe_2$ and high-temperature superconductors. The expected dipole transition between core states is hidden because of the self-consistent nature of the vortex potential. Instead the vortex itself moves and has a resonance at the frequency of the transition.

The description of quasiparticle levels in vortex cores of superconductors has been known for some time. Caroli, de Gennes, and Matricon[1] and Bardeen *et al.*[2] calculated the energies and wave functions of these discrete levels using the Bogoliubov–de Gennes (BdG) equation. This was a basis for theories of dissipative vortex motion based on the idea of a normal core such as those of Bardeen and Stephen,[3] Nozières and Vinen (NV),[4] and others.[5] Kramer and Pesch[6] used the Eilenberger equation to calculate the density of states in the core. Their approach has proven useful in qualitatively explaining[7] scanning-tunneling-microscope experiments on $NbSe_2$ by Hess *et al.*[8] These experiments, however, probe the density of states at a scale ~ 0.1 meV, whereas the separation of core levels is ~ 10 mK. Caroli and Matricon[9] discussed the implications of discrete levels for ultrasound attenuation and nuclear magnetic relaxation. Transitions between these levels may have been observed recently in high-temperature superconductors.[10] The electromagnetic response is interesting from a practical point of view. Herein we focus on the low-temperature and clean limit, considering eigenfunctions and matrix elements of quasiparticle states and assuming the BdG equations and a local gap equation, $\Delta(\mathbf{r}) = V\langle c_\uparrow(\mathbf{r})\, c_\downarrow(\mathbf{r})\rangle$, ($c_\sigma$ is a spin σ electron operator) to be valid. The vortex response to an electromagnetic field will be considered from a purely microscopic point of view. Real materials have vortex pinning but undergo a crossover to unpinned behavior at frequencies of order of magnitude comparable to the core-level separation;[11] so a first step should be a study of unpinned vortices at those frequencies. Real superconductors are nonlocal and the interaction is retarded but the hope is that, since we deal with rigid motions and relatively low frequencies, some relevance to real materials remains.

In terms of eigenfunctions, $\psi_\mu(\mathbf{r})^T = (u_\mu(\mathbf{r}) \quad v_\mu(\mathbf{r}))$, the quasiparticle operators are

$$\begin{pmatrix} \gamma^\dagger_{\mu\uparrow} \\ \gamma^\dagger_{\mu\downarrow} \end{pmatrix} = \int d\mathbf{r} \begin{pmatrix} c^\dagger_\uparrow(\mathbf{r}) & c_\downarrow(\mathbf{r}) \\ c^\dagger_\downarrow(\mathbf{r}) & -c_\uparrow(\mathbf{r}) \end{pmatrix} \psi_\mu(\mathbf{r}). \tag{1}$$

The Schrödinger equation for ψ is the BdG equation,

$$\epsilon\psi(\mathbf{r}) = \sigma^z \left[\frac{1}{2m}\left(\mathbf{p} - \sigma^z \frac{e}{c}\mathbf{A}\right)^2 - E_F\right]\psi(\mathbf{r}) + \begin{pmatrix} 0 & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & 0 \end{pmatrix}\psi(\mathbf{r}), \tag{2}$$

where $\Delta = |\Delta(\mathbf{r}-\mathbf{r}_0)|\exp[-i\theta(\mathbf{r}-\mathbf{r}_0)]$. $\theta(\mathbf{r}-\mathbf{r}_0)$ is the angle about the center of the vortex $\mathbf{r}_0$ measured from the $\hat{\mathbf{x}}$ axis. We consider a vortex parallel to $\hat{\mathbf{z}}$.

In the extreme-type-II limit with $H \ll H_{c2}$ the magnetic field that creates vortices may be ignored. Its importance compared to the phase of Δ is reduced by ξ^2/λ^2, where ξ is the coherence length and λ is the penetration depth.

