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 in the cuprates the effect of impurities on the longitudinal and Hall conductivities is of the same order of magnitude.

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Very recently, an interesting proposal has been advanced with the aim of explaining the anomalous magnetotransport data[1] in the cuprates. Namely, Varma and Abrahams (VA) have suggested that the marginal Fermi liquid (MFL) theory 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.[2] 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.[3] This peculiar type of scattering was argued in Ref. 2 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 Brief 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 $\mathbf{k}$ space whose boundary (the Fermi line) has a length $2\pi k_F$. We shall numerate the points on the Fermi line by a dimensionless length φ 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,[4] 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 $\mathbf{k}$-space) departure of the distribution function of the electrons, $f_{\mathbf{k}}$, from the equilibrium distribution, $f^0_{\mathbf{k}}$, be $f_{\mathbf{k}} = f^0_{\mathbf{k}} - (eE/k_F) g_{\mathbf{k}} \partial f^0_{\mathbf{k}} / \partial \varepsilon_{\mathbf{k}}$, where $\varepsilon_{\mathbf{k}}$ is the quasiparticle energy.

In the low-temperature limit the Boltzmann equation for quasielastic scattering on bosonic excitations and impurities reads[5]

$$\cos\psi(\varphi) + \beta g'(\varphi) = \oint \frac{d\varphi'}{2\pi} A(\varphi,\varphi')[g(\varphi) - g(\varphi')], \tag{1}$$

where $A(\varphi,\varphi')$ describes the scattering of the electrons between the points φ and φ' of the Fermi surface and $\beta = eB/\hbar k_F^2$ is a dimensionless magnetic field. $\psi(\varphi)$ is the angle between the normal to the Fermi line in the point φ and the x direction, $\cos\psi = \mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}/E v_{\mathbf{k}}$. Note that Eq. (1) is valid for a general shape of the Fermi surface with a nonconstant density of states (and, thus, a nonconstant $v_{\mathbf{k}}$) along the Fermi line. The information about $v_{\mathbf{k}}$ is contained in the dimensionless scattering function $A(\varphi,\varphi')$.[5]

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

$$A(\varphi,\varphi') = \Gamma_1 + A_2(\varphi,\varphi'),$$

where Γ_1 describes the scattering of the electrons on a hypothesized MFL mode. Since this scattering is supposed to be momentum independent, Γ_1 is a weak function of φ,φ', which we model by a constant. Within the MFL phenomenology, it is assumed that Γ_1 exhibits an anomalous scaling with temperature, $\Gamma_1 \propto T$.

The new ingredient introduced in Ref. 2 is the scattering on impurities outside the CuO_2 planes, which is described by the function $A_2(\varphi,\varphi')$. For the sake of simplicity, in what follows we shall assume the simplest possible form of $A_2(\varphi,\varphi')$ consistent with tetragonal symmetry, $A_2(\varphi,\varphi') = a(\varphi)a(\varphi')F(\varphi'-\varphi)$. Here $a(\varphi)$ is invariant under the symmetry operations of the CuO_2 plane and $F(\theta) = F(-\theta)$. We should like to point out that none of our conclusions is dependent on this particular form of $A_2(\varphi,\varphi')$.

VA argue that $F(\theta)$ is finite only for $|\theta| < \theta_c/2$ where $F(\theta) \approx F$. Since $\theta_c \sim (k_F d)^{-1}$ where d is the characteristic distance of the impurities from the CuO_2 plane, the actual numerical value of θ_c may be not too small. In what follows we consider two limiting cases: $\theta_c \ll 1$ (forward scattering) and $\theta_c = 2\pi$ (s-wave scattering). 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.

The physical (dimensionful) electron lifetime $\tau_{\mathbf{k}}$ can be calculated as $\tau_{\mathbf{k}}^{-1} = v_{\mathbf{k}} k_F \oint (d\varphi'/2\pi) A(\varphi,\varphi')$. On the other hand, according to angle-resolved photoemission spectroscopy (ARPES) measurements,[6] $\tau_{\mathbf{k}}^{-1} = v_{\mathbf{k}} k_F [\Gamma_1 + \Gamma_0 \cos^2 2\varphi]$. Thus, in order to fit the ARPES data, we have to take $a(\varphi)$

$=|\cos 2\varphi|$, $F=2\pi\Gamma_0/\theta_c$ and $a(\varphi)=\cos^2 2\varphi$, $F=2\Gamma_0$ for forward and *s*-wave impurity scattering, respectively.

