Vortex Dynamics and the Hall Anomaly: A Microscopic Analysis

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We present a microscopic derivation of the equation of motion for a vortex in a superconductor. A coherent view on vortex dynamics is obtained, in which *both* hydrodynamics *and* the vortex core contribute to the forces acting on a vortex. The competition between these two provides an interpretation of the observed sign change in the Hall angle in superconductors with mean free path l of the order of the coherence length ξ in terms of broken particle-hole symmetry, which is related to details of the microscopic mechanism of superconductivity.

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In recent years the interest in vortex motion in superconductors has revived, mainly due to the advent of high temperature superconductors (HTSC). As a consequence of the peculiar material properties, the physics of vortices in HTSC shows many new aspects not encountered in conventional superconductors [1]. A major theme is the sign change in the Hall effect in the superconducting state, as is observed in both HTSC [2,3] and conventional superconductors [3] for temperatures T just below T_C . This Hall anomaly cannot be understood within the framework of the conventional Bardeen-Stephen [4] or Nozieres-Vinen [5] theories for vortex motion that predict the Hall effect in the superconducting and normal state to have the same sign for all temperatures. Several attempts at a theoretical understanding of the phenomenon have been undertaken [6,7], but none of these seem to explain the experimental data. In Ref. [3] Hagen et al., comparing a number of experiments, conclude that the sign change of the Hall effect is an intrinsic vortex property that occurs if the electron mean free path l is of the order of the coherence length ξ . Within a phenomenological analysis, Feigel'man *et* al. [8] interpret the sign change in terms of broken particlehole symmetry and obtain good agreement with the experimental signatures [3] of this effect. It is the purpose of this Letter to report on a microscopic calculation of the dynamical single vortex properties that yields a unifying description of the physics involved and puts the results of the analysis of Ref. [8] on a firm theoretical basis.

Before presenting the microscopic theory, we discuss our main results for the vortex equation of motion and the resulting Hall force and angle. In general one expects the forces on a vortex to consist of two contributions, i.e., one from the electronic states in the vortex core and one from the hydrodynamic flow far away from the core. The vortex equation of motion has the form

$$[M_C + M_H]\mathbf{V} + \eta_C \mathbf{V} = \{\kappa_H \mathbf{V}_T - [\gamma_C + \gamma_H]\mathbf{V}\} \times \mathbf{z}.$$

Here V denotes the velocity of the vortex and V_T is the transport velocity due to an applied current density $\mathbf{j} = \kappa_H V_T / \Phi_0$ (we consider a film or layered structure,

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the extension to a 3D geometry is straightforward). The equation of motion includes a vortex mass M, a damping term η , and the Lorentz and Hall force coefficients κ and γ . We made a clear separation into core and hydrodynamic contributions by writing subscripts C and H, respectively. Extrinsic forces due to pinning and the interaction with other vortices add to the right-hand side of the above equation of motion; however, here we consider only intrinsic vortex properties. The coefficient for the Lorentz force, $\kappa_H = \pi n_s$, arises from the hydrodynamic flow around the vortex with the superfluid density described by n_s [9]. The mass terms were considered by Suhl in a Ginzburg-Landau approach [10]. The core contributions η_C and γ_C were calculated by Kopnin and coworkers [11], who found (we use $\hbar = c = k_B = 1$)

$$\eta_C = \pi n_e \frac{\omega_0 \tau_r}{1 + (\omega_0 \tau_r)^2}, \qquad \gamma_C = \pi n_e \frac{(\omega_0 \tau_r)^2}{1 + (\omega_0 \tau_r)^2},$$
(1)

where n_e denotes the electronic density, $\omega_0 \approx \Delta^2/\epsilon_F$ is the level spacing between the localized Caroli– de Gennes–Matricon (CdGM) states in the core [12], and τ_r is the relaxation time.

