Two regimes in conductivity and the Hall coefficient of underdoped cuprates in strong magnetic fields

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Abstract
We address recent experiments shedding light on the energy spectrum of under and optimally doped cuprates at temperatures above the superconducting transition. Angle resolved photoemission reveals coherent excitation only near nodal points on parts of the ‘bare’ Fermi surface known as the Fermi arcs. The question debated in the literature is whether the small normal pocket, seen via quantum oscillations, exists at higher temperatures or forms below a charge order transition in strong magnetic fields. Assuming the former case as a possibility, expressions are derived for the resistivity and the Hall coefficient (in weak and strong magnetic fields) with both types of carriers participating in the transport. There are two regimes. At higher temperatures (at a fixed field) electrons are dragged by the Fermi arcs’ holes. The pocket being small, its contribution to conductivity and the Hall coefficient is negligible. At lower temperatures electrons decouple from holes behaving as a Fermi gas in the magnetic field. As the mobility of holes on the arcs decreases in strong fields with a decrease of temperature, below a crossover point the pocket electrons prevail, changing the sign of the Hall coefficient in the low temperature limit. Such behavior finds its confirmation in recent high-field experiments.

Keywords: superconductivity, cuprates, pseudogap phase, Hall effect

1. Introduction
An understanding of high temperature superconductivity (HTSC) in cuprates is a pressing issue both on the theoretical side of the problem and for practical implications. While in superconductors of the ‘old’ generation it was at least known that superconductivity emerges from the normal Fermi liquid phase, HTSC is preceded by the so-called pseudogap phase with many abnormal properties. The most unexpected feature revealed in angle resolved photoemission (ARPES) experiments is that coherent electronic excitations exist only on the Fermi arcs along the ‘bare’ Fermi surface, separated from each other by large energy gaps [1].

It was absolutely unclear how to interpret even such basic experimental data as those for resistivity or the Hall coefficient. The importance of the question was probably realized for the first time when it turned out that the Hall coefficient [2] in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) manifests an activation temperature dependence [3].

In 2007 the discovery of quantum oscillations (QOs) in underdoped (UD) $\text{ortho II} \ Y\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) [4] showed the presence of small Fermi liquid (FL) pocket(s).
Low frequency QOs in high magnetic fields were found in HgBa₂CuO₄₊ₓ (Hg1201) as well [6].

So far, ARPES experiments have been performed on two-layer Bi₂Sr₂CaCu₂O₈ (Bi2212), single-layer Bi₂Sr₂CuO₆ (Bi2201) and LSCO (see the recent review [7]). As yet, ARPES is not available for Hg1201 and YBCO because of problems with the surface [8]. The consensus is that, except for minor details, ARPES findings bear the general character and reflect the basic physics.

It is all the more remarkable that the recent experiments [9] added new and convincing evidence in support of the Fermi arcs concept. In brief, it was pointed out in [9] that the characteristic for temperature dependence of resistivity of clean Hg1201 (and a few other cuprate compounds) is the contribution proportional to the square of the temperature, as if in a Fermi liquid. In [9] the latter was related to free carriers on the Fermi arcs.

In turn, non-monotonic temperature and field dependence of the Hall and Seebeck coefficients in YBCO and Hg1201 in experiments [11, 12] below \( T \approx 100–150 \) K was considered as due to the contribution from electrons on the pocket.

These results pose a question about the interrelation between pocket(s) and the Fermi arcs. Currently, one highly debated issue in the literature concerns the nature of the pocket, that is, whether the pocket is a band feature and is omnipresent in the spectrum, including at higher temperatures, or whether it emerges below a charge order (CDW) transition. As to the latter, according to [13, 14], a CDW ordering indeed occurs in the relevant intervals of temperature and magnetic field.

Let us emphasize that most QO experiments have been performed in high fields and at not too high temperatures (\( T < 10 \) K). We investigate conductivity and the Hall coefficient assuming that carriers of both types participate in the transport properties in the whole temperature range of the pseudogap phase. We adopt the view [5] that only one small pocket exists in UD YBCO that lies away from a Fermi arc.

