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Citation	Physical Review B - Condensed Matter And Materials Physics, 1999, v. 60 n. 5, p. 3080-3083
Issued Date	1999
URL	http://hdl.handle.net/10722/43279
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## Sign reversal of the mixed-state Hall resistivity in type-II superconductors

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(Received 16 November 1998; revised manuscript received 22 February 1999)

Taking into account pinning, thermal fluctuations, and vortex-vortex interactions, we develop a unified theory to explain the sign reversal of the mixed-state Hall resistivity  $\rho_{xy}$  in both high- $T_c$  and low- $T_c$  superconductors. Molecular dynamics simulations show that besides the pinning forces, either the thermal fluctuations in the high- $T_c$  superconductors or the vortex-vortex interactions in the low- $T_c$  ones play an important role in the sign reversal of  $\rho_{xy}$ . From a calculated phase diagram for vortex motion, we find that the abnormal Hall effect always occurs in the plastic flow state of vortices. [S0163-1829(99)11629-1]

Since the discovery of high- $T_c$  superconductors, much attention has been paid to the anomalous Hall effect in the mixed state. One of the most controversial phenomena is a sign reversal of the Hall resistivity  $\rho_{xy}$  in the mixed state below  $T_c$  as temperature or magnetic field is varied. Such a sign reversal of  $\rho_{xy}$  has been observed in most of the high- $T_c$  superconductors.<sup>1–9</sup> Besides, this sign reversal effect has also been found in some conventional superconductors<sup>10,11</sup> and some relatively low- $T_c$  cuprate materials.<sup>12–15</sup> Another issue that has attracted special attention is the scaling behavior,  $\rho_{xy} \sim \rho_{xx}^{\beta}$ , between the Hall resistivity  $\rho_{xy}$  and the longitudinal resistivity  $\rho_{xx}$ . It was reported that the scaling exponent  $\beta$  is between 1.5 and 2.0 in high- $T_c$  superconductors.<sup>1,3,6,8,9</sup>

The sign reversal of  $\rho_{xy}$  is not expected within the stan-dard theories of flux motion,<sup>16</sup> which predict the same Hall sign in the mixed state and in the normal state. A number of theoretical models $^{17-20}$  have been proposed to account for the puzzling Hall effect, but it seems difficult for them to explain simultaneously both the sign reversal and the scaling law. Wang, Dong, and Ting (WDT) (Ref. 21) developed a unified theory for the anomalous mixed-state Hall effect by taking into account the backflow current due to pinning and the thermal fluctuation effect. Their theory has successfully explained the sign reversal of  $\rho_{xy}$  and the scaling behavior in high- $T_c$  superconductors. The WDT model appears to be especially applicable for the high- $T_c$  superconductors where there exist the strong pinning and thermal fluctuation,<sup>3,9,22</sup> both of them being indispensable factors.<sup>24</sup> However, the sign reversal of the mixed-state Hall effect has been found not only in the high- $T_c$  superconductors, but also in some low- $T_c$  superconducting materials, such as cuprate superconductors NdCeCO,<sup>12,13</sup> BSLCO,<sup>14</sup> and LSCO,<sup>15</sup> and conven-tional superconductors Nb (Ref. 10) and MoSi.<sup>11,12</sup> In these low- $T_c$  materials, the thermal fluctuation effect should be weak and so the interaction between vortices would be more

important. It is a puzzle for the WDT model how to account for the anomalous mixed-state Hall effect in low- $T_c$  superconductors, for the interaction between vortices was not included in their model. As a result, it is highly desirable to set up a more unified theory of the mixed-state transport, which includes the pinning, the thermal fluctuations, and the interactions between vortices, so as to be simultaneously suitable for the high- $T_c$  and low- $T_c$  superconductors.

In this paper, based on the WDT model, we develop a more complete theory particularly by taking into account the vortex-vortex interactions. Using the molecular dynamics simulations, we find that not only the thermal fluctuations in the high- $T_c$  superconductors but also the interactions between vortices in the low- $T_c$  ones, along with the pinning, can result in the sign reversal of  $\rho_{xy}$ . More interestingly, we connect the abnormal Hall effect with the melting transition of the vortex lattice and show that the sign reversal of  $\rho_{xy}$ always occurs in the "plastic" vortex flow region where pinning is relevant. This theoretical result is found in agreement with recent experiments.<sup>23</sup> Calculated results show that the vortex-vortex interactions, which were usually omitted in theoretical treatments,<sup>21,24</sup> have a significant impact on the vortex motion, in particular for low-temperature superconductors.