Forward scattering on impurities. In this case $\theta_c \ll 1$ and it is useful to define a (dimensionless) transport scattering rate

$$\Gamma_2(\varphi)=a^2(\varphi)\langle F(\theta)(1-\cos\theta)\rangle=\frac{\theta_c^2}{24}\Gamma_0\cos^2 2\varphi,$$

where we have introduced the Fermi surface averages as $\langle\cdots\rangle=(1/2\pi)\oint d\varphi\ldots$. Making use of $\Gamma_2(\varphi)$, the Boltzmann equation (1) simplifies to

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

where the primes denote derivatives with respect to φ. 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.[5]

We assume that $\beta \ll 1$ and we expand g in powers of β to first order in β, $g=g_0+g_1$, where $g_n \propto \beta^n$. 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 $\tilde{\tau}_1\Gamma_2$, where $\tilde{\tau}_1=\Gamma_1^{-1}$. 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

$$g_0=\tilde{\tau}_t\cos\psi-\tilde{\tau}_1^2(\Gamma_2\psi')'\sin\psi, \tag{3}$$

$$g_1=\beta\tilde{\tau}_1^2[h'+\tilde{\tau}_1(\Gamma_2 h')''+\tilde{\tau}_1(\Gamma_2 h'')'], \tag{4}$$

where $\tilde{\tau}_t^{-1}=\tilde{\tau}_1^{-1}+\Gamma_2(\psi')^2$ is the transport lifetime introduced in Ref. 2 and $h(\varphi)=\cos\psi$. The factor ψ' is determined by the shape of the Fermi line. For a circular Fermi line, $\psi'=1$. For noncircular Fermi lines, ψ' oscillates around 1, being smaller (larger) in the flat (curved) parts of the Fermi line.[7]

Following Ref. 5, we calculate the longitudinal and Hall conductivities $\sigma=(2e^2/h)\langle g_0(\varphi)\cos\psi(\varphi)\rangle$ and $\sigma_H=-(2e^2/h)\langle g_1(\varphi)\sin\psi(\varphi)\rangle$, respectively. 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 $\langle\cos 2\psi F(\varphi)\rangle=\langle\sin 2\psi F(\varphi)\rangle=0$, 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 Γ_2 and making use of the above identities, we find

$$\sigma=\frac{e^2}{h}\langle\tilde{\tau}_t\rangle, \tag{5}$$

$$\sigma_H=\frac{e^2}{h}\beta\langle\tilde{\tau}_t^2\psi'\rangle. \tag{6}$$

Note that Eq. (5) is in complete agreement with VA, whereas Eq. (6) contains only the ''customary'' term of VA, while their ''new'' term is absent in our result. This difference can be traced back to the difference of our Eq. (2) with respect to the analogous Eq. (16) of VA, which in our language reads

$$\cos\psi+\beta g'=\Gamma_1 g-2\Gamma_2' g'-\Gamma_2 g''.$$

s-wave scattering on impurities. For $\theta_c=2\pi$ the scattering function $A_2(\varphi,\varphi')$ satisfies the criterion for the validity of the relaxation-time approximation, $\oint A_2(\varphi,\varphi')g(\varphi')=0$ for all φ. Thus there is no difference between single-particle and transport scattering rates and $\Gamma_2(\varphi)=\Gamma_0\cos^2 2\varphi$. The Boltzmann equation simplifies to

$$\cos\psi+\beta g'=[\Gamma_1+\Gamma_2(\varphi)]g. \tag{7}$$

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 $\tilde{\tau}_1\Gamma_2$, we find that Eqs. (5) and (6) apply, but with $\tilde{\tau}_t^{-1}=\tilde{\tau}_1^{-1}+\Gamma_2$. Thus, if $\psi'\approx 1$ (which is the case in the cuprates[8]), the impurity effects are formally the same in both limiting cases (provided they are expressed in terms of the transport scattering rate Γ_2). Note, however, that because of the absence of the small factor $\theta_c^2/24$ in Γ_2, *s*-wave impurity scattering cannot fit the ARPES and transport data simultaneously, and it is only of methodological interest.

In a previous paper we have shown that magnetotransport is completely different in systems with dominant forward and *s*-wave scattering.[5] Thus our present result might come as a surprise. However, there is nothing mysterious about it. In the model of Ref. 2, 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 cannot 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.[9] 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,[10] and the temperature dependence of the transport coefficients can be determined making use of the relaxation-time approximation.

Anisotropic $\tilde{\tau}_1$. Let us consider briefly the effect of a possible anisotropy of $\tilde{\tau}_1$. After all, within MFL theory one requires that it is the *T*-dependent part of the physical lifetime, $\tau_{1\mathbf{k}}$, which is isotropic and thus, if the Fermi velocity is not constant around the Fermi line, then $\tilde{\tau}_{1\mathbf{k}}=\tau_{1\mathbf{k}}v_{\mathbf{k}}k_F$ should be anisotropic as well. For a nonconstant $\tilde{\tau}_1$, the longitudinal and Hall conductivities read, again to leading nontrivial order in $\tilde{\tau}_1\Gamma_2$,