The model of holes on the Fermi arcs interacting via short-range interactions has been examined in the framework of the kinetic equation in [10] for interacting holes on the Fermi arcs. Below, the model is generalized to include electrons on the pocket and extended to the case of strong magnetic fields. Looking ahead, our results do not contradict [11, 12]; more importantly, in our opinion, the results give support to the notion of such a pocket as a band feature.

In its most general form the kinetic equation is

\[
\frac{d n}{d t} = I_{\text{col}}. \tag{1}
\]

On the left, the total derivative \( (d n / d t) \) accounts for variations of the Fermi distribution of the quasiparticles in their motion in the real and the momentum space in the presence of external fields. The right-hand term, the collision integral \( I_{\text{col}} \), is responsible for the relaxation processes.

2. Results from the model of Fermi arcs

Consider first carriers on the Fermi arcs. In weak constant electric and magnetic fields the kinetic equation (1) is presented in the commonly accepted form

\[
e \left( \vec{E} + \frac{1}{c} [\vec{v} \times \vec{H}] \right) \vec{V}_{F} n(\vec{p}) = I_{\text{coll}}. \tag{2}
\]

Changes \( n_{1} \) of the Fermi distribution function \( n(\vec{p}) \) are also small. At a non-zero current the system of charged carriers moves as a whole with a drift velocity \( \vec{u} \). Correspondingly, the left-hand side (LHS) in (2) reduces to

\[
e \left( (\vec{E} \cdot (\vec{v} - \vec{u})) - \frac{1}{c} (\vec{v} \times \vec{H}) \cdot \vec{u} \right) \frac{\partial n_{0}}{\partial \varepsilon}. \tag{3}
\]

(Here \( (\partial n_{0} / \partial \varepsilon) \) is the derivative of the equilibrium Fermi function: \( \vec{v} = d \varepsilon (\vec{p} / d \varepsilon) \).) Similarity, the collision integral on the right-hand side (RHS) of equation (3) should be expanded over small \( n_{1} \). The balance between LHS and RHS gives expressions for the quadratic resistivity term and for the Hall coefficient, correspondingly [10],

\[
\rho^{2D}(T) = \left( \frac{\pi}{e^{2}} \right) \frac{4 \pi^{2}}{3 \Delta \varphi^{2}} \left( V(1; 2) \right)^{2} 
\times \left( \frac{\Delta}{\varepsilon_{F}} \right) \left( \frac{T}{\varepsilon_{F}} \right)^{2} \tag{4}
\]

and

\[
R_{H} = \frac{1}{\varepsilon_{F} \tau_{\text{eff}}} > 0. \tag{5}
\]

Here \( V(1; 2) \) is the renormalized matrix element of the electron–electron interaction, \( m^{*} = Z^{-1} m \) is the renormalized mass. The combination \( \varepsilon_{F}^{*} = \rho_{2D}^{2} / 2 m^{*} \) is defined as the renormalized Fermi energy.

In equation (4), \( \Delta = \varepsilon_{F} p_{F} [(K / 4 p_{F}) - 1], K^{1} \) is the projection of the Umklapp vector \( \vec{K} = (2 \pi / a, 2 \pi / a) \) on the diagonal in the Brillouin zone (BZ). Processes with Umklapp scattering are critical for relaxation of the momentum and, hence, for non-zero resistivity. Unlike ordinary metals with large Fermi surfaces, for the system of narrow Fermi arcs the resistivity is obtained in the explicit form of equation (4); \( \Delta \varphi \) is the arc width. For the isotropic energy spectrum the effective number of carriers is \( n_{\text{eff}} = \frac{\Delta \varepsilon}{\varepsilon_{F}^{2}} \). Here \( c_{z} \) is the lattice constant in the perpendicular-to-plane direction, \( s \) is the number of CuO₂ planes per unit cell. Note in passing that each parameter in (4) and (5) can be found experimentally. In fact, the position of the nodal points \( p_{F} \) is known from ARPES; the Fermi arc width \( \Delta \varphi \) follows directly from the experimental value of \( R_{H} \). (The nodal points usually lie rather close to the \((\pm \pi / 2, \pm \pi / 2)\)-points [7].)