The eigenfunctions for fixed k_z, $\mu \ll k_{F\perp}\xi$, and the radial coordinate $r \ll \xi$ are

$$\psi_\mu(\mathbf{r}) = \left(\frac{k_F}{2\pi\xi L_z}\right)^2 e^{ik_z z} \begin{pmatrix} e^{i(\mu-\frac{1}{2})\phi} J_{\mu-\frac{1}{2}}(k_{F\perp}r) \\ e^{i(\mu+\frac{1}{2})\phi} J_{\mu+\frac{1}{2}}(k_{F\perp}r) \end{pmatrix}, \tag{3}$$

where $\mu = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$ and $\perp$ refers to the $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ directions (we assume at least cylindrical symmetry). They fall off exponentially for $r > \xi$. The energies as calculated by Kramer and Pesch,[6] who accounted for some self-consistency effects due to the gap equation, are

$$\epsilon_\mu = \frac{2\mu\Delta_0^2}{k_F v_F \cos^2\Theta} \ln\left(\frac{\pi}{2}\xi_0 \cos\Theta/\xi_1\right), \quad \cos\Theta \equiv k_{F\perp}/k_F. \tag{4}$$

The logarithmic factor is not important here and is ignored hereafter, but see Ref. 12.

Consider a long-wavelength electromagnetic wave, $\mathbf{A}' \perp \hat{\mathbf{z}}$, with polarization at angle θ_0 to $\hat{\mathbf{x}}$. We treat the perturbation $-\frac{e}{mc}\mathbf{A}'\cdot\mathbf{p}$ to first order in A'. If the matrix elements with respect to low-energy states are not very sensitive to the exact behavior of the wave functions at the core boundary, then they may be estimated, using standard Besselfunction identities, to be $\int \psi^\dagger_{\mu\pm1}(-\frac{e}{mc}\mathbf{A}'\cdot\mathbf{p})\psi_\mu = (e\hbar k_{F\perp}A'/2mc)\exp[\mp i(\theta_0+\frac{\pi}{2})]$.

Consider a vortex with velocity $\mathbf{v}_L \perp \hat{\mathbf{z}}$ and a background superfluid velocity $\mathbf{v}_S$. These velocities will be assumed uniform along the length of the vortex. This is valid if the distance the electromagnetic wave penetrates the superconductor (the shorter of the London penetration depth and skin depth) is long compared to the coherence length. We shall consider a background supercurrent or gauge field of the form

$$\mathbf{A}'(t) \equiv -(mc/e)\mathbf{v}_S(t) = \mathbf{E}ct + \mathbf{A}'_0. \tag{5}$$

$\mathbf{E}$ is the applied electric field.

Let us now outline the ensuing calculation. The time dependence of the quasiparticle states under the applied field and the moving vortex will be calculated and written in terms of a density matrix. The motion of the vortex will be inferred, using the gap equation, by identifying changes in the off-diagonal components of the density matrix with that due to a displaced vortex. Because this calculation involves self-consistency in the vortex velocity there is a slight subtlety. Given initial ($t=0$) values of $\mathbf{v}_L$ and $\mathbf{v}_S$, as considered below, in general, they will not be consistent. In general, $\mathbf{v}_L$ is obtained by integrating the equation of motion for a given $\mathbf{v}_S(t)$. We shall first derive the acceleration of the vortex at $t=0$ and then find the equation of motion for all time by beginning in a well-defined equilibrium state ($\mathbf{v}_L=\mathbf{0}$, $\mathbf{v}_S=\mathbf{0}$, $\mathbf{r}_0=\mathbf{0}$ at $t=0$) and, given a time dependence $\mathbf{v}_S(t)$, calculating the resulting motion to all orders in t.