The key point in the determination of the Hall angle $\alpha_{\text{Hall}} (\tan \alpha_{\text{Hall}} = \gamma/\eta)$ is to find the hydrodynamic contribution γ_H . For comparison we review the similar procedure for uncharged bosons like ⁴He, where the vortex core has no internal structure and the Hall force arises from the first order time derivative $\bar{\psi}i\partial_t\psi$ in the Lagrangian density [13]. With $\psi = \sqrt{n} e^{i\varphi}$, *n* the mean particle density, the corresponding contribution to the Lagrangian is $\delta \mathcal{L} = -n\dot{\varphi}$. In the presence of a vortex at **R**, the phase configuration is $\varphi(\mathbf{r}, \tau) = \varphi_v(\mathbf{r} - \mathbf{R}(\tau))$ with $\varphi_v(\mathbf{r}) = \arctan(y/x)$. The Euler-Lagrange equation yields a Hall force $\mathbf{F}_{\text{Hall}} = -2\pi n \mathbf{V} \times \mathbf{z}$, or $\gamma_H = 2\pi n$ for bosons. If no normal fluid component is present at T = 0, the Hall and Lorentz force combine into the Galilei invariant Magnus force $\mathbf{F}_M = \kappa(\mathbf{V}_T - \mathbf{V}) \times \mathbf{z}$ [9].

A hydrodynamic contribution to the Hall force in a superconductor arises also from a first order time derivative

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in the Lagrangian. This is most clearly seen in a time dependent Ginzburg-Landau (TDGL) approach, where a term $\delta \mathcal{L} = (N'_e/2\Lambda N_e)\bar{\Delta}i\partial_t\Delta$ appears in the Lagrangian density [14]. This term depends on the electronic band structure through the derivative of the density of states N_e at the Fermi level $N'_e = \partial_{\mu} N_e(\mu)|_{\mu=\epsilon_F}$ and is thus related to particle-hole asymmetry. Here Λ is the strength of the attractive BCS model interaction. Note that in BCS theory $2N'_e/\Lambda N_e = N_e \partial_\mu \ln T_C$. The same procedure as for ⁴He leads to a small hydrodynamic contribution $\gamma_H =$ $\pi (N'_e/\Lambda N_e) |\Delta|^2$ of order $n_e (\Delta/\epsilon_F)^2 (N'_e \simeq n_e/\epsilon_F^2)$. Its exact magnitude and sign depend on the (experimentally accessible) details of the electronic band structure. Although core physics is lacking in a TDGL approach [6], we will see in the following that TDGL does predict the correct hydrodynamic contribution γ_H . A hydrodynamic contribution to γ is a general property of superconductors with broken particle-hole symmetry, also for temperatures far below T_C .

Defining $n_{\Delta} = N'_e \Delta^2 / \Lambda N_e$, the total Hall force constant for a superconductor at $\omega_0 \ll T \ll \Delta$ becomes (see also the detailed discussion in Ref. [8])

$$\gamma = \pi n_e (\omega_0 \tau_r)^2 / [1 + (\omega_0 \tau_r)^2] + \pi n_\Delta.$$
 (2)

The first term describes the contribution arising from the quasiparticles bound to the core. Close to the superconducting-normal transition the scattering states have to be included [15] and the term crosses over to the normal state Hall term; it therefore has the normal state sign. The second term is the hydrodynamic contribution. With $\omega_0 = \Delta^2/\epsilon_F$ and $n_\Delta/n_e \approx \Delta^2/\epsilon_F^2$, the core term is dominant in the clean limit $l > \xi(T)$, whereas the hydrodynamic contribution determines the Hall angle in the dirty case. A sign change in the Hall effect occurs if the hydrodynamic term has a negative sign, i.e., $N'_e < 0$. Within a free-electron based BCS theory we have $N'_e \ge 0$ and no sign change occurs. However, a simple modification of the electronic dispersion can drive N'_{e} negative, resulting in sign changes of the Hall effect as described below [e.g., consider the dispersion $\epsilon_k = k^2/2m + k^4/4m^2\epsilon_0$ in two dimensions: the corresponding density of states is $N_e(\epsilon) = m/\pi (1 + 2\epsilon/\epsilon_0)$ and $N'_e = -(2\pi/m\epsilon_0)N_e^2(\epsilon) < 0$ accordingly]. With $N'_{e} < 0$ the Hall effect has the normal state sign in the clean limit and the opposite one in the dirty limit. Furthermore, the two contributions have a different temperature dependence through $\Delta(T)$, allowing for multiple sign changes. Our interpretation of the sign changes in HTSC (Bi- and Tl-based compounds) is as follows: At low temperatures the clean limit is realized with $l > \xi(T)$ and the Hall effect has the normal state sign; with increasing temperature, τ_r and Δ decrease until the second term in Eq. (2) dominates and a first sign change occurs when $l \sim \xi(T)$. At even higher temperatures, close to T_C , the normal quasiparticles take over and a second sign change back to the normal state sign occurs. Note that the low-temperature sign change may be invisible if pinning is strong enough, which is probably the case for Y-Ba-Cu-O. This analysis provides a natural interpretation for the experimental findings as summarized by Hagen *et al.* [3].