Rigorously speaking, expression (5) for the Hall coefficient applies only in the weak-field regime \( \omega_{c} \tau_{\text{col}} \ll 1 \) \( (\omega_{c} = (eH / m^{*} c)) \) [10]. (The notation \( \tau_{\text{col}} \) stands for the mean scattering time.) Meanwhile, the order of magnitude \( \tau_{\text{col}} \) in (4) is \( \tau_{\text{col}} \propto \varepsilon_{F} / T^{2} \), i.e., \( \tau_{\text{col}} \) is large in clean samples. For instance, at \( T = 100 \) K the magnetic field should be much smaller than 3–5 T for (5) to apply. Data for \( R_{H} \) in Hg1201, YBCO and LSCO in the whole temperature range have been obtained only in higher fields (see [2, 11] and [12]).
3. The role of the electronic pocket

The Hall coefficient equation (5) is temperature independent. Meanwhile, the notable feature in the Hall data [2, 11, 12] is the temperature dependence, \( R_H(T) \) (hence, the same for \( \Delta \varphi(T) \)).

Two mechanisms come to mind in regard to the \( T \)-dependence of the Hall effect. The first one is a temperature dependence of the Fermi arcs’ width that is seen in ARPES experiments [15–18]. For the model this means an increase in the number of carriers with temperature increase.

Recall that the notion of two scattering times [19] was introduced to reconcile the resistivity linear in temperature and the \( T^2 \)-dependence of the Hall angle: \( \cot(\theta_H) \propto T^2 \) above \( T^*(\chi) \). Here we concentrate on the universal experimental regime of the \( T^2 \)-resistivity [9]. Increase of the arc width with temperature (i.e. of the number of carriers) causes deviations from quadratic dependence in the arc width with temperature (i.e. of the number of carriers) causes deviations from quadratic dependence in the arc width with temperature. Consequently, the matrix elements that determine \( 1/\tau_{eh} \) have the same order of magnitude. This makes it possible from the analysis of the kinetic equation to derive the following estimate for \( 1/\tau_{eh} \):

\[
\frac{1}{\tau_{eh}} \approx \text{const} \times \left( \frac{m_e}{m^*} \right) \left( \frac{p_F}{p_{Fe}} \right) \frac{T^2}{\delta E} \tag{10}
\]

with a const \( \sim 1 \). The factor \( p_F/p_{Fe} \gg 1 \) in (10) shows that \( 1/\tau_{eh} \gg 1/\tau_{FA} \). From (7) the conductivity follows:

\[
\sigma_{3D}(T) = e^2 \left( \frac{n_{eff}}{m^*} - \frac{n_e}{m_e} \right) \tau_{FA} \tag{11}
\]

where the second term is the contribution from \textit{electrons dragged} by holes (hence the negative sign). In (11) \( n_e \) is the electronic density. Comparison between \( n_{eff} = \Delta \varphi sp_F^2/\pi c^2 \), the effective density of holes on the Fermi arcs, and \( n_e = (p_F/2\pi)^2 \) shows that \( n_{eff} \gg n_e \) \( (m^* \sim m_e; p_F/p_{Fe} \gg 1) \), i.e. the contribution of electrons to the conductivity in this regime is very small.

