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LETTER TO THE EDITOR

Motion of vacancies in a pinned vortex lattice: origin of the Hall anomaly

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Abstract. Physical arguments are presented to show that the Hall anomaly is an effect of the vortex many-body correlation rather than that of an individual vortex. Quantitatively, the characteristic energy scale in the problem, the vortex vacancy formation energy, is obtained for thin films. At low temperatures a scaling relation between the Hall and longitudinal resistivities is found, with the power depending on sample details. Near the superconducting transition temperature and for small magnetic fields the Hall conductivity is found to be proportional to the inverse of the magnetic field and to the quadratic of the difference between the measured and the transition temperatures.

The ubiquitous occurrence of the Hall anomaly in the mixed state of both conventional and oxide superconductors, the sign change of the Hall resistivity below the superconducting transition temperature and the smallness of the Hall angle, has defied a consistent explanation so far [1]. A straightforward application of the Magnus force cannot explain this phenomenon. This failure leads to the frustration of questioning the Magnus force as the only transverse force in the vortex dynamic equation. The transverse force has been subsequently modified into various forms [2]. Following the general properties of a superconductor, on the other hand, recent theoretical work on vortex dynamics has shown that there is no transverse force other than the Magnus force, a result of the topological constraint and the momentum conservation [3, 4]. One can further show that the Magnus force is equivalent to the spectral flow process [5]. An apparent conflict between the theoretical reasonings and the experimental measurements naturally arises.

In this letter we attempt to solve this puzzle by showing that the Hall anomaly can be understood based on the vortex vacancy motion in a pinned vortex lattice, and emphasize that the anomaly is a property of the vortex many-body correlation rather than that of an individual vortex. We will demonstrate that vacancies can have the lowest energy scale, and that they dominate the thermal activation contributions to the vortex motion at low temperatures. The present vacancy model for the Hall anomaly is also consistent with other measurement such as the Nernst effect. In the following we present our arguments leading to the model, and discuss its predictions and validity conditions. For simplicity, we will consider an isotropic s-pairing superconductor with one type of charge carrier in two dimension. In this situation vortices (or straight vortex lines) can be viewed as point particles [6].

The vortex dynamic equation for a jth vortex of unit length in the sample takes the form of the Langevin equation identical to that of a charged particle in the presence of a magnetic field:

$$m\ddot{\boldsymbol{r}}_j = q\frac{\rho_s}{2}h(\boldsymbol{v}_{s,t} - \dot{\boldsymbol{r}}_j) \times \hat{z} - \eta\dot{\boldsymbol{r}}_j + \boldsymbol{F}_p + \boldsymbol{f} \quad (1)$$

with an effective unit length mass m, a pinning force $\boldsymbol{F}_p$, a vortex viscosity η, and a fluctuating force $\boldsymbol{f}$. In equation (1) $q = \pm 1$ is the vorticity, h the Planck constant, ρ_s the superfluid electron number density at temperature T, and $\hat{z}$ the unit vector in z-direction. If there is a temperature gradient, the thermal force $\boldsymbol{F}_T = -s_\phi \nabla T$ should be added in at the right hand of equation (1), with s_ϕ the entropy carried by a vortex. The term associated with the total superconducting electron velocity $\boldsymbol{v}_{s,t} = \boldsymbol{v}_s + \boldsymbol{v}_{s,in}$ and the vortex velocity $\dot{\boldsymbol{r}}$ at the right side of equation (1) is the Magnus force. Although $\boldsymbol{v}_{s,t}$ is due to all other vortices, here we split it into two parts, with $\boldsymbol{v}_s$ corresponding to the rearrangement of vortices due to the externally applied supercurrent and $\boldsymbol{v}_{s,in}$ accounting for the rest contribution describing the vortex interaction without external current. In the following we will assume $\boldsymbol{v}_s$ is small such that this splitting is valid.

