Anomalous Hall Effect in $YBa_2Cu_3O_7$

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The temperature dependence of the normal state Hall effect and magnetoresistance in $YBa_2Cu_3O_7$ is investigated using the nearly antiferromagnetic Fermi liquid description of planar quasiparticles. We obtain a direct (nonvariational) numerical solution of the Boltzmann equation and find that highly anisotropic scattering at different regions of the Fermi surface gives rise to the measured anomalous temperature dependence of the resistivity and Hall coefficient while yielding the quadratic temperature dependence of the Hall angle observed for both clean and dirty samples.

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Eight years of experiments on increasingly pure samples of $YBa_2Cu_3O_7$ (YBCO) have demonstrated that, while angle-resolved photoemission spectroscopy experiments suggest that the planar quasiparticles possess a well-defined Fermi surface (FS), none of the spin [1] and charge [2] properties are those of a Landau Fermi liquid (FL). N. M. R. experiments show that there are strong antiferromagnetic (AF) correlations between neighboring Cu^{2+} spins and that the spin-spin correlation function is strongly peaked at $\mathbf{Q} = (\pi, \pi)$, while transport measurements yield a planar resistivity which is approximately linear in temperature. The resistivity and optical properties are consistent with a quasiparticle spectrum for which the $\mathrm{Im}\Sigma(\mathbf{p}, \omega)$ is linear in the $\max(\omega, T)$ (Ref. [3]), for $\mathbf{p}$ close to the FS, while the effective mass enhancement is believed to be about 2. One of us has suggested that the above anomalies can be traced to a strong magnetic interaction between the quasiparticles [4]. The resulting system is called a nearly antiferromagnetic Fermi liquid (NAFL).

While the NAFL model has been shown to be consistent, both qualitatively and quantitatively, with many experiments, including NMR, optical conductivity, resistivity, the superconducting transition temperature, and the role played by impurity scattering [4], a major challenge for the NAFL approach has been explaining anomalous transport in an applied magnetic field, where experiments show that the Hall resistivity is a strong function of temperature, yet the cotangent of the Hall angle has a very simple behavior $\cot\Theta_H = A + BT^2$. This has been explained in terms of spin-charge separation [5] and has been considered as major support for that approach.

In this Letter we report on calculations based on the NAFL model of the Hall conductivity σ_H and resistivity ρ, using standard Boltzmann transport theory. Recently Hlubina and Rice (HR) [6] explored this approach by solving the Boltzmann equation (BE) using a variational method [7]. Here we study the solution of the BE in a finite magnetic field B. We use the same band parameters as HR and Monthoux and Pines (MP) [8], $t = 0.25$ eV and $t' = -0.45t$. The hole concentration (doping) is either 0.25 or 0.15. Note that for the parameters chosen the Fermi velocity varies very little along the FS, and therefore the presence of the van Hove singularities near the Fermi surface plays only a marginal role. We assume that the effective *magnetic* interaction between *conduction* quasiparticles is given by [9,10]

$$V^{\mathrm{eff}}(\mathbf{q}) = g^2\chi(\mathbf{q}, \omega) = \frac{g^2 A}{\omega_{\mathrm{SF}} + \omega_{\mathrm{SF}}\xi^2(\mathbf{q} - \mathbf{Q})^2 - i\omega}, \tag{1}$$

where the spin fluctuation (SF) energy $\omega_{\mathrm{SF}} = T_0 + \beta T$, g is the coupling constant, and ξ is the magnetic correlation length in units of the lattice constant a. For optimally doped YBCO the dimensionless parameter $A \approx 1.1$, $g = 0.64$ eV, $T_0 \approx 110$ K, and $\beta = 0.55$, and the energy $\omega_{\mathrm{SF}}\xi^2 \approx 880$ K is very nearly independent of temperature [8].

In Boltzmann theory one seeks the displacement $\delta f_{\mathbf{k}} = f_{\mathbf{k}} - f_0 = -\Phi_{\mathbf{k}}\, \partial f_0/\partial\epsilon$ of the FS in an external field, where f_0 is the equilibrium Fermi distribution function. The transport coefficients are found straightforwardly from $\mathbf{j} = e\sum_{\mathbf{k}} \mathbf{v}\delta f_{\mathbf{k}}$. We introduce the dimensionless quantities $\mathbf{u}_{\mathbf{k}} \equiv \mathbf{v}_{\mathbf{k}}\hbar/at$, $b = B/B_0$, where $B_0 = \hbar c/ea^2 \approx 4300$ T. We assume that $\mathbf{E} = E\hat{\mathbf{x}}$ and $\mathbf{B} \parallel \hat{\mathbf{z}}$. Then the BE can be written as