Suppose the field in Eq. (5) is turned on at $t=0$. Let us calculate the quasiparticle density matrix to order t^2. We use $\langle\ \rangle_0$ to denote the (diagonal) values at $t=0$. Using matrix elements of $\mathbf{A}'$, the off-diagonal density matrix elements are

$$\langle\gamma^\dagger_\mu\gamma_{\mu-1}\rangle(t) = [\langle\gamma^\dagger_\mu\gamma_\mu\rangle_0 - \langle\gamma^\dagger_{\mu-1}\gamma_{\mu-1}\rangle_0]\left\{-i\frac{W}{\hbar}t - \frac{t^2}{2\hbar^2}[i\hbar W' + W(\epsilon_{\mu-1}-\epsilon_\mu)]\right\}, \tag{6}$$

where $W = (e\hbar k_{F\perp}A'_0/2mc)\exp i(\theta_0+\frac{\pi}{2})$ and W' is the same as W except with A'_0 replaced by cE. Terms of order W^2 (such as the change in the diagonal density matrix element) are ignored by taking the amplitude of the perturbation to be sufficiently small.

The significance of these density-matrix elements is clarified by considering a displaced vortex in terms of the underlying quasiparticles. The inverse of Eq. (1) substituted into the gap equation is

$$\Delta(\mathbf{r}) = V\sum_{\mu,\nu}\left[\left(\delta_{\mu\nu} - \sum_\sigma\langle\gamma^\dagger_{\nu\sigma}\gamma_{\mu\sigma}\rangle\right)v^*_\nu(\mathbf{r})u_\mu(\mathbf{r}) + \text{other terms}\right]. \tag{7}$$

Suppose the quasiparticles are displaced by δr_0 at angle ϕ_0 to $\hat{\mathbf{x}}$. The occupation is taken to be diagonal before displacement, $\langle\gamma^\dagger_{\nu\sigma}\gamma_{\mu\sigma}\rangle = \delta_{\mu\nu}f(\epsilon_\nu)$, where $f(\epsilon)$ is the Fermi function. Then, in the undisplaced eigenbasis, to linear order in δr_0,

$$\delta\Delta(\mathbf{r}) = -V\delta r_0 k_{F\perp}\sum_\nu\{\, e^{i\phi_0}[f(\epsilon_\nu) - f(\epsilon_{\nu+1})]v^*_{\nu+1}(\mathbf{r})u_\nu(\mathbf{r}) \tag{8}$$

$$+e^{-i\phi_0}[f(\epsilon_\nu) - f(\epsilon_{\nu+1})]v^*_\nu(\mathbf{r})u_{\nu+1}(\mathbf{r})\}. \tag{9}$$

Comparing with Eq. (6), it is clear that the term of order t may be produced by a rigid translation of the vortex core at velocity $\delta r_0/t = -(e/mc)A'_0$ in the direction $\phi_0 = \theta_0$. It is simply the velocity by which the gauge field boosts the group velocity of all waves.

Returning to Eq. (6), the first term of order t^2 corresponds to an acceleration proportional to the electric field, and Eq. (9) shows that it is $\dot{\mathbf{v}}_S$. The second piece is trickier. Because $\epsilon_{\mu-1}-\epsilon_\mu$ can depend on k_z and (for large μ) μ, the t^2 term does not correspond to a rigid acceleration of the vortex core except in the limit of low temperature and strong mass anisotropy, $m_z \gg m_\perp$. There $\epsilon_{\mu-1}-\epsilon_\mu = 2\Delta_0^2/k_F v_F$ (independent of μ) and making the identification with a rigid displacement leads to an acceleration

$$\frac{2\delta r_0}{t^2} = -\frac{2\Delta_0^2 e A'_0}{\hbar k_F v_F mc} \tag{10}$$

in a direction $\phi_0 = \theta_0 + \frac{\pi}{2}$ perpendicular to $\mathbf{v}_S$. This corresponds to the Lorentz force.