In vector notation the Hall coefficient \( R_H(T) \) is defined by the relation

\[
\vec{E} = \rho \vec{J} + R_H \vec{H} \times \vec{J}. \tag{12}
\]

Here \( \rho \) is the resistivity and \( \vec{J} \) is the longitudinal current. The two drift velocities \( v_{p,H} \) and \( \vec{v}_{FA,H} \) for electrons and holes in the presence of the magnetic field are found from the kinetic equations after substituting into equation (3) for the Lorentz forces:

\[
-|e|E = \frac{|e|}{c} H_{FA} \quad \text{(for holes)}; \tag{13a}
\]

\[
|e|E = -\frac{|e|}{c} H_{p} \quad \text{(for electrons).} \tag{13b}
\]

Calculations of the Hall currents are similar to those for the two electrical currents. The Hall coefficient of the two-component system is

\[
R_H(T) = \frac{1}{c|e|n_{eff}} \times \left\{ 1 + \left( \frac{n_e}{n_{eff}} \right) \left( \frac{m^*}{m_e} \right) \right\} \tag{14}
\]

(\text{Note that the small contributions from electrons in (11) and (14) have different signs.})
Pockets have been seen in e-doped Nd_{2−x}Ce_xCuO_4 [21]. With the estimate \( E_F \sim 50 \text{ meV} \) in hole-doped cuprates and the ARPES resolution of typically 10 \text{ meV}, observation of the pocket in photoemission experiments looks, in principle, feasible, although difficult. We recall again that it is the surface quality that plagues ARPES in YBCO and Hg1201. Doping in LSCO produces more disorder. (Two-layer Bi2212 has other problems related to superstructure.) Currently, ARPES experiments are mostly focused on the vicinity of the ‘bare’ Fermi surface. In our model the pocket lies away from the Fermi arcs. To repeat, the main experimental difficulties lie in the preparation of good crystalline surfaces.

4. Interplay between holes and electrons in strong magnetic fields

As mentioned above, formally, there are restrictions on the strength of the magnetic field. For holes it reads \( \omega_c \tau_{\text{PA}} \propto (\omega_c / T)(e_F / T) \ll 1 \).

The argument is given below that expression (5) applies for the Hall coefficient of holes even if that restriction is not fulfilled. At the same time, for electrons the restriction \( \omega_c \tau_e \ll 1 \) \( (\omega_c \equiv (eH/m_e c)) \) at a fixed value of the magnetic field is violated at temperatures considerably lower than for carriers on the Fermi arcs due to the factor \( p_{\text{ec}} / p_{\text{eh}} \ll 1 \) in \( \omega_c \tau_e \approx \omega_c (p_{\text{ec}} / p_{\text{eh}}) \tau_{\text{PA}} \). Thus, at high enough temperatures the contribution from holes on the Fermi arcs prevails over that from electrons.

Thereby, while holes on the Fermi arcs can already be in the strong field regime for electrons, the new physics sets in only at \( \omega_c \tau_e \approx \omega_c (p_{\text{ec}} / p_{\text{eh}}) \tau_{\text{PA}} \approx 1 \). Below, the pocket decouples from holes on the Fermi arcs and its contribution to \( R_{\text{H}}(T) \) finally becomes that of free electrons in a magnetic field and scattering on impurities finally becomes the only mechanism of relaxation. To the best of the authors’ knowledge no rigorous theoretical expression for \( R_{\text{H}}(T) \) is available in general except in the limit of strong magnetic field.

For the (diagonal or symmetric) component of conductivity in high fields estimates give [22] \( \sigma^S \sim \sigma_0 (\omega_c \tau_e)^{-2} \), where \( \sigma_0 \) is the conductivity in the absence of the field. For holes on the Fermi arcs \( \sigma^S_{\text{PA}} \approx (n_{\text{eff}} e^2 / \omega_c^2 m_e^*) (T^2 / \varepsilon_F) \), while for electrons \( \sigma^S_p \approx (n_e e^2 / \omega_c^2 m_p) \tau_{\text{imp}}^{-1} \). One sees directly that at low temperatures the electronic mobility will exceed the mobility of carriers on the Fermi arcs. Comparison of the two expressions defines the temperature scale \( T_0 \). \( T_0^2 \approx (n_e / n_{\text{eff}}) (\varepsilon_F / \tau_{\text{imp}}) \) (by the order of magnitude it can be rewritten as \( T_0^2 \approx (p_{\text{ec}} / p_{\text{eh}}) (E_F / \tau_{\text{imp}}) \)).