$$\Phi_{\mathbf{k}} = eE\left[u_x - b\left(u_y \frac{\partial\Phi_{\mathbf{k}}}{\partial k_x} - u_x \frac{\partial\Phi_{\mathbf{k}}}{\partial k_y}\right)\right] f_0(\mathbf{k})/I(\mathbf{k}, T), \tag{2}$$

where the linearized collision term is given by

$$I(\mathbf{k}, T) = \frac{g^2}{t^2}\int d\epsilon' \int \frac{dk'}{2\pi^2|\mathbf{u}_{\mathbf{k}'}|}\, n(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) \times \mathrm{Im}\chi(\mathbf{k} - \mathbf{k}', \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})\left(\frac{\Phi_{\mathbf{k}'}}{\Phi_{\mathbf{k}}} - 1\right) f_0(\mathbf{k}'). \tag{3}$$

We solve Eqs. (2) and (3) numerically on a fine mesh in momentum space with typically 200×200 points in the Brillouin zone (BZ), taking into account the appropriate umklapp processes [11]. We have verified that our results for the longitudinal and Hall conductivity practically do not vary for mesh sizes larger than 100×100. The difference between the calculated Hall conductivity at mesh sizes 100 and 200 is of order 1% at all temperatures, while the accuracy of our results for the longitudinal resistivity is considerably better. Our principal results are given in Figs. 1–3. The input parameters in the figures are as specified above, unless stated otherwise.

As may be seen in Fig. 1 our calculated result for the resistivity as a function of temperature is very similar to HR for the same doping value, and quantitatively it is even close to MP at lower temperatures. Unlike MP, both HR and the present calculation show a nonlinearity in $\rho(T)$ [see inset (a) in Fig. 1], which has not been observed in experiments, and which is due to normal FL-like scattering: For sufficiently low temperatures, in this model, the resistivity is proportional to T^2 with crossover to linear in T resistivity. As indicated in insets of Fig. 1, if the lifetime effects are neglected, the crossover temperature is approximately equal to 200 K in this model. However, a different choice of band parameters, or the hole concentration, can shift the crossover temperature to much lower values.

Our results for the Hall conductivity (Fig. 2) are in qualitative agreement with the experiments [12], for temperatures above the aforesaid crossover temperature. The inset of Fig. 2 compares the Hall resistivity ρ_H with experiment. More than *qualitative* agreement cannot be expected, since we have neglected any effects associated with CuO chains and/or planar mass anisotropy, both of which influence the experimental results. Figure 3 is our main result: It shows that $\cot\Theta_H$ obeys the simple form $A + BT^2$ over the entire temperature range.

We now consider the physical origin of these results. In a FL the temperature variation of the Hall angle is the same as that of the resistivity, if one assumes a uniform (temperature) dependence of scattering along the FS. However, this is not the case for a NAFL, where the effective interaction (1) depends strongly on the momentum transfer $\mathbf{q}$. As the calculations of HR and MP show the quasiparticle lifetime $\tau_{\mathbf{k}}$ is highly anisotropic, because the scattering is very strong for points $\mathbf{k}$ and $\mathbf{k}'$ such that $\mathbf{k} - \mathbf{k}' = \mathbf{q} \approx \mathbf{Q}$. As may be seen in Fig. 4, there are only a small number of such *regions* on the FS, called "hot spots" by HR. Nevertheless, as HR have shown [6] for $\epsilon_{\mathbf{k}} \gg T_0$ the *average* quasiparticle lifetime is linear in the excitation energy $\epsilon_{\mathbf{k}}$. In addition, the $\mathbf{k}$ dependence of τ is found to be large only away from hot spots on the Fermi surface, in regions where the scattering is no longer anomalous. It is the combination of these features which is responsible for the peculiar temperature dependence of both resistivity and the Hall angle.

For our orientation of $\mathbf{E}$, with $B = 0$, $\Phi_{\mathbf{k}}(B = 0) \equiv \Phi_{\mathbf{k}}^0$ can be written as $u_x/I_0(\mathbf{k}, T)$, where I_0 is given by Eqs. (2) and (3), while in a weak field B one has $\Phi_{\mathbf{k}}(B) \approx \Phi_{\mathbf{k}}^0 - (b/I_0)[u_y(\partial\Phi_{\mathbf{k}}^0/\partial k_x) - u_x(\partial\Phi_{\mathbf{k}}^0/\partial k_y)]$. The conductivity σ_0 and the Hall conductivity σ_H are averages of $u_x\Phi_{\mathbf{k}}$ and $u_y\Phi_{\mathbf{k}}$ around the FS; since I_0 possesses the symmetry of the crystal lattice, the contribution of $\Phi_{\mathbf{k}}^0$ to σ_H vanishes identically. Thus σ_0 is an average of u_x^2/I_0 and σ_H is an average of $u_y(b/I_0)[u_y\nabla_x(u_x/I_0) - u_x\nabla_y(u_x/I_0)]$ around the FS. The integral over ϵ' in Eq. (3) can be done analytically for $\mathbf{k}$ on the FS. It equals $\pi T[(2\omega_{k-k'})^{-1} + \sum_n(-1)^n(\omega_{k-k'} + n\pi T)^{-1}]$, where

