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Sign Change of the Flux Flow Hall Effect in HTSC*

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A novel mechanism for the sign change of the Hall effect in the flux flow region is proposed. The difference δn between the electron density at the center of the vortex core and that far outside the vortex causes the additional contribution to the Hall conductivity $\delta\sigma_{xy} = -\delta nec/B$. This contribution can be larger than the conventional one in the dirty case $\Delta(T)\tau < 1$. If the electron density inside the core exceeds the electron density far outside, a double sign change may occur as a function of temperature.

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The sign change of the Hall effect in the mixed state of the high temperature superconductors (HTSC) is the most puzzling and controversal phenomenon in the physics of magnetic properties of these materials [1]. In spite of the numerous attemps to explain this anomaly even the origin of the sign reversal in the Hall resistivity remains unclear [1]. The sign change of the Hall resistivity had also been observed in the conventional superconductors and thus is not a pecularity of the HTSC [1,2]. Comparing experimental data for different materials, Hagen *et al.* [1] argued that the sign change is an intrinsic property of the vortex motion, and moreover that the sign reversal occurs in the range of parameters where the transport mean free path l becomes of the order of the vortex core size ξ.

In the present paper we propose an explanation of the sign reversal in the Hall resistivity . We show that the sign change may follow from the difference δn between the electron density at the center of the vortex core and the density far outside the core.

In order to describe the Hall effect one has to find a transverse force experienced by the vortex moving with the velocity $\mathbf{v}_L$ under the applied transport current $\mathbf{j}$. There are two contributions to the transverse force. The first one arises from the nondissipative momentum transfer from the moving vortex to infinity. This contribution consists of the Magnus and Iordanskii [3] forces. The second contribution stems from the momentum transfer from the vortex to the normal excitations in the vortex core. The subsequent absorption of this transfered momentum by the thermal bath due to scattering of the normal excitations leads to dissipation and the longitudinal Bardeen - Stephen friction force.

In order to understand both contributions let us derive the dynamic term in the adiabatic action for a moving vortex. The effective action for a superconductor should depend on the phase of the order parameter χ in the following gauge invariant combinations: $S = S(\nabla\chi - 2e\mathbf{A}/\hbar c, \partial\chi/\partial t + 2e\phi/\hbar c)$, where $\mathbf{A}$ and ϕ are the vector and scalar potentials, respectively. By variation of the action with respect to the phase one gets the current conservation law:

$$\frac{\delta S}{\delta\chi(\mathbf{r},t)} = -\frac{\hbar}{2e}\nabla\mathbf{j} + \frac{\partial}{\partial t}\frac{\delta S}{\delta\partial\chi/\partial t} = 0, \qquad (1)$$

where we use the definition of the electric current density $\mathbf{j} = c\delta S/\delta\mathbf{A}(\mathbf{r},t)$. Because of the continuity equation $\nabla\mathbf{j}/e + \partial n/\partial t = 0$ (n is the particle density) for the particle current, we immediately see that the effective action has to contain the following topological term:

$$S_t = -\hbar\int dV dt \frac{n}{2}\frac{\partial\chi}{\partial t}. \qquad (2)$$

The factor 1/2 is due to pairing, and is absent for the superfluid Bose system. This topological term is irrelevant if $n = const$ and χ is a single valued function but in the presence of vortices it is just the term in action which determines their dynamics. Let us consider for simplicity the two dimensional case. Expressing the phase in the presence of a vortex as a sum of a singular $\Theta(\mathbf{r} - \mathbf{R}_L(t)) = arg(\mathbf{r} - \mathbf{R}_L(t))$, ($\mathbf{R}_L(t)$ is the vortex line position) and a regular contribution, $\chi = \Theta(\mathbf{r} - \mathbf{R}_L(t)) + \chi_r(\mathbf{r},t)$, and taking only the singular contribution into account one can rewrite the topological term in the action as

$$S_t = \frac{\hbar}{2}\int d^2r dt n\nabla\Theta\dot{\mathbf{R}}_L = \int dt\mathbf{a}(\mathbf{R}_L)\mathbf{v}_L. \qquad (3)$$