It is evident that in the mixed state of any real superconductor the many-body correlation between vortices and the pinning effect cannot be ignored. The competition between them is the source of the rich static and dynamical properties of flux phases [7, 8]. We will take the Abrikosov lattice as the known manifestation of the many-body correlation for the starting point to advance our arguments. The vortex pinning is also important in our reasoning, though several quantitative results obtained below do not explicitly depend on it. If there were no pinning for vortices, the whole vortex lattice would move together under the influence of an externally applied current in the same manner as that of independent vortices. Hence, one would get the same sign of the Hall resistivity in both superconducting and normal states. In the presence of pinning centres in the sample as well as the edge pinning, the vortex lattice will be pinned down. In such a situation the motion of the vortex lattice is made possible by various kinds of defect motions due to thermal fluctuations. We will argue below that at low temperatures the dominant contribution to the motion is due to vortex vacancies, and the Hall anomaly occurs.

For two vortices separated by a distance r, which is less than the effective magnetic screening length $\lambda_\perp = \lambda_L^2/d(d < \lambda_L, \lambda_\perp = \lambda_L$ if $d > \lambda_L)$ but greater than ξ_0, the interaction potential is $V_0(r) = 2d(\Phi_0/4\pi\lambda_L)^2 \ln(r/\xi_0)$ [7]. Here $\lambda_L^2 = m^* c^2/8\pi\rho_s e^2$ is the London penetration depth, m^* the effective mass of a Cooper pair, ξ_0 the coherence length of the superconductor, and d the thickness of the superconductor film. The energy scale $\epsilon_0 \equiv d(\Phi_0/4\pi\lambda_L)^2$ sets both the scale for the strength of vortex interaction and the scale for the strength of a strong pinning centre. The energy for a dislocation pair separated by a distance larger than the vortex lattice constant is given by $V_d(r) = (\epsilon_0/2\sqrt{3}\pi)\ln(r/a_0)$ [9, 7], with a_0 an order of the the vortex lattice constant. The energy scale $\epsilon_0/2\sqrt{3}\pi$ for the dislocation pair here is about ten times smaller than ϵ_0 for the vortex interaction and pinning centres. It is energetically favourable to have dislocation pairs in the lattice. Hence, for temperature $T \ll \epsilon_0$ we can ignore the contribution from the vortices hopping out of pinning centres and the creation of vortex–antivortex pairs. The vortex lattice is then effectively pinned down. Because vacancies and interstitials can be viewed as the smallest dislocation pairs [11], we immediately have the estimated energy scale for vacancy formation energy ϵ_v as, by putting $r \sim 2a_0$ in $V_d(r)$,

$$\epsilon_v \sim \frac{1}{2\sqrt{3}\pi}\left(\frac{\Phi_0}{4\pi\lambda_L}\right)^2 d. \tag{2}$$

This result is valid for an intermediate magnetic field B: $H_{c1} < B < H_{c2}/2$. For thicker films the thickness in equation (2) will be replaced by a crossover thickness d_c due to the z-direction correlation, whose precise value is a complex and unknown function of various parameters such as the magnetic field, the pinning, the temperature, and anisotropy. In the case d_c is finite, its estimation in the high magnetic field limit is as follows. Ring type vacancy excitations are possible in thicker films. Its energy scale is determined by the smallest ring, which should be the size of the vortex lattice constant. In this case d_c is an order of the vortex lattice constant, $d_c \sim a_0$. However, because of the large anisotropy in the HTcS materials, d_c can be the order of the CuO layer spacing close to the superconducting transition temperature T_{c0}.

It is clear from the above analysis that vacancies and interstitials have the lowest excitation energy scales. We note that the value in equation (2) is consistent with the variational and numerical calculations [12], with about a factor 2 smaller, and also with the estimation from the dislocation core energy [13]. Using the shear modulus results for $B \leqslant H_{c1}$ [7] and $H_{c2}/2 < B \leqslant H_{c2}$ [9, 7] we have obtained the corresponding vacancy formation energies as $(2/9\pi)^{1/2}(b_0/\lambda_L)^{3/2}\mathrm{e}^{-b_0/\lambda_L}\epsilon_0$ with $b_0^2 = \Phi_0/B$, and $0.7/\sqrt{3}\pi(1 - B/H_{c2})^2\epsilon_0$, respectively.

Now we argue that the vacancy formation energy is even lower than that of an interstitial. The experimental observations at low magnetic fields have shown the abundance of vacancies comparing with interstitials [14]. The natural explanation is that the the vacancy formation energy is lower than that of interstitials, therefore by thermal fluctuations vacancies have a higher density. The theoretical calculations have also confirmed the lower vacancy formation energy [15]. This phenomenon of the vacancy formation energy is lower than that of interstitials has also been observed in other crystalline structures [11]. We conclude that vacancies will dominate thermal fluctuation contributions to resistivities at low enough temperatures for low magnetic fields [16].