At high temperatures higher-energy levels become important. The level spacing decreases with increasing energy so higher-energy quasiparticles have a smaller acceleration and lag behind the core. The term $\epsilon_{\mu-1}-\epsilon_\mu$ contains a factor $(1/\cos^2\Theta)$ that is the k_z dependence. This factor is not actually divergent. Expression (4) for the energies is valid only for small energies. The ϵ_μ are bounded by Δ_0, and so $\epsilon_{\mu-1}-\epsilon_\mu$ must go to zero as $\Theta\to\pi/2$. In real materials such as $NbSe_2$ the Fermi surface is open, which restricts $\cos\Theta$. Below, for simplicity, we assume that the system has an anisotropic mass and that the lack of rigid acceleration is not important.

Assuming rigid motion we see that the applied field, instead of causing dipole transitions, causes the density matrix to evolve off-diagonal elements corresponding to vortex motion (after applying the gap equation). In the new displaced set of basis functions the density matrix is again diagonal. The vortex does not stand still and allow a dipole transition to take place, as does the core of an atom. *The vortex is a self-consistent potential.*

The moving vortex itself affects the density matrix. Suppose the vortex has velocity $\mathbf{v}_L$ at an angle ϕ_0 to $\hat{\mathbf{x}}$. The matrix element

$$W_{\mu\nu} = \int d\mathbf{r}\ \psi_\mu^\dagger(\mathbf{r}) \begin{pmatrix} 0 & \delta\Delta(t) \\ \delta\Delta^*(t) & 0 \end{pmatrix} \psi_\nu(\mathbf{r}) \qquad (11)$$

may be rewritten using Galilean invariance. Let $\delta\psi_\mu(\mathbf{r})$ be the change in $\psi_\mu(\mathbf{r})$ upon displacement of the vortex by $\delta\mathbf{r}_0$. Then substituting $\delta\psi$ and $\delta\Delta$ into the BdG equation, subtracting the undisplaced piece, keeping terms to first order in δr_0, and integrating by parts results in $W_{\mu\nu} = (\epsilon_\nu - \epsilon_\mu)\int d\mathbf{r}\psi_\mu^\dagger(\mathbf{r})\delta\psi_\nu(\mathbf{r})$. Writing $\delta\psi(\mathbf{r}) = t\mathbf{v}_L \cdot \nabla\psi(\mathbf{r})$, and using standard identities,

$$W_{\mu\nu} = -\frac{v_L t k_{F\perp}}{2i}\delta_{\mu,\nu\mp1}(\epsilon_\nu - \epsilon_\mu)e^{\pm i(\phi_0 + \frac{\pi}{2})}. \qquad (12)$$

Treating this to linear order and integrating from 0 to t gives an acceleration $(2\delta r_0/t^2) = (v_L/\hbar)(\epsilon_\nu - \epsilon_{\nu+1}) = -(\Delta_0^2/E_F\hbar)v_L$ in a direction at an angle $+\pi/2$ to $\mathbf{v}_L$.

This together with Eq. (10) gives an acceleration $(\Delta_0^2/\hbar E_F)(\mathbf{v}_L - \mathbf{v}_S) \times \hat{\mathbf{z}}$ corresponding to the Magnus force given in Ref. 4 as $(hn/2)(\mathbf{v}_S - \mathbf{v}_L) \times \hat{\mathbf{z}}$, where n is the (superfluid) electron density. Taking $n = k_{F\perp}^2 k_{Fz}/\pi^3$ and the in-plane coherence length $\xi_\perp = \hbar v_{F\perp}/\pi\Delta$, one may extract a "mass" of the vortex $M \sim m_\perp(k_{F\perp}\xi_\perp)^2$ per unit length k_{Fz}^{-1}. This expression is perhaps a microscopic justification for a "normal core" of size ξ, even at low temperatures when there is a gap in the single-particle density of states. This mass should be contrasted with the very different definition of mass discussed recently by Duan and Leggett.[13] Here the mass corresponds to the inertia of the electrons in the core of the vortex.