We now continue with an outline of the microscopic derivation of the vortex equation of motion, starting from a model Hamiltonian H that includes a short range attractive BCS interaction, as well as a long range repulsive Coulomb interaction (see Ref. [16] for more details). We express the grand canonical partition function as an imaginary time path integral over the electronic fields ψ and the gauge field A_{α} ($\alpha = \tau, x, y, z$),

$$Z = \int \mathcal{D}^2 \psi \, \mathcal{D} A_\alpha \exp\{-S\}, \qquad (3)$$

with Euclidean action

$$S = \int d^{3}\mathbf{r} \int_{0}^{\beta} d\tau \{ \overline{\psi}_{\sigma} [\partial_{\tau} - ieA_{0} + \xi(\nabla - ie\mathbf{A})] \psi_{\sigma} - \Lambda \overline{\psi}_{\uparrow} \overline{\psi}_{\downarrow} \psi_{\downarrow} \psi_{\uparrow} + ieA_{0}n_{i} + [\mathbf{E}^{2} + \mathbf{B}^{2}]/8\pi \}.$$

Here $\xi(\nabla) \equiv -\nabla^2/2m - \mu$ describes a single conduction band, and en_i denotes the background charge density of the ions. The idea is to construct an effective action for the vortex coordinate **R** only, by integrating out the electronic degrees of freedom. Our approach is inspired by the one of Simanek [17]. In addition to the analysis of Ref. [17] we treat carefully the hydrodynamics of the problem and also avoid approximations for the matrix elements in the vortex core (see below).

A Hubbard-Stratonovich transformation introduces the energy gap Δ as an order parameter field and after performing the trace over the field ψ (see Refs. [18,19] for a survey of the technique used) we arrive at

$$Z = \int \mathcal{D}^{2} \Delta \mathcal{D} A_{\alpha} \exp(\operatorname{Tr} \ln \mathcal{G}^{-1} - S_{0}),$$

$$\mathcal{G}^{-1} = \begin{pmatrix} \partial_{\tau} - ieA_{0} + \xi(\nabla - ie\mathbf{A}) & \Delta \\ \overline{\Delta} & \partial_{\tau} + ieA_{0} - \xi(\nabla + ie\mathbf{A}) \end{pmatrix}, \quad (4)$$

$$S_{0} = \int dx \left[\frac{1}{\Lambda} |\Delta|^{2} + \frac{\mathbf{E}^{2} + \mathbf{B}^{2}}{8\pi} + ien_{i}A_{0} \right]$$

and $\int dx = \int_0^{\beta} d\tau \int d^3 \mathbf{r}$. The only remainder of the electrons is the Nambu-Gor'kov Green's function G. The Euler-Lagrange equations obtained by varying A_0 and **A** describe Thomas-Fermi and London screening, respectively. They read [20]

$$\nabla \cdot \mathbf{E} = 4\pi i e [n_e(\mu + i e A_0, \Delta) - n_i],$$

- $\partial_\tau \mathbf{E} + \nabla \times \mathbf{B} = 4\pi \mathbf{j}_e.$ (5)