We show next that in the pinned vortex lattice a vacancy behaves as a vortex with a vorticity $-q$ and an interstitial as a vortex with $+q$, respectively. Let $\boldsymbol{u}$ be the displacement vector at position $\boldsymbol{r}$, with a point defect, vacancy or interstitial, at $\boldsymbol{r}_0$. According to equation (1) the transverse force acting on the defect is, measured from the pinned perfect vortex lattice,

$$\boldsymbol{F}_M^d = q\frac{\rho_s}{2}h\int \mathrm{d}^2\boldsymbol{r}\,\delta\rho(\boldsymbol{r})(\boldsymbol{v}_s - \dot{\boldsymbol{u}}) \times \hat{z}. \tag{3}$$

Here the vortex density $\delta\rho$ deviated from a perfect lattice is determined by the dilatation $\boldsymbol{\nabla}\cdot\boldsymbol{u}$: $\delta\rho = \boldsymbol{\nabla}\cdot\boldsymbol{u}/S_0$, with S_0 the area of a unit cell in the vortex lattice. By definition,

$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = \mp S_0\delta^2(\boldsymbol{r} - \boldsymbol{r}_0) \tag{4}$$

with '$-$' for a missing vortex, a vacancy, and '$+$' for an extra vortex, an interstitial. Using equations (3) and (4), we have the desired transverse force on the defect as

$$\boldsymbol{F}_M^d = \mp q\frac{\rho_s}{2}h(\boldsymbol{v}_s - \dot{\boldsymbol{r}}_0) \times \hat{z}. \tag{5}$$

This is identical to the dynamics of a hole or a particle in a semiconductor in the presence of a magnetic field, with a pinned perfect vortex lattice as a filled valence band and a vacancy in real space as a hole in the energy space. Equation (5) shows that both a vacancy and an interstitial will move along the direction of the applied supercurrent $\boldsymbol{v}_s$. This implies that vortices defining vacancies move against the direction of $\boldsymbol{v}_s$, a result of the many-body correlation and pinning. This leads us to our main conclusion that at low enough temperatures the sign of the Hall resistivity is different from its sign in the normal state because of the dominance of vacancies. Quantitatively, vacancies and interstitials may be considered as independent particles moving in the periodic potential formed by the vortex lattice and a random potential due to the residue effect of pinnings. The potential height of the periodic potential as well as that of the random potential is an order of ϵ_v. Assuming the vacancy (interstitial) density $n_v(n_i)$ in a steady state, the longitudinal resistivity is

$$\rho_{xx} = \frac{h}{2e^2} \sum_{l=v,i} \frac{\eta_l \rho_s h/2}{\eta_l^2 + (\rho_s h/2)^2} \frac{n_l}{\rho_s} \tag{6}$$

and the Hall resistivity

$$\rho_{yx} = \frac{h}{2e^2} \sum_{l=v,i} q_l \frac{(\rho_s h/2)^2}{\eta_l^2 + (\rho_s h/2)^2} \frac{n_l}{\rho_s} \tag{7}$$

with $q_v = -q$ and $q_i = q$. Here $\eta_{v,i}$ are the effective vacancy and interstitial viscosities, related to their diffusion constants in the periodic potential due to the vortex lattice by the Einstein relation between the diffusion constant and the mobility. It should be pointed out that contributions of other vortex motions to resistivities such as vortex–antivortex pairs, which are omitted here for their smaller activation probabilities, are additional to those of vacancies, and that the including of the normal fluid (quasiparticle) contributions is straightforward [17].

Under the driving of a temperature gradient, the effective thermal force felt by a vacancy is opposite in sign to the force felt by an interstitial or a vortex in direction but equal in magnitude, $\boldsymbol{F}_T^v = +s_\phi \nabla T$. This can be seen by repeating the demonstration from equations (3) to (5). Then the Nernst effect due to vacancies has the same sign as that of vortices or interstitials. Therefore our model gives that in the Hall anomaly regime there is no sign change for the Nernst effect, and furthermore, the Nernst effect is more pronounced because of the additive contributions due to both vacancies and interstitials. This is in agreement with the experimental observations [17].