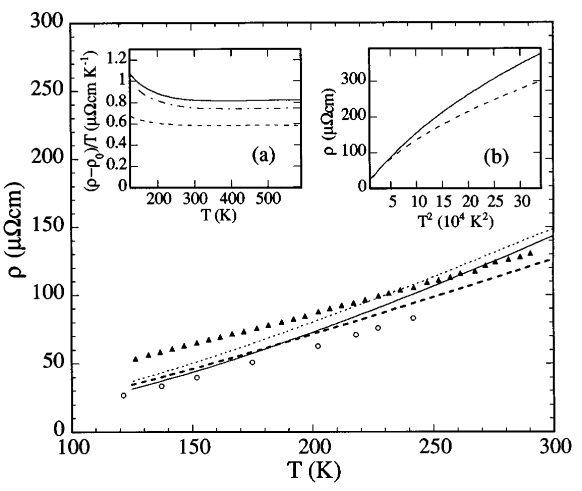

FIG. 1. The resistivity as a function of temperature at two doping levels ($n_h = 0.25$ solid line, $n_h = 0.15$ dashed line). The dotted line shows the result of HR [6], the open circles show the result of MP [8], and triangles the experimentally obtained ρ_{aa} (Ref. [12]). Insets: (a) $(\rho - \rho_0)/T$, where ρ_0 is the residual resistivity, as a function of T, for $\omega_{\mathrm{SF}}\xi^2 = 880$ and 970 K (dash-dotted line); (b) ρ as a function of T^2.

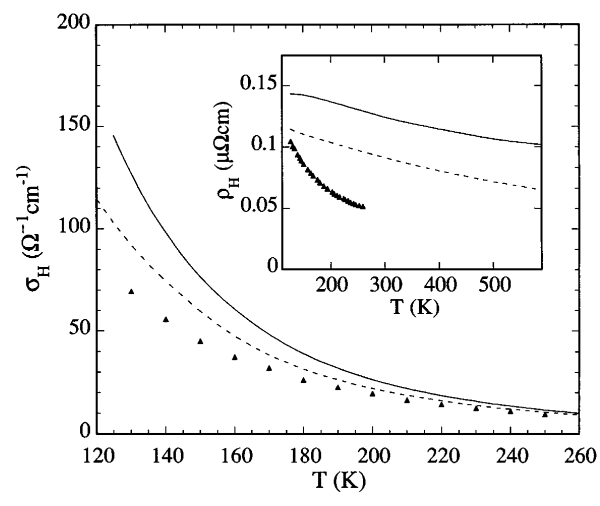

FIG. 2. NAFL results for the Hall conductivity σ_H (inset shows the Hall resistivity) as a function of temperature at $B = 1$ T. The solid (dashed) line shows the calculated result at doping level 0.25 (0.15), while the triangles show the experimental results of Ref. [12].

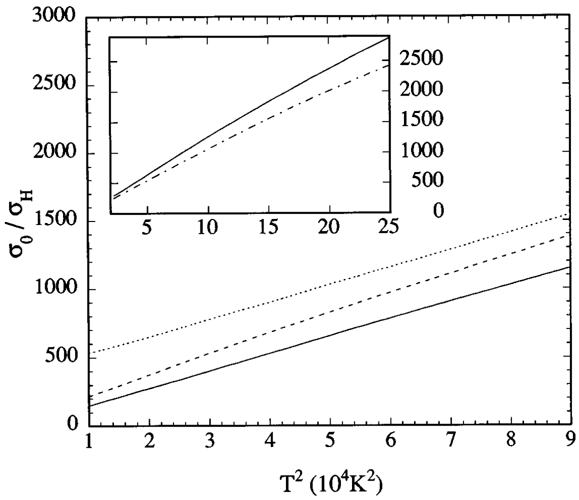

FIG. 3. Cotangent of the Hall angle as a function of temperature. The solid and dotted lines show clean and dirty samples, respectively, at doping level $n_h = 0.25$. The dashed line shows the clean result at $n_h = 0.15$. Inset: results at higher temperature for $\omega_{\rm SF}\xi^2 = 880$ and 970 K (dash-dotted line).

