Hall effect in the cuprates: the role of forward scattering on impurities

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We solve the Boltzmann equation for electrons moving in a two-dimensional plane of square symmetry in the presence of a transverse magnetic field \(B\). We assume that there are two sources of scattering: a large momentum-independent scattering on a collective mode of the electron system, and a smaller momentum-dependent forward scattering on impurities. We show that the effect of impurities on the longitudinal and Hall conductivities is of the same order of magnitude.

Very recently, an interesting proposal has been advanced with the aim of explaining the anomalous magnetotransport data in the cuprates. Namely, it has been suggested that the marginal Fermi liquid theory (MFL) which correctly predicts the temperature dependence of the resistivity of the optimally doped cuprates, \(\rho \propto T\), can be modified by taking into account the scattering on impurities away from the CuO\(_2\) planes. It has been argued previously that such impurity scattering should be of very special type, allowing the electron to change its momentum by only a small fraction of the Fermi momentum. This peculiar type of scattering was argued in Ref. 1 to lead to corrections to the Hall conductivity of the pure MFL system, \(\sigma_H \propto T^{-2}\), which are in agreement with the experimentally observed scaling \(\sigma_H \propto T^{-3}\). In this Report we explore this idea in more detail. In particular, we ask whether within such modified MFL approach, both the resistivity and the Hall conductivity data can be explained on equal footing.

Let us first introduce the model under study. We consider electrons moving in a two-dimensional plane of square symmetry. We assume that the Fermi sea is a simply connected region in k space whose boundary (the Fermi line) has a length \(2\pi k_F\). We shall enumerate the points on the Fermi line by a dimensionless length \(\varphi\) defined by \(d\varphi = dk/k_F\), where \(dk\) is an element of the Fermi line. We set \(\varphi = 0\) along the \(x\) axis of the plane (which is assumed to coincide with one of the crystallographic axes of the plane).

Within standard transport theory, we want to study the transport properties of the electron gas in an applied electric field \(\mathbf{E}\) parallel to the plane and a magnetic field \(\mathbf{B}\) perpendicular to the plane. Because of the square symmetry of the problem, the linear response coefficients do not depend on the direction of \(\mathbf{E}\) and we take it to be parallel to the \(x\) axis of the plane. Let the local (in \(k\)-space) departure of the distribution function of the electrons, \(f_k\), from the equilibrium distribution, \(f_k^0\), be \(f_k = f_k^0 - (e\mathbf{E}/k_F)g_k\partial f_k^0/\partial \varepsilon_k\), where \(\varepsilon_k\) is the quasiparticle energy.

Let us introduce the local Fermi energy \(\varepsilon_F(k) = v_kK_k\), where \(v_k\) is the local Fermi velocity and \(K_k\) is the local radius of curvature of the Fermi line. Then for temperatures \(T \ll \text{min}[\varepsilon_F(k)]\) the Boltzmann equation for quasielastic scattering on bosonic excitations and impurities reads:

\[
\cos \psi(\varphi) + \beta g'(\varphi) = \frac{d\varphi'}{2\pi} A(\varphi, \varphi') [g(\varphi) - g(\varphi')],
\]

where \(A(\varphi, \varphi')\) describes the scattering of the electrons between the points \(\varphi\) and \(\varphi'\) of the Fermi surface and \(\beta = eB/hk_F^2\) is a dimensionless magnetic field. \(\psi(\varphi)\) is the angle between the normal to the Fermi line in the point \(\varphi\) and the \(x\) direction, \(\cos \psi = \mathbf{E} \cdot \mathbf{v}_k/Eck\). Note that Eq. (1) is valid for a general shape of the Fermi surface with a non-constant density of states (and, thus, a non-constant \(v_k\)) along the Fermi line. The information about \(v_k\) is contained in the dimensionless scattering function \(A(\varphi, \varphi')\).

In Ref. 2 the following scattering function has been proposed to describe the magnetotransport in the cuprates:

\[
A(\varphi, \varphi') = \Gamma_1 + \Gamma_2 \left( \frac{\varphi + \varphi'}{2}, \varphi' - \varphi \right),
\]

where \(\Gamma_1\) describes the scattering of the electrons on a hypothesized MFL mode. Since this scattering is supposed to be momentum-independent, \(\Gamma_1\) is a weak function of \(\varphi, \varphi'\), which we model by a constant. The physical (dimensionful) electron lifetime \(\tau_k\) is related to \(\Gamma_1\) via \(\tau_k^{-1} = v_kk_F\Gamma_1\). Within the MFL phenomenology, it is assumed that \(\Gamma_1\) exhibits an anomalous scaling with temperature, \(\Gamma_1 \propto T\).