The quantity $\mathbf{a}(\mathbf{R}_L) = \frac{\hbar}{2}\int d^2r n(\mathbf{r} - \mathbf{R}_L)\nabla\Theta(\mathbf{r} - \mathbf{R}_L)$ has the meaning of the 'vector potential' of a fake constant magnetic field. To see this, one calculate

$$\nabla\times\mathbf{a} = \frac{\hbar}{2}\oint n\nabla\Theta d\mathbf{l} = \pi\hbar(n_\infty - n_0), \qquad (4)$$

where we replaced the surface integral by the two contour integrals at infinity and around $\mathbf{r} = \mathbf{R}_L$, with n_∞ and n_0 being the particle densities far outside the vortex core and on the core axis respectively. This term in action describes a particle (the vortex) moving in an 'effective magnetic field' [4] resulting in the transverse force

$$\mathbf{F}_\perp = \mathbf{v}_L\times\mathbf{z}\pi\hbar(n_\infty - n_0), \qquad (5)$$

analogous to the Lorentz forced experienced by a particle moving in a magnetic field ($\mathbf{z}$ is the unit vector along the vortex axis). Note that this force is independent of charge and is not of electromagnetic origin. For superfluid Helium an additional factor 2 appears with n being the density of the Helium atoms.

For the Galilean invariant case $n_0 = 0$, $n_\infty = n_s$, and the force (5) is just the Magnus force. Based on a similar Berry phase type of arguments Ao and Thouless [5] arrived at the conclusion that the relevant density in Eq.(5) is always n_s rather than n. We believe that this difference arises because in their arguments they use a 'superfluid wave function' $\Psi_s^2 \propto n_s$, which is ill defined at finite temperatures or in the presence of disorder, where the difference between n_s and n occurs.

In general there are two major differerences between the (5) and the Magnus force; first, n_∞ is the total density rather than the superfluid one and thus this part is the sum of the Magnus and Iordanskii [3] forces. Second, and most important is that there is an additional term proportional to the density at the vortex axis. In our derivation of the Eq. (4) we have excluded the vortex axis from the integration, since $n\nabla\Theta$ has a singularity there if $n_0 \neq 0$, and our adiabatic action is not applicable very close to the core axis. The fact that $n_0 \neq 0$ means that not all the particles participate in the superfluid motion and there are normal excitations inside the vortex core [6]. As the Magnus force arises from the nondissipative transfer of the momentum from the vortex to infinity, the other term $-n_0\hbar \mathbf{v}_L \times \mathbf{z}$ is due to the transfer of momentum from the condensate to the normal excitations inside the vortex core. This term is just the term obtained by Volovik [7] who, starting from the BCS theory, derived an effective action describing the transfer of the momentum from the condensate to the fermionic modes in the vortex core. The subsequent absorption of this momentum by the heat bath due to the scattering of these excitations on the impurities leads to the Bardeen Stephen dissipation. Thus the hidden assumption in the derivation of the Eq. (5) was that impurity scattering is so strong that all the momentum transfered to the normal excitation is absorbed by the heat bath. However, for BCS superconductors we have $n_\infty - n_0 \ll n_\infty$ and the Magnus force is compensated almost completely [7]. In this case the impurity scattering should be considered in more details. Such a calculations have been done long ago [8] without the account for the nonzero $n_\infty - n_0$ difference. Our goal is to take into account both effects simulteneously and show that their combination can lead to a change of the overall sign of Hall conductivity.

An accurate treatment of the scattering processes in the adiabatic action approach is complicated and is left for future investigations. Instead we consider a simple phenomenological model which is similar to the original model of Noziéres and Vinen [9], but differs in that we take into account both the impurity scattering and the change in density. To this end we consider a model of the fully normal core with a carrier density n_0 and a sharp boundary at a radius $r_c \simeq \xi$ with the superconductive material having a density n [10,9]. We denote the velocity of the normal carriers inside the core in the laboratory frame as $\mathbf{v}_c$ and look at the transfer of the momentum in the system. The conservation of the momentum $d\mathbf{P}/dt = 0$ in the electron system, with a transport current $\mathbf{j}_T$, and electric as well as magnetic fields present reads

$$\mathbf{j}_T \times \mathbf{B}/c + ne\mathbf{E} - mn_0\mathbf{v}_c f(B/H_{c2})/\tau = 0 \qquad (6)$$