Before exploring of consequences of equations (6) and (7) we discuss the qualitative implications of the present model. In the above picture, to obtain a maximum contribution of vacancies, we need the vortex lattice to define vacancies and sufficiently strong pinnings to prevent the sliding of the vortex lattice. The existence of a whole lattice structure is nevertheless unnecessary. Sufficiently large local crystalline structures, like lattice domains, will be enough to define vacancies. Therefore vacancy-like excitations in a vortex liquid state can exist, because of the presence of large local orderings. Whether or not this is also true for a vortex glass state depends upon the details. For example, a further lowering of temperature may quench a vortex system into a glass state with no local crystalline structure. Then vacancies will disappear and the sign of the Hall resistivity will change again. On the other hand, for a fixed temperature if the pinning is too strong, for example, the (random) pinning centre density is much larger than the vortex density, vortices will be individually pinned down and the local lattice structure required for the formations of vacancies and interstitials will be lost. This suggests that the Hall anomaly only exists in a suitable range of pinnings and magnetic fields, that is, for $B_l < |B| < B_u$ with the lower and upper critical fields determined by pinning as well as by temperature.

Now we study the limiting cases of equations (6) and (7). At low temperatures the motions of vacancies and interstitials in the vortex lattice are thermal hopping: $\eta_v = \eta_0 \mathrm{e}^{a_v \epsilon_v / K_B T}$ and $\eta_i = \eta_0 \mathrm{e}^{a_i \epsilon_v / K_B T}$, with a_v, a_i (presumably $a_v < a_i$) numerical factors of order unity and η_0 insensitive to temperature. In this limit, the vacancy (interstitial) density $n_v = n_0 \mathrm{e}^{-b_v \epsilon_v / k_B T}$ ($n_i = n_0 \mathrm{e}^{-b_i \epsilon_v / k_B T}$), with $b_v = 1(b_i > 1)$ for the thermally activated vacancies (interstitials) and $b_v(b_i) = 0$ for the pinning centre induced vacancies (interstitials). In the following we further assume that $\eta_v, \eta_i \gg \rho_s h/2$, corresponding to the Hall angle $|\tan\theta| = |\rho_{yx}/\rho_{xx}| \ll 1$ common in experiments. Under this assumption, we obtain the Hall angle as

$$\tan\theta = -q\frac{\rho_s h}{2\eta_0}\frac{\mathrm{e}^{-(2a_v+b_v)\epsilon_v/k_BT} - \mathrm{e}^{-(2a_i+b_i)\epsilon_v/k_BT}}{\mathrm{e}^{-(a_v+b_v)\epsilon_v/k_BT} + \mathrm{e}^{-(a_i+b_i)\epsilon_v/k_BT}}$$
$$= \begin{cases} -q\dfrac{\rho_s h}{2\eta_0}\dfrac{\gamma}{2}\dfrac{\epsilon_v}{k_BT} & k_BT \geqslant \epsilon_v \\ -q\dfrac{\rho_s h}{2\eta_0}\mathrm{e}^{-a_v\epsilon_v/k_BT} & k_BT < \min\{1,\gamma\}\epsilon_v. \end{cases} \quad (8)$$

Here $\gamma = 2a_i + b_i - 2a_v - b_v$. The high temperature limit $k_BT \geqslant \epsilon_v$ is achieved near the superconducting transition temperature T_{c0}, but the thermal creation of a vortex–antivortex pair is still improbable, because the relevant energy scale ϵ_0 is about ten times bigger than ϵ_v. In the low-temperature limit both longitudinal and Hall resistivities vanish exponentially. We obtain a scaling relation between them as

$$\rho_{yx} = A\rho_{xx}^{\nu} \quad (9)$$

with $A = -q(\rho_s h/2\eta_0)^{b_v/(a_v+b_v)}(2e^2\rho_s/hn_0)^{a_v/(a_v+b_v)}$, and the power

$$\nu = \frac{2a_v + b_v}{a_v + b_v} \quad (10)$$

varying between 1 and 2, depending on the detail of a sample which determines the numerical factors a_v and b_v. If all vacancies are produced by pinnings, we have $b_v = 0$ and $\nu = 2$. In this case A is independent of B because n_0 is. In the other limit, if all vacancies are produced by thermal activations, and if $a_v \ll 1$, we have $b_v = 1$ and $\nu \simeq 1$. In this case A will be independent of B if η_0 is.