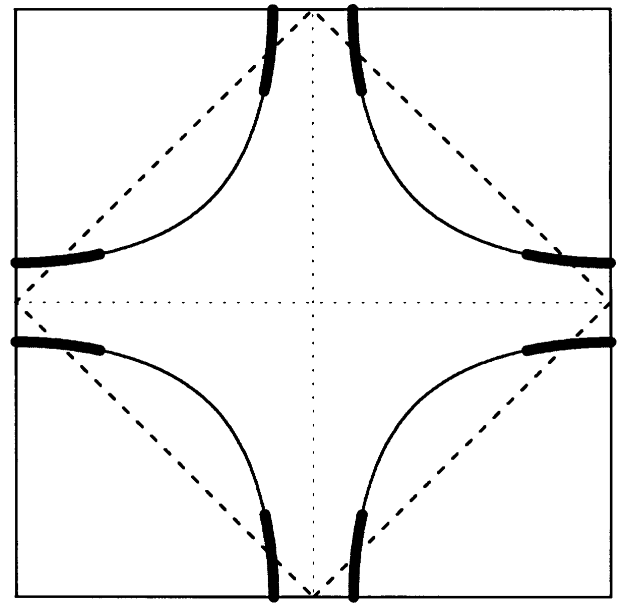

FIG. 4. The FS of YBCO (solid line) and the magnetic BZ (dashed line). The hot spots are the thick regions near the intercepts of the two lines.

$\omega_q = \omega_{\rm SF} + \omega_{\rm SF}\xi^2(\mathbf{q} - \mathbf{Q})^2$, and can be approximated by $\pi T^2/2\omega_{\mathbf{k}-\mathbf{k}'}(\omega_{\mathbf{k}-\mathbf{k}'} + \pi T)$. When $T_0 \ll T \ll \omega_{\rm SF}\xi^2$ we find, for $\mathbf{k}$ near the middle of a hot spot, that $\Phi_{\mathbf{k}}^0$ is independent of $\mathbf{k}$, $\Phi_{\mathbf{k}}^0 \sim u_x/\sqrt{T/\omega_{\rm SF}\xi^2}$. $\Phi_{\mathbf{k}}^0$ becomes $\mathbf{k}$ dependent away from a hot spot and is given by $\Phi_{\mathbf{k}}^0 \sim u_x s^3/(T/\omega_{\rm SF}\xi^2)^2$, where s is the distance along the FS between $\mathbf{k}$ and the center of the nearest hot spot. Experiment shows that for YBCO $\xi \sim 2$ in temperature region $100 < T < 300$ K (Ref. [13]). This means that the hot regions are fairly large: Under these circumstances, $\mathbf{k}$ is never too far from a hot spot (see Fig. 4). Since $\Phi_{\mathbf{k}}$ must have a maximum somewhere in between two hot spots along the FS, the s dependence of $\Phi_{\mathbf{k}}$ is significantly altered: For $s \sim \sqrt{T/\omega_{\rm SF}}/\xi$ we now have $\Phi_{\mathbf{k}} \sim s/(T/\omega_{\rm SF}\xi^2)^2$ over most of the FS. As a result $\sigma_0 \sim 1/T$, and $\rho \sim g^2(T/\omega_{\rm SF}\xi^2)$. As shown in the inset of Fig. 1, a 10% change in $\omega_{\rm SF}\xi^2$ yields a change of slope in resistivity of about 10%. Note that so far we have only included the fact that $\xi \sim 1$ and that the hot regions are symmetrically placed on the FS. It is important to note that the contribution of the equidistant regions from two adjacent hot spots is still $\sim(T/\omega_{\rm SF}\xi^2)^2$. This is why one finds a nonlinearity in $\rho(T)$ at lower temperatures, which vanishes as T becomes larger than T_0 (see Fig. 1), and the hot spots spread as $s \sim \sqrt{T}$. Our result is also consistent with the anisotropy of the self-energy found earlier [8].