The first two terms describe the momentum transfer due to the Lorentz- and the electric field forces. The third term accounts for the momentum transfer due to the impurity scattering (τ and m are the transport time and the effective mass respectively). For $B > H_{c2}$, $f(B/H_{c2}) = 1$, $ne\mathbf{v}_c = \mathbf{j}_T$ and the equation (6) gives the Drude formulas for the longitudinal and Hall conductivities. For $B \ll H_{c2}$ the impurity scattering happens only in the vortex core and $f \propto B/H_{c2}$. If the carrier density n_0 inside the core is equal to that outside the core n, than the transport current $\mathbf{j}_T$ is equal to $n_0 e\mathbf{v}_c$ and we obtain [9] $\omega_0\tau\mathbf{z} \times (\mathbf{v}_L - \mathbf{v}_c) = \mathbf{v}_c$, where we introduced $\omega_0 = eB/mcf(B/H_{c2})$ ($\omega_0 \simeq \Delta^2/E_F$ at $B \ll H_{c2}$). The same result can be obtained by writing the steady state equation for the normal excitation inside the vortex core [11]. Solving this equation one finds

$$\mathbf{v}_c = \frac{\omega_0\tau}{1+(\omega_0\tau)^2}\mathbf{z} \times \mathbf{v}_L + \frac{(\omega_0\tau)^2}{1+(\omega_0\tau)^2}\mathbf{v}_L, \qquad (7)$$

which coincides with the result of the microscopic calculations in the relaxation time approximation [8]. If, however, $n_0 \neq n$ then $n_0 e\mathbf{v}_c$ can not be equal to the $\mathbf{j}_T$. In the reference frame moving with the vortex the current conservation gives $n_0 e\tilde{\mathbf{v}}_c = \tilde{\mathbf{j}}_T$. Going to the laboratory frame we have $n_0 e\mathbf{v}_c = \mathbf{j}_T + \delta n e\mathbf{v}_L$, where $\delta n = n_0 - n_\infty$ Inserting in Eq.(6) one sees that the equation for $\mathbf{v}_c$ (7) remains unchanged and

$$\mathbf{j}_T = \frac{en_0\omega_0\tau\mathbf{z} \times \mathbf{v}_L}{1+(\omega_0\tau)^2} + e\left(\frac{n_0(\omega_0\tau)^2}{1+(\omega_0\tau)^2} - \delta n\right)\mathbf{v}_L. \qquad (8)$$

where the first term in r. h. s. is the Bardeen Stephen longitudinal conductivity and the second term is the Hall conductivity. The δn term rewritten as the transverse force is just the term which we derived in Eq. 5 considering the adiabatic action. From these topological arguments (see also [7]) it follows that δn in Eqs. (8) is not some averaged change in density but is the difference between the electron density on the axis of the vortex core and that far outside the core. The transverse force can be rewritten as $\pi\hbar(n - \frac{n_0}{1+(\omega_0\tau)^2})\mathbf{v}_L \times \mathbf{z}$, where the first term is the Magnus force and the second one is the force due to impurity scattering which cancells the Magnus force almost completly in conventional situation [8,7].

From the Eq. (8) we obtain the Hall conductivity

$$\sigma_{xy} = \frac{n_0 ec}{B}\frac{(\omega_0\tau)^2}{1+(\omega_0\tau)^2} - \frac{\delta nec}{B} \qquad (9)$$

The additional contribution to the flux flow Hall conductivity $\delta\sigma_{xy} = -\delta nec/B$ is our main result.

The above considerations are valid for a model uncharged superconductor, and in that case $\delta n/n \sim (\Delta/E_F)^2$ [7]. In real superconductors the Coulomb screening is always present, and suppresses strongly any inhomogenities in the charge density distribution, and the total charge of the vortex becomes zero. We will see, however, that the screening has no effect on the value of the Hall conductivity, though the latter can't be expressed any more in terms of the density difference δn. In order to account for the screening effect we supplement the superconductive Lagrangian $\mathcal{L}_{sc}$ by the Coulomb terms: $\mathcal{L}_{tot} = \mathcal{L}_{sc} + \mathcal{L}_C$, where

$$\mathcal{L}_C = \frac{1}{8\pi}\sum_q \mathbf{E}_{\parallel}(\mathbf{q})\mathbf{E}_{\parallel}(-\mathbf{q})\varepsilon(\mathbf{q}) \qquad (10)$$