The new ingredient introduced in Ref. 2 is the scattering on impurities which is described by the function \(A_2(\varphi, \theta)\). The authors of Ref. 2 argue rather convincingly that this type of scattering is effective only for \(\theta < \theta_c\), i.e., the scattering is in the forward direction.

Since \(\theta_c \sim (k_Fd)^{-1}\) where \(d\) is the characteristic distance of the impurities from the CuO\(_2\) plane, the actual numerical value of \(\theta_c\) may be not too small. Therefore, in what follows we shall consider two limiting cases: \(\theta_c \ll 1\) and \(\theta_c \sim 2\pi\). We show that in both limits the impurity contribution leads to effects of the same order of magnitude, when expressed in terms of the impurity transport lifetime.

**Forward scattering on impurities.** In this case \(\theta_c \ll 1\) and, as shown in Ref. 3, it is useful to define a (dimensionless) transport scattering rate:

\[
\Gamma_2(\varphi) = \int \frac{d\theta}{2\pi} A_2(\varphi, \theta)(1 - \cos \theta).
\]
Note that the scattering rate $\Gamma_2(\varphi)$ is not assumed to be constant. Rather, the authors of Ref. [3] suggest that $\Gamma_2(\varphi)$ should be large along the Cu-O-Cu bonds and small along the $(\pm \pi, \pm \pi)$ directions, in order to make the single particle lifetime compatible with the lifetime anisotropy deduced from the ARPES experiments on the cuprates. [4]

Making use of the scattering rate $\Gamma_2(\varphi)$, the Boltzmann equation (2) simplifies to

$$\cos \psi + \beta g' = \Gamma_1 g - (\Gamma_2 g')', \tag{2}$$

where the primes denote derivatives with respect to $\varphi$. In Eq. (2), scattering on MFL fluctuations is treated in the relaxation-time approximation, whereas scattering on impurities is described within the recently developed scheme for forward scattering. [3]

We assume that $\beta \ll 1$ and we expand $g$ in powers of $\beta$ to first order in $\beta$, $g = g_0 + g_1$, where $g_0 \propto \beta^0$. We assume furthermore that $\Gamma_1 \gg \Gamma_2$ for $T > 100$ K and we calculate $g_0$ and $g_1$ to the lowest nontrivial order in $\tau_1 \Gamma_2$, where $\tau_1 = \Gamma_1^{-1}$. These assumptions are checked at the end of the calculation, when we compare our results to the experimental data on the cuprates. With the above simplifications, we find

$$g_0 = \tau_1 \left[ h + \tau_1 (\Gamma_2 h')' \right], \tag{3}$$

$$g_1 = \beta \tau_1 \left[ h' + \tau_1 (\Gamma_2 h'')' + \tau_1 (\Gamma_2 h'')' \right], \tag{4}$$

where we have introduced an auxiliary function $h(\varphi) = \cos \psi$. In agreement with Ref. [3], a term proportional to the second derivative of $\Gamma_2$ appears in Eq. (4).

Following Ref. [3] we calculate the longitudinal and Hall conductivities, respectively, as follows:

$$\sigma = \frac{2e^2}{h} \int \frac{d\varphi}{2\pi} g_0(\varphi) \cos \psi(\varphi), \tag{5}$$

$$\sigma_H = -\frac{2e^2}{h} \int \frac{d\varphi}{2\pi} g_1(\varphi) \sin \psi(\varphi). \tag{6}$$

In taking the integrals, we repeatedly make use of the trigonometric relations $\cos^2 \psi = (1 + \cos 2\psi)/2$ and $\sin^2 \psi = (1 - \cos 2\psi)/2$ and of the identity

$$\int \frac{d\varphi}{2\pi} \cos 2\psi F(\varphi) = \int \frac{d\varphi}{2\pi} \sin 2\psi F(\varphi) = 0,$$

which holds for any function $F(\varphi)$ compatible with square symmetry. In fact, under the transformation $\varphi \to \varphi + \pi/2$, $F(\varphi)$ does not change, whereas $\psi(\varphi + \pi/2) = \psi(\varphi) + \pi/2$ and hence $\cos 2\psi$ and $\sin 2\psi$ change sign.