At lower temperatures the Hall coefficient is

\[
R_{\text{H}}(T) = -\frac{1}{c|c| n_e}.
\]

Rewriting \( \omega_c \tau_e \approx \omega_c (p_{\text{ec}} / p_{\text{eh}}) \tau_{\text{PA}} \approx 1 \) as \( T^2 \approx (p_{\text{ec}} / p_{\text{eh}}) \) \( \omega_c E_F \) defines the approximate position of the Hall coefficient maximum:

\[
T_{\text{max}} \approx \sqrt{(p_{\text{ec}} / p_{\text{eh}}) \omega_c E_F}.
\]

5. Hall coefficient for holes on Fermi arcs

We return to holes on the Fermi arcs in the opposite limit \( \omega_c \tau_{\text{col}} \gg 1 \) and show that the expression (5) for \( R_{\text{H}}(T) \) is correct in the limits of both weak and strong magnetic fields.

Assuming tetragonal symmetry for the CuO_2-plane in cuprates, the Hall coefficient in strong fields can be defined as \( R_{\text{H}}H \equiv 1 / \sigma_{xy} \) (below we use the system of coordinates with the \( x, y \)-axes along the two diagonals of the BZ). For normal metals in the strong field limit the value of the non-diagonal conductivity component \( \sigma_{xy} \) is known to depend critically on whether electrons at the Fermi surfaces in the magnetic field move along closed or open trajectories (see e.g. [22]). In particular, in the former case,

\[
\sigma_{xy} = -\frac{|e|c}{H} n.
\]

(Here \( n \) is the number of carriers for a closed Fermi surface.)

Returning to equation (1), in strong magnetic fields \( \omega_c \tau_{\text{col}} \gg 1 \) the collision integrals obviously should be omitted. Finding the distribution functions for carriers placed in the strong magnetic field and a weak electric field reduces to solving the equations of motion, as given by Liouville’s theorem,

\[
\frac{dn}{dt} = 0.
\]

The approach to solving (18) was elaborated in [23]. (See the summary of the method in [22].)

Unlike weak fields, as in equation (3), the charges now move along trajectories bent by the strong magnetic field. Because of this, presenting the distribution functions in terms of the Cartesian momentum components, \( p_x, p_y \), is not convenient. Instead, in [23] it was suggested to go over to new variables: energy \( \varepsilon \) and time variable \( \tau \) defined via the relation

\[
dr = c \frac{d\varepsilon}{\varepsilon} (c/eH).
\]

(Here \( ds \) is the element of ‘length’ along the Fermi surface: \( ds^2 \equiv dp_x^2 + dp_y^2, v_x^2 = v_x + v_y \).) Equation (8) means that in a strong field, \( \hat{H} \) carries move along the Fermi surface with high speed.

For a weak electrical field equation (18) takes the form [22, 23]

\[
\frac{dn}{d\varepsilon} \approx -\frac{dn_0}{d\varepsilon} (\hat{E} \cdot \vec{v}) + \frac{\partial n_1}{\partial \tau} \approx 0.
\]

(The collision integrals were discarded.) As for \( n_1 \), the latter is presented [22, 23] in the form

\[
n_1 = (\partial n_0 / \partial \varepsilon) e(\hat{E} \cdot \vec{g}).
\]

The equation for \( \vec{g} \) is

\[
\frac{\partial \vec{g}}{\partial \tau} = \vec{v}.
\]

It is important that the solution of (22) cannot contain a constant vector \( \vec{g}_0 \). (Such a term would result in a meaningless constant shift of the distribution function (21)). The further calculations for the Fermi arcs model are, in some sense, even simpler than in [23].
In fact, there is no dilemma now concerning motion along either open or closed trajectories in the momentum space: carriers cannot go away from arcs because on both sides of the arc the distribution function is restricted by large energy gaps. In [22] the ‘time’ \( \tau \) for a carrier was formally defined by its initial position on the Fermi surface. The actual physical meaning of such a procedure [23] is that it indirectly characterizes carriers by their velocities \( d \mathbf{s} / d \tau \) along the Fermi surface, as follows from equation (19). As the Fermi arcs are separated from each other by large energy gaps where the distribution function is zero, the time variables \( \tau \) of equation (19) can be introduced for each Fermi arc independently.