Both the electronic density n_e and current density \mathbf{j}_e are expressed through the electron Green's functions. For instance, $n_e = -\text{Tr} [\sigma_3 G] = \frac{1}{2} \int d\xi N_e(\xi + \mu + \mu)$ ieA_0) $[1 - \xi\sqrt{\xi^2 + \Delta^2}]$. The electronic density is a function of the electrochemical potential $\mu + ieA_0$ and in the presence of particle-hole asymmetry also of the energy gap Δ [8,21]. Because of charge neutrality $n_e(\mu, 0) = n_i$. Expanding in A_0 and Δ we find $n_e = n_i + ieA_0N_e + n_{\Delta} + \cdots$, with $n_{\Delta} = N'_e\Delta^2/\Lambda N_e$. Deviations of n_e from n_i are screened on the Thomas-Fermi length $\lambda_{\rm TF} = (4\pi e^2 N_e)^{-1/2}$ and yield a nonzero scalar potential A_0 determined by the screened Poisson equation $(-\nabla^2 + \lambda_{\rm TF}^{-2})A_0 = 4\pi i e n_{\Delta}$. Magnetic fields and currents are screened on the scale of the London penetration depth $\lambda_L = (4\pi n_s e^2/m)^{-1/2}$. In the following we concentrate on strong type II superconductors with $\lambda_L \gg \xi$.

Varying $\overline{\Delta}$ yields the BCS gap equation, which has a constant as well as vortex solutions. Here we concentrate on the single vortex solution $\Delta(x) = \Delta_v (\mathbf{r} - \mathbf{R}(\tau))$ with vortex coordinate \mathbf{R} and $\Delta_v = |\Delta_v|e^{i\varphi_v}$. For Δ_v we adopt the mean-field solution from Ref. [12]. Using n_{Δ_v} as a source, the screened Poisson equation defines also a single vortex solution A_{v0} for the scalar potential. In the limit of strong screening ($\lambda_{\text{TF}} \ll \xi$) $A_{v0} = 4\pi i e \lambda_{\text{TF}}^2 n_{\Delta_v}$. As a result, the electronic density in the vortex core does not differ from the density far away from the core.

We neglect fluctuations around the mean-field solutions $A_{\nu\alpha}(\mathbf{r} - \mathbf{R}(\tau))$ and $\Delta_{\nu}(\mathbf{r} - \mathbf{R}(\tau))$, since longitudinal fluctuations of the phase and A_0 are lifted to the plasma frequency, transverse fluctuations of **A** have a gap proportional to the superfluid density, and fluctuations of $|\Delta|$ are at least at energy 2Δ [18]. Thus, the path-integral measure $\int \mathcal{D}^2 \Delta \mathcal{D} A_{\alpha}$ reduces to $\int \mathcal{D} \mathbf{R}$.

Using a gauge transformation $eA_0 \rightarrow eA_0 - \dot{\varphi}/2 \equiv Q_0$ and $e\mathbf{A} \rightarrow e\mathbf{A} - \nabla \varphi/2 \equiv \mathbf{Q}$, the energy gap Δ can be chosen real and manifestly gauge invariant quantities, such as the superfluid velocity \mathbf{Q}/m , appear in \mathcal{G}^{-1} . The dynamics of a vortex can now be studied by expanding Tr $\ln \mathcal{G}^{-1}$ to second order in $Q_{\nu\alpha}$ and in the vortex displacement $\delta \Delta = -\mathbf{R}(\tau) \cdot \nabla \Delta_{\nu}(\mathbf{r})$ around the static vortex solution. Furthermore, due to the singular gauge transformation a source term $\nabla \times \nabla \varphi_{\nu}/2e = \Phi_0 \delta(\mathbf{r} - \mathbf{R})$ appears in the London equation that determines the magnetic field \mathbf{B}_{ν} around a vortex.

We express the unperturbed Nambu-Gor'kov Green's function in the presence of one vortex in Bogoliubov-de Gennes eigenstates U_{λ} with energy E_{λ} as

$$\mathcal{G}_{\nu}(\mathbf{r},\mathbf{r}';\boldsymbol{\omega}_{\mu}) = \sum_{\lambda} \frac{U_{\lambda}(\mathbf{r})U_{\lambda}^{\dagger}(\mathbf{r}')}{i\tilde{\boldsymbol{\omega}}_{\mu} + E_{\lambda}}, \qquad U_{\lambda} = \begin{pmatrix} u_{\lambda} \\ v_{\lambda} \end{pmatrix}.$$
(6)

In the relaxation time approximation that we use, $\tilde{\omega}_{\mu} = \omega_{\mu} + \text{sgn}(\omega_{\mu})/2\tau_r$, where the ω_{μ} are fermionic Matsubara frequencies.