Integrating per parts so as to remove the derivatives of the function $\Gamma_2$ and making use of the above identities, we find the resistivity $\rho = \sigma^{-1}$ and the Hall angle $\Theta_H = \sigma_H/\sigma$,

$$\rho = \frac{h}{e^2} \frac{1}{\tau_1} + \int \frac{d\varphi}{2\pi} \Gamma_2(\varphi)(\psi')^2, \tag{7}$$

$$\Theta_H = \beta \tau_1 \left[ 1 + \tau_1 \int \frac{d\varphi}{2\pi} \Gamma_2(\varphi)(\psi')^2 (1 - 2\psi') \right]. \tag{8}$$

The factors $\psi'$ are determined by the shape of the Fermi line. For a circular Fermi line, $\psi' = 1$. For non-circular Fermi lines, $\psi'$ oscillates around 1, being smaller (larger) in the flat (curved) parts of the Fermi line.[4]

$s$-wave scattering on impurities. If $\theta_c \sim 2\pi$, electrons can scatter on an impurity to all directions. In this so-called s-wave scattering case the scattering function $A_2[(\varphi + \varphi')/2, \varphi' - \varphi]$ becomes a function of the incoming momentum only, i.e. $A_2 \to \Gamma_2(\varphi)$ and the standard relaxation-time approximation applies both to MFL scattering and to impurity scattering. Thus the Boltzmann equation simplifies to

$$\cos \psi + \beta g' = \left[ \Gamma_1 + \Gamma_2(\varphi) \right] g. \tag{9}$$

Note the difference of this equation with respect to Eq. (2).

Assuming again that $\Gamma_1 \gg \Gamma_2$ and calculating $g_0$ and $g_1$ to the lowest nontrivial order in $\tau_1 \Gamma_2$, we find results identical to Eqs. (3,4), with the only change that we should write $\Gamma_2(\varphi)$ instead of $\Gamma_2(\varphi)(\psi')^2$. Thus, if $\psi' \approx 1$ (which is the case in the cuprates), the impurity effects are virtually the same in both limiting cases (provided they are expressed in terms of the transport scattering rate $\Gamma_2$).

In a previous paper we have shown that magnetotransport is completely different in systems with dominant forward and $s$-wave scattering.[3] Thus our present result might come as a surprise. However, there is nothing mysterious about it. In the model of Ref. [3] the dominant scattering is on the MFL mode. This scattering is of $s$-wave type and as such is well describable by the relaxation-time approximation. The impurity scattering is only a small perturbation which can not manifest itself too differently in the limiting cases of forward and $s$-wave scattering. In some sense, this is similar to the analysis of impurity scattering at low temperatures in nearly antiferromagnetic systems.[3] In that case, impurities are the $s$-wave scatterer and antiferromagnetic fluctuations are the anomalous scatterer. If the $s$-wave scattering dominates (which happens typically at low temperatures), then it is not necessary to search for full solutions of the Boltzmann equation as would be the case in a clean system.[3] and the temperature dependence of the transport coefficients can be determined making use of the relaxation-time approximation.

Anisotropic $\tau_1$. Let us consider briefly the effect of a possible anisotropy of $\tau_1$. After all, within MFL theory one requires that it is the physical lifetime, $\tau_k$, which is isotropic and thus, if the Fermi velocity is not constant around the Fermi line, then $\tau_{1k} = \tau_k v_F k F$ should be anisotropic as well. For a non-constant $\tau_1$, the longitudinal and Hall conductivities read, again to leading non-trivial order in $\tau_1 \Gamma_2$. 

2
\[
\sigma = \frac{e^2}{h} \beta \int \frac{d\varphi}{2\pi} \left[ \tilde{\tau}_1 - \Gamma_2 \tilde{T}_1 \right],
\]
(10)
\[
\sigma_H = \frac{e^2}{h} \beta \int \frac{d\varphi}{2\pi} \tilde{\tau}_1 \left[ \tilde{\tau}_1 \psi' - 2\Gamma_2 \tilde{T}_2 \right].
\]
(11)

For forward impurity scattering we find \( \tilde{T}_1 = \tilde{\tau}_1^2(\psi')^2 + \tilde{\tau}_1^2(\psi')^2 + \tilde{\tau}_1^2 \psi'' + 2(\tilde{\tau}_1)^2 \psi' - \tilde{\tau}_1 \tilde{\tau}_1^2 \psi' \), whereas for s-wave scattering on impurities \( \tilde{T}_1 = \tilde{\tau}_1^2 \) and \( \tilde{T}_2 = \tilde{\tau}_1^2 \psi' \).