Consider an infinite slab of superconductor with a magnetic field applied perpendicular to the surface, forming flux lines along the magnetic field direction. The rigid flux lines and straight columnar pins are assumed parallel to the *z* direction (unit vector  $\hat{\mathbf{n}}$ ), and so the three-dimensional (3D) flux lines can be modeled as a 2D vortex lattice on the *x*-*y* plane with randomly distributed point pinning centers, the vortex quantum given by  $\Phi_0 = hc/2e$ . In the presence of interactions between vortices, we can write down the force balance equation for the *i*th vortex located at  $\mathbf{r}_i$  as  $\mathbf{F}(\mathbf{r}_i) + \mathbf{f}_{drag}(\mathbf{r}_i) + \mathbf{F}_{th}(\mathbf{r}_i) + \mathbf{F}_{pin}(\mathbf{r}_i) + \mathbf{F}_{vv}(\mathbf{r}_i) = 0$ . Here the first

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four terms, in order, are the the Magnus force, the general drag force,<sup>21</sup> thermal noise, and pinning forces acting on the *i*th vortex. The last term  $\mathbf{F}_{vv}(\mathbf{r}_i)$  is the interacting force from the other vortices, which was absent in the WDT theory. Since rigorous analytical analysis on the above force balance equation is extremely difficult, the direct numerical simulations are highly desirable. By the aid of the expressions for  $\mathbf{F}(\mathbf{r}_i)$  and  $\mathbf{f}_{drag}(\mathbf{r}_i)$ ,<sup>21</sup> the force balance equation can be rewritten as

$$\eta \mathbf{v}_{i} = \mathbf{F}_{L} - \beta_{0}(1 - \bar{\gamma})\mathbf{F}_{L} \times \hat{\mathbf{n}} - \beta_{0}(1 + \bar{\gamma})\mathbf{F}_{pin}(\mathbf{r}_{i})$$
$$\times \hat{\mathbf{n}} + \mathbf{F}_{pin}(\mathbf{r}_{i}) + \mathbf{F}_{vv}(\mathbf{r}_{i}) + \mathbf{F}_{th}(\mathbf{r}_{i}). \tag{1}$$

Here  $\mathbf{v}_i = d\mathbf{r}_i/dt$  is the velocity of the *i*th vortex at  $\mathbf{r}_i$  and  $\eta = \Phi_0 H_{c2} / \rho_n$  is the usual viscous coefficient, with  $\rho_n$  the normal-state resistivity,  $H_{c2} = \Phi_0/2\pi\xi^2$  the upper critical field and  $\xi$  the superconducting coherence length.  $\mathbf{F}_L = \mathbf{J}$  $\times \Phi_0$  is the Lorentz force with J the applied current along the x direction. In our simulations the driving current is fixed as J=2 A/cm<sup>2</sup>, which is very close to that used in the experiments.<sup>2,3</sup> The transverse term  $\mathbf{F}_{pin} \times \hat{\mathbf{n}}$  is produced by the backflow current inside the normal core. We wish to point out here that the existence of this term is not in conflict with the obsevation on the average of the pinning force from symmetry considerations in Ref. 19, where it is merely observed that after averaging over the pinning force, the terms perpendicular to the average velocity of vortex motion cancel each other out and so do not appear in the expression of the disorder-averaged pinning force  $\langle \mathbf{F}_{pin}(\mathbf{r}_i) \rangle$ . This indicates that the average of the pinning force should be antiparallel to the average velocity of vortex motion, but the transverse term is never symmetry forbidden in the original force balance equation for vortices with normal cores.<sup>21</sup>  $\beta_0$  $=\mu_m H_{c2}$  with  $\mu_m = \tau e/mc$  the mobility of the charge carrier, and  $\bar{\gamma} = \gamma (1 - \bar{H}/H_{c2})$  with  $\bar{H}$  the average magnetic field over the normal core of the vortex and  $\gamma$  the parameter describing the contact force on the surface of the core.  $\gamma$  is a rapidly varying function of temperature around a characteristic temperature  $T_0$ , and has the following asymptotic behavior:  $\gamma \sim 0$  for  $\xi/l \ll 1$  and  $\gamma \sim 1$  for  $\xi/l \ge 1$  with *l* the mean free path of the carrier.<sup>17</sup> In order to simulate this temperature dependence, it may be assumed that  $\gamma$ =  $1/\{\exp[\alpha_0(t_0-t)]+1\}$  where  $t_0 = T_0/T_c$  and  $t = T/T_c$  are reduced temperatures, and  $\alpha_0 \ge 1$ . In the simulated calculations, we choose  $t_0 = 0.9$  and  $\alpha_0 = 100$ , the calculated result being found insensitive to their values.