The result of the expansion is an effective action $S_{\text{eff}}[\mathbf{R}] = S_C + S_H$ for the coordinate **R** of one vortex, consisting of a hydrodynamic part

$$S_{H} = \int dx \left(\frac{\mathbf{E}_{\nu}^{2} + \mathbf{B}_{\nu}^{2}}{8\pi} + \frac{1}{2} \Pi_{\alpha\beta} Q_{\nu\alpha} Q_{\nu\beta} - in_{\Delta_{\nu}} Q_{\nu0} \right),$$
(7)

and a core part

$$S_{C} = \frac{1}{2\beta^{2}} \sum_{\lambda\lambda'} \sum_{\mu,n} \frac{(\mathbf{R}_{\omega_{n}} \cdot \mathbf{W}_{\lambda\lambda'}) (\mathbf{R}_{-\omega_{n}} \cdot \mathbf{W}_{\lambda'\lambda})}{(i\tilde{\omega}_{\mu} + E_{\lambda}) (i\tilde{\omega}_{\mu+n} + E_{\lambda'})},$$
$$\mathbf{W}_{\lambda\lambda'} = \int d^{2}r U_{\lambda}^{\dagger} \begin{bmatrix} 0 & \nabla \Delta_{v} \\ \nabla \bar{\Delta}_{v} & 0 \end{bmatrix} U_{\lambda'}, \qquad (8)$$

and the ω_n denote bosonic Matsubara frequencies.

First we discuss *the hydrodynamic contribution* S_H . The kernel $\Pi_{\alpha\beta}$ is the polarization bubble and describes both longitudinal and transverse screening [22]. The transverse part of the polarization term in Eq. (7) is $\Pi_T =$ $n_s(T) (\delta^{ab} - k^a k^b/k^2) + \cdots$, where a, b = x, y, z and " \cdots " indicates higher order terms in **k** and ω . The longitudinal part of the polarization term in Eq. (7) is $\Pi_L = N_e + \cdots$. Using the equation of motion (5) for the fields and $n_e(\mu, \Delta_\nu) - n_i = n_{\Delta_\nu}$, the hydrodynamic part of the effective action can be rewritten as

$$S_{H} = \frac{1}{8\pi} \int dx [\mathbf{E}_{\nu}^{2} + \mathbf{B}_{\nu}^{2} + \lambda_{L}^{2} (-\partial_{\tau} \mathbf{E}_{\nu} + \nabla \times \mathbf{B}_{\nu})^{2} + \lambda_{\mathrm{TF}}^{2} (\nabla \cdot \mathbf{E}_{\nu})^{2} + 16\pi^{2} \lambda_{\mathrm{TF}}^{2} n_{\Delta_{\nu}}^{2} + 4\pi i n_{\Delta_{\nu}} \dot{\varphi}_{\nu}].$$
(9)

The last term is the most important one for our discussion as it yields the hydrodynamic contribution to the Hall coefficient $\gamma_H = \pi n_\Delta = \pi N'_e \Delta^2 / \Lambda N_e$. This result coincides with that of the TDGL approach. The only other dynamic term in Eq. (9) is the transverse part of the \mathbf{E}^2 term that yields a small electromagnetic mass [10,16]. All other terms are nondynamic and contribute to the line energy of a vortex [1].