$$\sigma=\frac{e^2}{h}\langle\tilde{\tau}_t\rangle, \tag{8}$$

$$\sigma_H=\frac{e^2}{h}\beta[\langle\tilde{\tau}_t^2\psi'\rangle+2\langle\tilde{\tau}_t^3\Gamma_2\psi' X_2\rangle], \tag{9}$$

where $\tilde{\tau}_t^{-1}=\tilde{\tau}_1^{-1}+\Gamma_2 X_1$. For forward impurity scattering we find

$$X_1=(\psi')^2+(\tilde{\tau}_1'/\tilde{\tau}_1)^2,$$

$$X_2=\tilde{\tau}_1''/\tilde{\tau}_1-(\tilde{\tau}_1'/\tilde{\tau}_1)^2-(\tilde{\tau}_1'/\tilde{\tau}_1)(\psi''/\psi'),$$

whereas for *s*-wave scattering on impurities $X_1=1$ and $X_2=0$. Note that in agreement with VA, Eq. (9) represents a sum of a ''customary'' and a ''new'' term. This is qualitatively different from the relaxation-time approximation result, where only the ''customary'' term appears. However, our result differs from that given by VA, as already noted in the special case $\tilde{\tau}_1=\text{const}$.

Discussion. Let us apply the above results to the cuprates. Taking $k_F\approx 0.74$ Å^{-1} we find $\hbar k_F^2/e\approx 3.6\times 10^4$ 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 $\tilde{\tau}_1(\varphi)=\tau^*(1-\delta\cos 4\varphi)$ with $0<\delta<0.1$, taking into account the slightly smaller Fermi velocity along the Cu-O-Cu bonds.[6] The shape of the Fermi line is modeled 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.[8] Finally, we take $\Gamma_2(\varphi)=\Gamma^*\cos^2 2\varphi$, as required by the recent ARPES experiments.[6] Within MFL theory it is assumed that $\tau^*\propto T^{-1}$ and $\Gamma^*=(\theta_c^2/24)\Gamma_0$ is independent of temperature. Making use of Eqs. (8) and (9), we obtain to leading nontrivial order in $\tilde{\tau}_1\Gamma_2$ for the resistivity $\rho=\sigma^{-1}$ and the Hall angle $\theta_H=\sigma_H/\sigma$

$$\rho=\frac{h}{e^2\tau^*}[1+\tau^*\Gamma^* f_1], \tag{10}$$

$$\theta_H=f_2\beta\tau^*\left[1+\tau^*\Gamma^*\left(f_1-\frac{2f_3}{f_2}\right)\right], \tag{11}$$

where f_1, f_2, f_3 are functions of ϵ and δ.

The resistivity data require that at $T\approx 100$ K, $\tau^*\Gamma^* f_1\approx 1/8$, since the ratio of the resistivity at 100 K to its 0 K extrapolated value is ≈ 9.[2] Thus the relative weight of the contribution to θ_H coming from impurity scattering is $R=(1-2f_3/f_1f_2)/8$. In Fig. 1 we plot the value of R as a function of ε for various δ. Since we never find $R\gg 1$, we conclude that the mechanism proposed in Ref. 2 cannot explain simultaneously the resistivity and the Hall data on the cuprates. Finally, let us point out that in the most promising paramater region (i.e., where R is maximal) $\tau^*\Gamma^* f_1\approx 1/8$ implies that $\tau^*\Gamma^*\approx 0.1$. This justifies *a posteriori* our assumption $\tilde{\tau}_1\Gamma_2\ll 1$ already at $T=100$ K. At higher temperatures, $\tilde{\tau}_1\Gamma_2$ becomes even smaller.

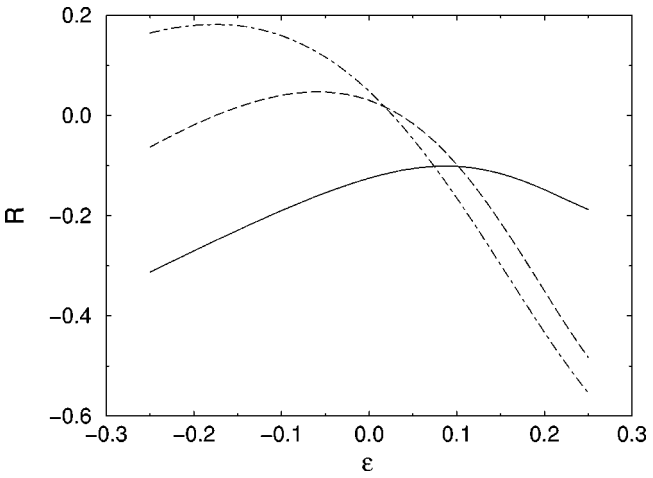

FIG. 1. The relative weight R of the impurity contribution to θ_H at $T=100$ K as a function of ϵ for δ=0,0.1,0.2 (bottom to top curves at $\epsilon=-0.25$).

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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