Another useful quantity is the Hall conductivity $\sigma_{xy} = \rho_{yx}/(\rho_{xx}^2 + \rho_{yx}^2)$. Under the same assumption of $\eta_v, \eta_i \gg \rho_s h/2$ we obtain the Hall conductivity due to vacancies and interstitials, from equations (6) and (7), as

$$\sigma_{xy} = -q\frac{2e^2}{h}\frac{\rho_s}{n_0}\frac{\mathrm{e}^{-(2a_v+b_v)\epsilon_v/k_BT} - \mathrm{e}^{-(2a_i+b_i)\epsilon_v/k_BT}}{\left[\mathrm{e}^{-(a_v+b_v)\epsilon_v/k_BT} + \mathrm{e}^{-(a_i+b_i)\epsilon_v/k_BT}\right]^2}$$
$$= \begin{cases} -q\dfrac{2e^2}{h}\dfrac{\rho_s}{n_0}\dfrac{\gamma}{4}\dfrac{\epsilon_v}{k_BT} & k_BT \geqslant \epsilon_v \\ -q\dfrac{2e^2}{h}\dfrac{\rho_s}{n_0}e^{+b_v\epsilon_v/k_BT} & k_BT < min\{1,\gamma\}\epsilon_v. \end{cases} \quad (11)$$

As discussed above, here $0 \leqslant b_v \leqslant 1$ and $\gamma \sim O(1)$. Near the superconducting transition temperature T_{c0}, $\rho_s = \rho_{s0}(1 - T/T_{c0})$ and $\epsilon_v = \epsilon_{v0}(1 - T/T_{c0})$ because of the London penetration depth in equation (2). We may further assume $n_0 = B/\Phi_0$, with Φ_0 the flux quantum. From equation (11) we obtain

$$\sigma_{xy} = \alpha_1\frac{(1 - T/T_{c0})^2}{B} \quad (12)$$

with $\alpha_1 = -q(2e^2/h)\rho_{s0}\Phi_0\gamma\epsilon_{v0}/4k_BT_{c0}$. Taking $\rho_{s0} = 10^{21}$ cm^{-3}, $\gamma = 1$, and $\epsilon_{v0}/k_BT_{c0} = 50$, we find $|\alpha_1| \sim 20\,T\,\mu\Omega^{-1}$ cm^{-1}.

Two points should be noted. (1) A naive accounting of the many-body correlation and pinning may not lead to the sign change in the Hall resistivity: Since vortex interaction terms cancel each other when summing over all vortices, one would like to conclude that there is no many-body correlation effect on the sign of the Hall resistivity. If this claim were correct, the same argument would lead to no sign change for the Hall resistivity in a hole semiconductor, and no such phenomena as the quantum Hall effect. This absence of

Hall anomaly is the result of the underestimation of the many-body correlation. (2) There might be a tendency to mix up antivortices and vacancies. As discussed above, the creation energy of an antivortex is about ten times larger than that of a vacancy, which makes it energetically unfavourable. Furthermore, since an antivortex feels the same thermal force as a vortex, $\boldsymbol{F}_T = -s_\phi \nabla T$, it has an opposite sign contribution to that of a vortex for the Nernst effect, in conflict with experiments [1].

In conclusion, we have demonstrated that within the vortex dynamics equation the Hall anomaly can be explained. What has been missed in previous models is a proper consideration of the competition between the many-body correlation and pinning. We have proposed the model of vacancy motion in a pinned lattice as a concrete realization: the characteristic energy in the model, the vacancy formation energy, is obtained; and vacancies move along an applied supercurrent as the origin for the Hall anomaly. The model leads to an exponential tail and the scaling relation at low temperatures, and no sign change for the Nernst effect. Near the superconducting transition temperature and for small magnetic fields the Hall conductivity is found to be proportional to the inverse of the magnetic field and is quadratic in the temperature different from the transition. For thin enough films the activation energy in the low-temperature limit has a linear film thickness dependence.

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