To treat dissipation we assume that core states maintain equilibrium with the lattice and that the linear-in-t change in the single-particle states (in the lattice frame of reference) also decays as an exponential $\exp(-t/\tau)$. τ is related to the transport lifetime, although there are differences in matrix element and phase space that can be elucidated in a microscopic theory. Given the velocity $\mathbf{v}_L$, then to linear order in t the off-diagonal component of the density matrix is, in a basis fixed to the lattice at $t = 0$,

$$\langle\gamma_\mu^\dagger\gamma_{\mu-1}\rangle = \langle\gamma_\mu^\dagger\gamma_\mu\rangle(1 - \langle\gamma_{\mu-1}^\dagger\gamma_{\mu-1}\rangle)[-(k_{F\perp}v_L/2)e^{i\phi_0}]t \qquad (13)$$

$$+\langle\gamma_{\mu-1}^\dagger\gamma_{\mu-1}\rangle(1 - \langle\gamma_\mu^\dagger\gamma_\mu\rangle)[(k_{F\perp}v_L/2)e^{i\phi_0}]t. \qquad (14)$$

The result is an additional contribution to the second derivative of the off-diagonal element,

$$\frac{d^2}{dt^2}\langle\gamma_\mu^\dagger\gamma_{\mu-1}\rangle = -\frac{1}{\tau}\frac{d}{dt}\langle\gamma_\mu^\dagger\gamma_{\mu-1}\rangle + (\text{previous terms}). \qquad (15)$$

This produces a contribution $-(1/\tau)\mathbf{v}_L$ to the vortex acceleration. Collecting terms, the equation of motion is

$$\dot{\mathbf{v}}_L = \dot{\mathbf{v}}_S + \frac{\Delta_0^2}{\hbar E_F}(\mathbf{v}_L - \mathbf{v}_S) \times \hat{\mathbf{z}} - \frac{1}{\tau}\mathbf{v}_L. \qquad (16)$$

In the above derivation we applied $\mathbf{v}_S$ instantaneously to a vortex stationary for $t < 0$. That produced $\mathbf{v}_L = \mathbf{v}_S$ at $t = 0$, which is an insufficiently general initial condition. We now show that Eq. (16) is valid at all times. We begin at $t = 0$ in a well-defined state, $\mathbf{v}_L = \mathbf{v}_S = \mathbf{0}$, and displacement $\mathbf{r}_0 = \mathbf{0}$. Given the Taylor expansion of $\mathbf{v}_S$, we may calculate, using the above technique, the displacement to any order t^n because we need know only $\mathbf{v}_S$ to order $n-1$ and $\mathbf{v}_L$ to order $n-2$. The gap equation applied to the order n displacement of the quasiparticles gives $\mathbf{v}_L$ to order $n-1$ and thus continues the calculation. The result to fourth order is

$$\mathbf{r}_0(t) = \frac{1}{2}\dot{\mathbf{v}}_S(0)t^2 + \frac{1}{3!}[\ddot{\mathbf{v}}_S(0) - \tau^{-1}\dot{\mathbf{v}}_S(0)]t^3 \qquad (17)$$

$$+\frac{1}{4!}\{-\tau^{-1}\Omega_0[\dot{\mathbf{v}}_S(0) \times \hat{\mathbf{z}}] - \tau^{-1}\ddot{\mathbf{v}}_S(0) + \tau^{-2}\dot{\mathbf{v}}_S(0)\}t^4 + \cdots, \qquad (18)$$

where $\Omega_0 \equiv \Delta_0^2/\hbar E_F$. This calculation is fully consistent and equivalent to taking the derivatives of Eq. (16) and evaluating them at $t = 0$. Since the equation is linear and velocities can be calculated to all orders in t, this equation is valid for all $t > 0$.

Equation (16) at zero frequency was introduced by deGennes and Matricon.[14] The dissipation acts on $\mathbf{v}_L$ rather than $\mathbf{v}_S$ as in the NV equation. This has the drawback of not allowing for small conductivities observed in experiments on flux flow[15] (not to mention that there has never been a satisfactory explanation of the Hall effect). The present derivation is valid in the clean, low-temperature limit where the levels are clearly separated. Our result agrees with the NV equation of motion in that limit[16] but cannot be extended to the dirty limit.