Discussion. Let us apply the above results to the cuprates. Taking \( k_F \approx 0.74 \text{ Å}^{-1} \) we find \( \hbar k_F^2/e \approx 3.6 \times 10^4 \text{ T} \), confirming our assumption that \( \beta \ll 1 \) for laboratory fields. In what follows, we shall assume the simplest nontrivial angular variations of the quantities \( \tilde{\tau}_1(\varphi), \psi(\varphi), \) and \( \Gamma_2(\varphi) \). The dimensionless MFL lifetime is assumed to vary along the Fermi line according to \( \tilde{\tau}_1 = \tau_0(1 - \delta \cos 4\varphi) \) with \( 0 < \delta < 0.1 \), taking into account the slightly smaller Fermi velocity along the Cu-O-Cu bonds. The shape of the Fermi line is modelled by \( \psi(\varphi) = \varphi - \epsilon \sin 4\varphi \) with \( 0 < \epsilon < 0.25 \), in accordance with a flat Fermi line at \( \varphi = 0 \) and equivalent directions. Finally, we take \( \Gamma_2(\varphi) = \Gamma_0 \cos^2 2\varphi \), as required by the recent ARPES experiments. Within MFL theory it is assumed that \( \tau_0 \propto T^{-1} \) and \( \Gamma_0 \) is temperature-independent. Inserting the above expressions into Eqs. (10)(11), we obtain
\[
\rho = \frac{\hbar}{e^2} \left[ \frac{1}{\tau_0} + \Gamma_0 f_1 \right],
\]
(12)
\[
\theta_H = \tau_0 \beta \left[ 1 + 4\delta \epsilon + \tau_0 \Gamma_0 (f_1(1 + 4\delta \epsilon) + f_2) \right].
\]
(13)

For forward scattering on impurities we find, to linear order in \( \delta \),
\[
\begin{align*}
f_1(\epsilon, \delta) &= \frac{1}{2} (1 - 4\epsilon + 8\delta^2) - \frac{\delta}{2} (1 - 8\epsilon + 12\epsilon^2), \\
f_2(\epsilon, \delta) &= -(1 - 6\epsilon + 24\epsilon^2 - 24\epsilon^3) + 2\delta(5 - 44\epsilon + 36\epsilon^2 - 48\epsilon^3).
\end{align*}
\]

For s-wave impurity scattering we obtain (again to linear order in \( \delta \)) \( f_1(\epsilon, \delta) = (1 - \delta)/2 \) and \( f_2(\epsilon, \delta) = -(1 - 2\epsilon) + \delta(3 - 12\epsilon)/2 \).

Turning to the resistivity data, experiment requires that at \( T \approx 100 \text{ K}, \tau_0 \Gamma_0 f_1 \approx 1/9 \), since the ratio of the resistivity at 100 K to its 0 K extrapolated value is \( \approx 10 \). Note that since \( f_1 \approx 1/2 \), this justifies a posteriori our assumption \( \tilde{T}_1 \Gamma_2 \ll 1 \) already at \( T = 100 \text{ K} \). At higher temperatures, \( \tilde{T}_1 \Gamma_2 \) becomes even smaller.

As regards the Hall angle, the impurity contribution should dominate at \( T > 100 \text{ K} \), if the mechanism proposed in Ref. 2 has to apply. This requires \( \tau_0 \Gamma_0 f_1(1 + 4\delta \epsilon) + f_2 \gg 1 + 4\delta \epsilon \), or, taking into account the estimate of \( \tau_0 \Gamma_0 f_1 \) (at \( T = 100 \text{ K} \)) from the resistivity data, \( f_2 \gg 8f_1(1 + 4\delta \epsilon) \). This is, however, impossible for \( 0 < \delta < 0.1 \) and \( 0 < \epsilon < 0.25 \), as can be readily seen both for forward and s-wave impurity scattering.

Conclusions. Within standard transport theory we have shown that additional impurity scattering on top of a dominant isotropic scattering on a collective mode does indeed lead to corrections to the Hall number, as predicted in Ref. 2. However, the effect is sufficiently large only for impurity scattering comparable to the inelastic scattering, in which case also the impurity contribution to the resistivity becomes comparable to the inelastic (MFL) contribution. Thus the resistivity and the Hall number observed experimentally in the cuprates can not be explained simultaneously within the picture advanced in Ref. 2.

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