We now turn to *the core contribution* S_C in Eq. (8). Its origin is found in the transitions induced by the moving vortex between the CdGM states in the core labeled by λ and λ' and involving the matrix elements $W_{\lambda\lambda'}$. The energies are $E_{\lambda} = \lambda \omega_0$ with λ a half integer. The sums over states λ and λ' in Eq. (8) may be evaluated using the constant level separation $E_{\lambda} - E_{\lambda-1} = \omega_0$ [12] and properties of the matrix elements [11]. Explicitly we use the identity

$$U_{\lambda}^{\dagger} \begin{pmatrix} 0 & \nabla \Delta_{\nu} \\ \nabla \bar{\Delta}_{\nu} & 0 \end{pmatrix} U_{\lambda'} = (E_{\lambda'} - E_{\lambda}) U_{\lambda}^{\dagger} \nabla U_{\lambda'}, \quad (10)$$

together with the relations for the eigenstate wave functions $\nabla_x U_\lambda = (k_F/2) [U_{\lambda-1} - U_{\lambda+1}], \quad \nabla_y U_\lambda = (ik_F/2) [U_{\lambda-1} + U_{\lambda+1}]$; see Ref. [11] for a discussion of this point. Using the orthogonality relations, we find the selection rule that only neighboring states are connected by the matrix elements. We also restrict ourselves to the temperature range $\omega_0 \ll T$ where the sum over λ 's may be replaced by the integral $\int dE_\lambda/\omega_0$. The result for S_C can be written in the form

$$S_C = \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \{ K_C^+(\tau - \tau') \mathbf{R}(\tau) \cdot \mathbf{R}(\tau') + i K_C^-(\tau - \tau') \mathbf{z} \cdot [\mathbf{R}(\tau) \times \mathbf{R}(\tau')] \}.$$
(11)

In Fourier components the kernels K_C^{\pm} determining the | mass and damping (K^+) and Hall force (K^-) are

$$K_C^{\pm}(\omega_n) = \frac{\omega_0 k_F^2}{4} \left[\frac{i\omega_n}{i\bar{\omega}_n - \omega_0} \pm \frac{i\omega_n}{i\bar{\omega}_n + \omega_0} \right], \quad (12)$$

where $\bar{\omega}_n = \omega_n + \tau_r^{-1} \operatorname{sgn}(\omega_n)$. They are nonlocal in time, however, after analytic continuation to real frequencies they can be expanded in ω/ω_0 . The kernel $K_C^- \approx$ $-i\omega_n(k_F^2\omega_0^2\tau_r^2/2)/[1 + (\omega_0\tau_r)^2]$ yields the core contribution γ_C as quoted in Eq. (1), if we put $k_F^2 = 2\pi n_e$ in two dimensions. The kernel $K_C^+ \approx (|\omega_n| + \tau_r \omega_n^2) \times$ $(k_F^2\omega_0\tau_r/2)/[1 + (\omega_0\tau_r)^2]$ is proportional to $|\omega_n|$ for small frequencies, thus describing Ohmic dissipation [19,23]. Apart from the damping coefficient η_C it yields the core contribution to the vortex mass [11,17],

$$M_C = \frac{(\omega_0 \tau_r)^2}{\left[1 + (\omega_0 \tau_r)^2\right]} \left(\frac{\epsilon_F}{\Delta}\right)^2 m, \qquad (13)$$

which is large in the superclean limit with $\omega_0 \tau_r \gg 1$.

Thus, a complete description of intrinsic vortex properties can be obtained if both core and hydrodynamic contributions are included. The hydrodynamic part of the Hall force was neglected in Refs. [11,15,17], whereas the core physics cannot be described by a hydrodynamic theory such as TDGL [6]. In Ref. [24] the superconducting phase was coupled to the superfluid density in order to obtain a Galilei-invariant Magnus force $\mathbf{F}_M =$ $\kappa(\mathbf{V}_T - \mathbf{V}) \times \mathbf{z}$ from hydrodynamics only. Our analysis shows that the phase of the superconducting order parameter couples to the square of the order parameter, with a small coefficient that depends on particle-hole asymmetry; i.e., details of the electronic band structure are relevant. A Galilei-invariant Magnus force at T = 0 and $\tau_r = \infty$ in fermionic superconductors is provided by the vortex core rather than the hydrodynamic flow around the vortex.

In conclusion, we have presented a microscopic derivation of the equation of motion of a vortex in a superconductor. Our results relate the observed sign change in the Hall effect in superconductors with $l \sim \xi$ to broken particle-hole symmetry in the electronic band structure.

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