By taking the pinning centers as Gaussian potential wells,<sup>25</sup> the pinning force acting on the vortex at  $\mathbf{r}_i$  is given by

$$\mathbf{F}_{pin}(\mathbf{r}_i) = -F_p \sum_k \frac{\mathbf{r}_i - \mathbf{R}_k}{\xi} \exp\left(-\frac{|\mathbf{r}_i - \mathbf{R}_k|^2}{\xi^2}\right), \quad (2)$$

where  $\mathbf{R}_k$  stands for the location of the *k*th pinning.  $F_p = F_{p0}f_0(1-b)\kappa/4$  with  $\kappa = \lambda(T)/\xi(T)$ ,  $b = B/B_{c2}(T)$ , and  $f_0 = \Phi_0^2/8\pi^2\lambda^3(T)$ , where  $\lambda$  is the in-plane superconducting penetration depth.  $F_{p0}$  is a dimensionless parameter, which is used to adjust the magnitude of the pinning force. The intervortex interacting force is given by<sup>26</sup>

$$\mathbf{F}_{vv}(\mathbf{r}_i) = F_{vv0} f_0 (1-b)^{3/2} \sum_{j \neq i} \frac{(\mathbf{r}_i - \mathbf{r}_j)/\lambda}{|(\mathbf{r}_i - \mathbf{r}_j)/\lambda|^2}.$$
 (3)

The cut length of this long-range repulsive force will be taken as  $4\lambda(0)$ . The thermal noise force  $\mathbf{F}_{th}$  is assumed to be a Gaussian white noise. In our simulation, Eq. (1) will be solved using the discrete time step  $\Delta$ . The thermal noise term  $\Delta F_{th}/\eta$  can be simulated as<sup>25</sup>

$$\sqrt{\frac{2\Delta k_B T}{\eta p}} \sum_j \delta(t-t_j) \Omega(t_j) \Theta(p-q_j), \qquad (4)$$

where  $p = \Delta/\tau$  is the probability that the noise term acts on a given vortex with  $\tau$  the mean time between two successive noise pulses.  $\Omega(t_j)$  is a random number chosen from a Gaussian distribution of mean 0 and width 1.  $\Theta(x)$  is the unit step function with  $\Theta(x)=1$  for x>0 and  $\Theta(x)=0$  for x<0, and  $q_j$  is a random number uniformly distributed between 0 and 1.

Equation (1), along with Eqs. (2)–(4), is the basic equation to describe the flux motion in the presence of the pinning, thermal fluctuations, and vortex-vortex interactions. In our dynamics simulations, typical parameter values of the YBCO material are used:  $T_c = 90$  K,  $\xi(0) = 14$  Å,  $\lambda(0) = 1400$  Å, and  $\rho_n = 5 \times 10^{-5} \Omega$  cm, whereby we obtain  $\xi(t) = \xi(0)/\sqrt{1-t^2}$ ,  $\lambda(t) = \lambda(0)/\sqrt{1-t^4}$ , and  $H_{c2}(t) = H_{c2}(0)(1-t^2)$ . The other parameters used in the simulations are  $F_{\nu\nu0} = 0.0002$ , and  $F_{p0} = 0.0003$ . The sample size is fixed as  $4\lambda(0) \times 4.3\lambda(0)$ , with periodic boundary conditions. We have also employed the same numerical simulations on a sample of size  $16\lambda(0) \times 17.2\lambda(0)$ . The calculated result is found insensitive to the sample size provided that the densities of vortices and pinning sites remain unchanged.