where $\mathbf{E}_{\parallel}(\mathbf{q})$ is the Fourier-component of the longitudinal electric field, $\mathbf{E}_{\parallel}(\mathbf{r}) = -\nabla\phi$, and $\varepsilon(\mathbf{q})$ is the dielectric function, whose $q \to 0$ limit determines the screening length r_D, $\varepsilon(q) = 1 + 1/r_D^2 q^2$; normally $r_D \ll \xi_0$. A distribution of the electric potential around the vortex is determined now by the equation $\delta\mathcal{L}/\delta\phi(r) = -e\delta\tilde{n}(r) + (\phi/r_D^2 - \nabla^2\phi)/4\pi = 0$, whereas the charge density $e\delta n = -\nabla^2\phi/(4\pi) = e\delta\tilde{n} - \phi/(4\pi r_D^2)$, and we introduced for future convenience the notation $e\delta\tilde{n}(r) = -\delta\mathcal{L}_{sc}/\delta\phi(r)$. In the weak screening limit $r_D \gg \xi$ one would get $\delta n(r) \approx \delta\tilde{n}(r)$, whereas at $r_D \ll \xi$ the density is almost constant and $\delta n(r) \simeq \delta\tilde{n}(r)(r_D/\xi)^2 \sim n_0(\Delta/E_F)^4$ [12], whereas $\phi(r) = 4\pi r_D^2\delta\tilde{n}(r)$. The key point now is that the Hall conductivity can be expressed via the value of $\delta\tilde{n} = \delta\tilde{n}(0)$ which *does not depend on screening.* It follows from the fact that the Coulomb part of the Lagrangian $\mathcal{L}_C$ depends upon the longitudinal electric field only, and thus does not contain contribution from the singular vortex-induced phase $\chi_v(\mathbf{r}) = \Theta(\mathbf{r}-\mathbf{r}_L)$. Therefore the 'topological' contribution to the Hall conductivity is determined by the effective action S_t, Eq.(2), with $n(r)$ replaced by $\delta\tilde{n}(r)$, so the result, Eq.(9), is recovered up to the replacement of δn by $\delta\tilde{n} = \partial\Omega_{sc}/\partial\mu$ (where μ is a chemical potential). In leading order of $(Tc - T)$ $\delta\tilde{n}$ can be expressed via the experimentally accessible quantities:

$$\delta\tilde{n} = -\frac{H_c^2(T)}{4\pi}\frac{\partial ln(T_c - T)}{\partial\mu} \qquad (11)$$

We will show now that the δn term in the conductvity we found is just the term which was obtained in Time Dependent Ginzburg Landau (TDGL) model [13,14]. We will follow the approach developed in [15] where it was proposed that the imaginary part of the relaxation time can be obtained from the dependence of the transition temperature T_c on the chemical potential μ. Then the first term in the GL thermodynamic potential should be modified to $\Omega_{sc} = -\alpha(T_c + e\phi\partial T_c/\partial\mu - T)\psi^*\psi + \ldots$. Taking into account that we should always have the gauge invariant combination $(2e\phi - i\partial/\partial t)$ one obtains the imaginary part of the relaxation time in the TDGL [15,14] $\gamma_2 = -\frac{\alpha}{2}\partial T_c/\partial\mu$. Without Coulomb interaction the change in density can be obtained in the same way as before: $n = -\partial\Omega_{sc}/\partial\mu = const - 2\gamma_2|\psi(r)|^2$. Then the δn contribution to the Hall conductivity in Eq. (9) coincides with the result of [13,14] if the numerical parameter β ($-\alpha_2$ in notation of [13]) is equal to 1, which corresponds to the value of the TDGL parameter $u \ll 1$ [14]. For large values of u the analysis of [13,14] gives a similar result but with an additional coefficient of the order of unity in front of the 'δn' term. In these papers the condition of the local electroneutrality ($\nabla\mathbf{j} = 0$, i.e. $\delta n(r) = 0$) was imposed in order to take Coulomb screening into account. Actually for the consistent treatment of the Coulomb effects one should add a term ϕ^2/r_D^2 to the GL free energy and allow for local density variations. The microscopic calculation for superconductors with paramagnetic impurities [16] shows that these numerical corrections to 'δn' term become small for the low enough concentration of paramagnetic impurities.

The effect of the vortex charge on the Hall effect was recently considered by Khomskii and Freimuth [17]. Although the treatment of the static charge distribution in the vortex core is the same as ours, the transverse force and the Hall conductivity found in [17] are much smaller (by a factor $\sim B/H_{c2}$) and have *the opposite sign* as compared to our Eqs. (5,9), which explicitely contradicts well-known result for the Magnus force in the Galilean invariant case where $n_0 = 0$.