The actual shape of the FS is of little relevance to σ_0, provided it is large enough to allow for spin-fluctuation scattering at $\mathbf{Q}$ (Ref. [8]) and the Fermi velocity is finite everywhere on the FS, while the Hall coefficient depends strongly on details of both band structure and the effective interaction. In general, the FS of several high temperature superconducting (HTSC) families is rather flat near hot spots, and curved away from them. Since σ_H involves a gradient of $\Phi_{\mathbf{k}}$, it is plausible that in the regions where I_0 varies rapidly with s, this gradient is dominated by the gradient of I_0; moreover, the curved regions of the FS will contribute to the Hall effect mostly through the change in u_x. One easily finds that in the flat regions σ_H/σ_0 are proportional to $\partial\Phi_{\mathbf{k}}/\partial s \sim (\omega_{\rm SF}\xi/T)^2$, while in the curved regions σ_H/σ_0 is proportional to $\nabla u_x(\omega_{\rm SF}\xi^2/T)^2$. Therefore in both regions one finds $\sigma_0/\sigma_H \sim (T/\omega_{\rm SF}\xi^2)^2$, independent of the specific behavior of $\rho(T)$. This is indeed the case, as clearly shown in the inset of Fig. 3, where we have plotted $\cot\Theta_H$ for two values of ξ. The present theory assumes that $T \ll \omega_{\rm SF}\xi^2$; when this is no longer the case, $\cot\Theta_H$ exhibits a deviation from the above behavior. We have verified by explicit calculation that, for both hole concentrations, this occurs at approximately 700 K (Ref. [11]), and is responsible for the very slight bending of the two lines at very high temperatures.

An important test of the soundness of our approach is obtained by adding weak impurity scattering to the collision term in the BE. Impurity scattering might be expected to *add* a temperature independent term to I_0, so that $\cot\Theta_H$ should be proportional to $A + BT^2$, where the slope B is unchanged from the clean case. The results of our numerical calculations (Fig. 3) show that this is indeed the case: B is the same in clean and dirty cases to within 1%. These results are consistent with a number of experiments [14–16]. Another challenge for the NAFL model is the existence of a small orbital magnetoresistance (MR) in YBCO, which

Harris *et al.* find [17] does not obey the usual Köhler rule. In calculations of $\rho(B)$ at several temperatures we have verified this behavior [11]. Not to our surprise, the relative MR, $\Delta\rho/\rho$, is found to have very strong temperature dependence and is of order Θ_H^2, as is usually the case in FLs. The values we find are somewhat higher than those obtained experimentally [11].

In conclusion, we have shown that the energy and momentum dependence of the effective magnetic interaction in the NAFL model gives rise to an anomalous temperature dependence of both resistivity and the Hall conductivity, which are qualitatively in agreement with transport measurements on fully doped $YBa_2Cu_3O_7$. The anomalous behavior originates in the hot spots which have a region of influence, $\delta k \sim \sqrt{T}$: As long as χ is sharply peaked at $\mathbf{q} \approx \mathbf{Q}$, with $\xi \sim 1$, this inevitably leads to the quadratic temperature dependence of $\cot\Theta_H$, despite the fact that neither σ_0 or σ_H displays FL-like temperature behavior. The sensitivity of our results to ξ provides a natural explanation of the experimentally observed noticeable differences in the slope of resistivity for rather small variations in T_c (Ref. [2]). In addition, since our results depend for the most part on the symmetric placement of the hot spots on the FS, and the existence of strong AF correlations, we expect similar results will hold for other HTSCs.

There are several unresolved issues. We find a somewhat lower resistivity with a somewhat higher slope and a more negative intercept than that measured at lower temperatures. More importantly, the resistivity appears FL-like up to temperatures of order 200 K, in contrast with experiments. This discrepancy is not serious, since, as shown in Fig. 1, a relatively small change in band parameters or the hole concentration reduces the crossover temperature to the experimentally observed T_c. The slope depends strongly on the coupling constant g and the energy scale $\omega_{\mathrm{SF}}\xi^2$, which are known only to within 10% accuracy, while lifetime effects make the influence of the hot spots much more prominent and therefore less FL-like [8]. There are several possible explanations for the large negative intercept, which leads to a weaker temperature dependence than is seen in experiment. These include small impurity scattering, spin-pseudogap effects, and normal fermion scattering, all seen experimentally in NMR measurements [1,9]. Imperfections which alter the local magnetic order change the magnetic quasiparticle interaction [8], and therefore affect the resistivity, while shifting $\cot\Theta_H$ only marginally. Indeed, only the highest quality samples show small negative intercepts in $\rho(T)$ [18]. Our calculations show that, in addition to providing a residual resistivity, impurities act to remove the nonlinearity seen in Fig. 1 (Ref. [11]). The spin pseudogap effect, as well as superconducting fluctuations [19], produce a curvature of the resistivity slightly above T_c (Ref. [13]), while normal fermion scattering [9] reduces the Hall conductivity and somewhat increases the resistivity. We address these issues elsewhere [11].

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