One can now refer to equations (84) and (11) in [22]. The latter reads now as the sum over the four arcs:

\[
\sigma_{\alpha\beta} = \frac{2e^2H}{(2\pi)^2c} \sum_{\Delta\varphi} v_\alpha g_\beta d\tau dp_z.
\]

\[
\equiv \frac{2e^3H}{\pi^2c} \sum_{\Delta\varphi} v_\alpha g_\beta d\tau dp_z.
\] (23)

(Sgn \( \Delta\varphi \) in the integral reminds one that the integration in (23) is limited by one Fermi arc.) For definiteness, \( \sigma_{xy} \) is chosen as follows:

\[
\sigma_{xy} = \frac{2e^3H}{\pi^2c} \int_{\Delta\varphi} v_x g_y d\tau dp_z.
\] (24)

After writing out the equation

\[
\frac{dp}{d\tau} = \frac{e}{c} [\mathbf{H} \times \mathbf{v}]
\] (25)

in the \( x, y \)-components, solving equation (11) gives \( g_y = -(c/eH)p_z \) while \( v_x = (c/eH)(dp_x/d\tau) \); one finds that integration over the \( \tau \)-variable in (24) is actually integration over the momentum component \( p_x \):

\[
\sigma_{xy} = \frac{2e^3H}{\pi^2c} \int_{\Delta\varphi} v_x g_y dp_z
\]

\[
\equiv -\frac{2ec}{\pi^2H} \left( \frac{s}{c_z} \right) \int_{\Delta\varphi} p_x dp_y,
\] (26)

where the last integral is over the area \( \delta S \) limited by the single arc:

\[
\sigma_{xy} = -\frac{ec}{H} n_{\text{eff}}.
\] (27)

In the isotropic case \( \delta S = (p_B^2/2)\Delta\varphi \) and \( n_{\text{eff}} = (\Delta\varphi)p_B^2/e\pi^2c \) is defined as in equation (5). At \( \Delta\varphi \Rightarrow \pi/2 \) one gradually returns to the expression of the Hall constant for the closed Fermi surface [22]. In the anisotropic case the number of carriers is expressed in terms of the area \( \delta S \) limited by the single arc. (For holes, \((-e) \Rightarrow |e| \). One sees that introduction of the time variable \( \tau \) for the finite Fermi arc was nothing more than a convenient mathematical device.) Equations (26) and (27) conclude the proof.

6. Conclusions

In summary, the expressions for resistivity and the Hall coefficient were derived for two types of carriers participating in transport. There are two regimes depending on the strength of the magnetic field. At a fixed magnetic field and at higher temperatures electrons on the pocket are bound to holes on the Fermi arcs. Since the size of the pocket is small, its contribution to the conductivity and the Hall coefficient is negligible.

On lowering the temperature electrons decouple from holes and behave as a Fermi gas in the magnetic field. In the limit of low temperatures electrons contribute most to the Hall effect, changing the sign of the Hall coefficient. The result seems to agree with recent high-field experiments.

Contributions from holes on the Fermi arcs at higher temperatures prevail and the Hall coefficient \( R_H(T) \) determines the actual number of carriers on the arcs. Its decrease with increase of temperature reflects the increase of the widths of the Fermi arcs \( \Delta\varphi(T) \).

At higher temperatures the contribution to \( R_H(T) \) from holes on the Fermi arcs is proven to be rigorous in the limits of both weak and strong magnetic field. In the expression for the Hall coefficient the width of the Fermi arcs can not be small.

Regarding the nature of the electronic pocket, the results are consistent with the notion of its being a particular feature in the spectrum.

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