It is easily verified that the homogeneous solution of (16) corresponds to the circular motion, with a definite handedness, at frequency Ω_0 and decaying on a timescale τ. To obtain a prediction for the surface impedance, consider the particular solution for $\mathbf{v}_S(t) = \mathbf{v}_S(0)\exp(i\omega t)$. It is

$$v_{Ly} - v_{Sy} = \left[\frac{\Omega_0\tau v_{Sx} - (1 + i\omega\tau)v_{Sy}}{(1 + i\omega\tau)^2 + (\Omega_0\tau)^2}\right], \qquad (19)$$

and another equation with x, y interchanged and $\Omega_0 \to -\Omega_0$.

There are two contributions to the surface impedance. The first is transverse vortex motion in phase with the supercurrent. For clarity let $v_{Sy} = v_{Sx}\exp i\theta = v_S/\sqrt{2}$. There is an induced voltage per vortex $\hat{\mathbf{z}} \times \mathbf{v}_L(h/2e)$. The supercurrent density $v_S ne$ gives dissipation $N_v(hn/2)\text{Re}(v_{Lx}^* v_{Sy} - v_{Ly}^* v_{Sx})$, where N_v is the vortex density. Using Eq. (19),

$$\mathrm{Re}(v_{Lx}^{*}v_{Sy}-v_{Ly}^{*}v_{Sx}) = -v_S^2\Omega_0\tau\frac{1-(\omega\tau)^2+(\Omega_0\tau)^2}{[1-(\omega\tau)^2+(\Omega_0\tau)^2]^2+4(\omega\tau)^2} \quad (20)$$

$$+\sin\theta v_S^2\omega\tau\frac{1+(\omega\tau)^2-(\Omega_0\tau)^2}{[1-(\omega\tau)^2+(\Omega_0\tau)^2]^2+4(\omega\tau)^2}. \quad (21)$$

The first term has an (anti)resonance at $(\omega\tau)^2 = (\Omega_0\tau)^2 + 1$, while the second, polarization-dependent, term has a resonance there.

The second source is the current due to vortex motion, which is in phase and parallel with the applied electric field. A straightforward calculation gives the average current density due to vortex motion as $2v_L(k_{Fz}/\pi)(E_F/\Delta)^2N_ve$. With the electric field $\mathbf{E} = -(m/e)\dot{\mathbf{v}}_S$ the dissipation is $-2m(k_{Fz}/\pi)(E_F/\Delta)^2N_v\mathrm{Re}(v_{Ly}^{*}i\omega v_{Sy}+v_{Lx}^{*}i\omega v_{Sx})$. Using Eq. (19),

$$\mathrm{Re}(v_{Ly}^{*}i\omega v_{Sy}+v_{Lx}^{*}i\omega v_{Sx}) = v_S^2\omega^2\tau\frac{1+(\omega\tau)^2-(\Omega_0\tau)^2}{[1-(\omega\tau)^2+(\Omega_0\tau)^2]^2+4(\omega\tau)^2}. \quad (22)$$

This has a peak at $(\omega\tau)^2 \sim (\Omega_0\tau)^2+1$ and is not polarization dependent. By letting $\Omega_0 \to 0$, this term becomes simply the Drude expression for dissipation.

The expected polarization-dependent absorption is distributed, due to states with different k_z, over a range of frequencies. Precise details depend on the Fermi-surface shape. The temperature dependence should be weak. The current due to quasiparticles moving in and out of the vortex core can be neglected at low temperature because there is a discrete energy cost to make charge fluctuations in the core. The considerations of this paper may be valid even for pinned vortices. If some parts of a line are pinned, other parts between pins can move, provided they are excited at high enough frequency.

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