In order to separate different effects that system parameters have on the mixed-state Hall effect, in our simulations, we fix all the parameters and vary only one at a time. Figure 1 shows the reduced temperature dependence of  $\rho_{xy}$  and  $\rho_{xx}$ , where we take the vortex number as  $n_v = 320$ , corresponding to a magnetic field of about 2 T applied on the system, and the pinning center number as  $n_p = 40\,000$ . In the absence of the thermal fluctuation and the vortex-vortex interaction, both  $\rho_{xy}$  and  $\rho_{xx}$  decrease with decreasing t and drop down to zero at  $t \approx 0.97$ , below which they remain zero and no negative  $\rho_{xy}$  appears. As either the thermal fluctuation or the vortex-vortex interaction is taken into account, we can obtain significant flux motion as well as negative Hall resistivity in a narrow region below  $T_c$ , as shown in Figs. 1(a) and 1(b). The former labeled with open squares is just the numerical result of the WDT model, in which the joint effects of pinning and thermal fluctuation result in the flux motion and sign reversal of  $\rho_{xy}$ . The latter labeled with open triangles is a new result, indicating that the pinning and the interaction between vortices can also produce the flux motion and the sign reversal. It then follows that the repulsive interactions between vortices and thermal fluctuations play a similar role in the mixed-state Hall effect. For a vortex system with disordered pinning under consideration, both of them have depinning effects on the vortex dynamics. The present result is able to account for the anomalous sign reversal of  $\rho_{xy}$  observed in low- $T_c$  cuprates and conventional superconductors, as has been mentioned in the introductory remarks. This new mechanism is undoubtedly a valuable extension to the WDT theory, because thermal fluctuations are not strong enough in low- $T_c$  superconductors so that the WDT theory does not work there. Since the present work includes both thermal



FIG. 1.  $\rho_{xy}$  (a) and  $\rho_{xx}$  (b) vs reduced temperature  $T/T_c$  for  $F_{th}=F_{vv}=0$  ( $\bigcirc$ ),  $F_{th}=0$  and  $F_{vv}=0.0002$  ( $\square$ ), and  $F_{th0}=5.0$  and  $F_{vv}$  ( $\triangle$ ). Here H=2T and  $n_p=40\,000$ .

fluctuations and vortex-vortex interactions, it is a more unified theory suitable simultaneously to the high- $T_c$  and low- $T_c$  superconductors.

Taking into account the vortex-vortex interactions and the thermal fluctuations ( $F_{th0}$ =1.0), we obtain temperature dependence of  $\rho_{xy}$  and  $\rho_{xx}$  for different applied magnetic fields (different  $n_v$ ), as shown in Fig. 2(a) and its inset. For temperatures very close to  $T_c$  (t>0.97), the longitudinal resistivities  $\rho_{xx}$  for different *H* tend to the same behavior; but the transversal resistivities exhibit different values,  $\rho_{xy}$  having a larger value for a stronger magnetic field. As the temperature is lowered from  $T_c$ , the positive  $\rho_{xy}$  decreases gradually and will reverse its sign from positive to negative. It is found that with increasing the magnetic field *H*, the onset of the dissipation for either  $\rho_{xx}$  or  $\rho_{xy}$  shifts to lower temperatures and the negative Hall effect becomes weaker. These calculated results are in good agreement with the experimental observations on high- $T_c$  superconductors.<sup>3</sup>

From the present vortex dynamics simulations, we find that the moving behavior of the vortices plays a critical role in the sign reversal of  $\rho_{xy}$ . Many works have suggested that there exist three phases for the vortex motion in the mixed state: (i) no motion, pinned vortices; (ii) disordered, plastic flow; and (iii) coherently moving vortex lattice. Which one appears depends mainly on the temperature and the driving force.<sup>27</sup> At relatively low temperatures, the vortices completely pinned and there is no dissipation due to vortex motion, so that both  $\rho_{xx}$  and  $\rho_{xy}$  vanish. On the other hand, at



FIG. 2. (a)  $\rho_{xy}$  and  $\rho_{xx}$  (in inset) vs reduced temperature for different magnetic fields H=1 T ( $\bigcirc$ ), 2 T ( $\square$ ), and 3 T ( $\triangle$ ). (b) Temperature dependence of  $c_L^v$  for different H. (c) H vs  $T/T_c$  phase diagram including three phases of moving behavior for a driven vortex lattice. ( $\bigcirc$ ) indicates the boundaries of the negative  $\rho_{xy}$ region extracted from (a); ( $\square$ ) and ( $\triangle$ ) stand for the boundaries between the plastic flow liquid and elastic moving glass, respectively, obtained from the Linderman-like criterion  $c_L^v=0.1$  and the static structure factor  $S(\mathbf{k})$ .