The crucial point for the discussion is the sign of δn. Taking as an estimate $\delta n/n = \mathrm{sign}(\delta n)(\Delta/E_F)^2$ and $\omega_0 = \Delta^2/E_F \ll \tau^{-1}$ one arrives at

$$\sigma_{xy} \simeq \frac{n_0 ec}{B}\frac{\Delta^2}{E_F^2}((\Delta\tau)^2 - \mathrm{sign}(\delta n)). \qquad (12)$$

The new term we found is important in the dirty case $\Delta\tau < 1$ and can lead to the sign change if $\delta n > 0$ (the carrier density in the core is bigger than outside). Let us consider this case in more details in application to HTSC. In this materials $\Delta\tau > 1$ at low temperature and $\Delta\tau \to 0$ at T_c. Note that what enters in Eq. (5) is $\Delta(T)$ rather than $\Delta(0)$. Thus at low temperatures we can neglect this δn contribution and the sign of σ_{xy} is positive (as in the normal state). As the temperature approaches T_c, $\Delta\tau \sim 1$ and σ_{xy} becomes negative. Near $H_{c2}(T)\omega_0 \approx$ cyclotron freqyuency ω_c , thus the first term in Eq.(11) transforms to the normal state Hall conductivity σ_{xy}^n, whereas the 'δn' contribution goes to zero $\propto H_{c2} - H$, and the Hall effect changes sign back to the normal value in this region [14]. These are just the two sign changes observed in Bi and Tl based materials. In 90 K YBCO the low temperature sign change back to the normal sign is usually not observed since ρ_{xy} is unmeasurably small because of pinning. However in the experiments where pinning was suppressed either by a high current [18] or by high frequencies [19] the second sign change seems to be observed at low temperatures. The temperature dependence of the Hall conductivity (9) is in very good agreement with the data by Samoilov *et al.* [20] who found for TBCCO that the B^{-1}- term in the Hall conductivity changes sign around 83 K and at higher temperature is $\propto T_c - T$.

In the [21] the Hall angle evidence for the superclean regime in 60 K YBCO was reported. In this material Hall angle changes sign and becomes relatively large ($\Theta_H \simeq -1/2$) at low temperature. There are two quite different ways to treat these data in our scheme. The one taken in [21] is that in 60 K YBCO superclean limit is realized with $\omega_0\tau \gg 1$ and Magnus force has a 'wrong' sign due to the complicated structure of the Fermi surface. Another possible scenario is that this material is not the superclean but just moderately clean, with $\omega_0\tau \ll 1$, and has the same sign of $\delta\tilde{n}$ as in 90 K material, but with larger numerical value (due to the fact that 60 K compound is closer to the half filling and the dependence on chemical potential is sharper than for the 90 K compound). In order to estimate the value of $\delta\tilde{n}/n$ we note that the additional term in the Hall conductivity is $-\delta\tilde{n}ec/B$, whereas the normal state Hall resistivity is $\rho_{xy}^n = B/nec$. Multiplying these two quantities one can get an estimate for $\delta\tilde{n}/n$. Analysis of the experiments [21,20] gives $\delta\tilde{n}/n \simeq 10^{-3}$ for Tl compound and 0.03 and 0.07 for 90 K and 60 K YBCO respectively. Thus the difference between these two Y based materials seems to be much smaller than between Y and Tl based compounds. Then the experimental data [21] for the 60K YBCO can be understood under the assumption that at low temperatures $\omega_0\tau \simeq 0.1 \ll 1$, i.e. of the same order of magnitude as $\delta\tilde{n}/n$; in that case only the second term in (9) is important and the Hall angle acquires the value of the order unity (since the logitudinal conductivity contains factor $\omega_0\tau$), although the material can still be rather dirty. (note also, that 60 K material is traditionally considered as more dirty than the 90 K one). On the other hand, the 90 K YBCO is expected to have bigger low-T value of $\omega_0\tau$ and smaller (as estimated above) value of $\delta\tilde{n}/n$, which makes the observation of the second sign change in this material [18,19] quite natural. The proposed second scenario seems preferable to us since it does not involve any *ad hoc* hypothesis about the complicated Fermi-surface, and suggests an unified decription of both 60 K and 90 K compounds.

In the simple BCS model T_c depends upon the density of states and increases with increased density leading to the positive $\partial T_c/\partial\mu$ and thus $\delta n < 0$. However one can consider a simple tight binding model with large effective mass exponentially dependent upon the lattice constant. Then under compression carriers become lighter and T_c decreases leading to $\delta n > 0$. The case of HTSC is complicated by the fact that the normal state Hall effect has hole like sign, although from the simple electrons counting the Fermi surface should have an electron like shape. It would be tempting to relate δn term with the doping dependence of T_c via Eq. (11), which would lead to a conclusion that the sign change should occur for the overdoped materials. This is dangerous, however, since in some versions of the RVB-like theories [22] the doping dependence of T_c and superconducting energy away from T_c may have opposite signs.

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