temperatures very close to  $T_c$  where the vortices move coherently,  $\rho_{xx}$  tends to the same regardless of different magnetic fields and  $\rho_{xy}$  remains positive values, as shown in Fig. 2(a) as well as other experiments.<sup>2,28</sup> As a result, we propose that the sign-reversal  $\rho_{xy}$  always appears in the plastic vortex flow phase of the type-II superconductors.<sup>29</sup> In order to demonstrate this point, we study fluctuations of the vortex velocities near  $T_c$  by numerical simulations and use

the Linderman-like criterion to determine whether or not the vortices are in the plastic flow phase where the motion of vortices is incoherent. Let us introduce a dimensionless parameter  $c_L^v$  to describe the magnitude of the fluctuation of vortex velocities, which is defined as

$$c_L^{V2} = \langle |\mathbf{v}_i - \mathbf{v}_0|^2 \rangle / |\mathbf{v}_0|^2, \tag{5}$$

where  $\mathbf{v}_i$  denotes the velocity of the *i*th vortex,  $\mathbf{v}_0$  is the average velocity of all the vortices, and  $\langle \cdots \rangle$  stands for the steady-state average after abandoning the first 20 000 runs of the dynamics simulation. It is found from Fig. 2(b) that the calculated points for  $c_L^v > 0.1$  are mainly distributed in the region between t=0.93 and t=0.97. This indicates that in such a temperature range the velocities of the vortices are irregular and incoherent, exhibiting the feature of a plastic flow liquid. Comparing the result for  $c_L^v$  with the temperature dependence of  $\rho_{xy}$  in Fig. 2(a), we find that the negative  $\rho_{xy}$  appears just in the temperature range of the plastic flow state. In particular, the peaks of the  $c_L^v$  vs t curves in Fig. 2(b) always correspond to the maximum negative  $\rho_{xy}$  in Fig. 2(a), strongly suggesting a close link between the sign reversal of  $\rho_{xy}$  and the plastic flow of the vortices.

Figure 2(c) shows a schematic phase diagram of the driven vortex lattice in the mixed state. Two phase boundaries are obtained by setting  $c_L^v \approx 0.1$  within our calculating precision. The left phase stands for the completely pinned vortices, in which there is no vortex motion and  $c_L^v$  approaches zero. The right phase is the coherently moving vortex glass, where  $c_L^v$  is very small, indicating that the vortices move with nearly the same velocity and exhibit a coherent or elastic motion. The plastic flow region lies between the

above two phases. It is in this region that the negative Hall effect can be observed. In determining the phase boundary  $T_{p\leftrightarrow c}$  between the plastic liquid and the coherently moving glass, the Linderman-like criterion alone appears somewhat crude. An alternative approach is to calculate the static structure factor  $S(\mathbf{k})$ ,<sup>30,31</sup> which is defined as  $S(\mathbf{k})$  $= 1/N_v |\Sigma_{r_i} \exp[i\mathbf{k} \cdot \mathbf{r}_i(t)]|$ , with **k** the momentum vector and  $\mathbf{r}_{i}(t)$  the position of the *j*th vortex at time *t*. The essential feature of  $S(\mathbf{k})$  has been shown in Fig. 2 of Ref. 29, in which for the plastic flow state, the absence of ordering manifests itself by a central peak and a structureless ring, while for the elastic moving state with high velocity, there will be sixfold coordinated Bragg peaks representing some sort of solid ordering. From the calculated  $S(\mathbf{k})$ , the phase boundary  $T_{p\leftrightarrow c}$ can be determined to be a function of H, as shown by the open triangles in Fig. 2(c). This phase boundary is nearly consistent with that (open squares) obtained by the Linderman-like criterion  $c_L^{\nu} = 0.1$ , as well as the boundary curve (open circles) for the sign reversal of  $\rho_{xy}$  from positive to negative. A comparison between Figs. 2(a), 2(b), and 2(c) strongly supports our conclusion that the sign-reversal  $\rho_{xy}$ always appears in the plastic flow state of vortex motion. In the plastic flow phase, the competition between pinning and depinning must not be spatially uniform. It is either the thermal fluctuation or the vortex-vortex interaction that can provide such depinning effects for the plastic flow state of vortices. In addition, with the increase of the applied field H, the temperature region of the negative  $\rho_{xy}$  shifts toward the left, which is also consistent with experimental observations.

This work was supported by the National Natural Science Foundation of China and the RGC grant of Hong Kong.

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