



Hall effect in the normal state of high T_c cuprates

J. Bok ^{*}, J. Bouvier

Solid State Physics Laboratory—ESPCI, UPR 005 CNRS, 10 rue Vauquelin, 75231 Paris Cedex 05, France

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Abstract

We propose a model for explaining the dependence in temperature of the Hall effect of high T_c cuprates in the normal state, in various materials (LSCO, YBCO, BSCCO, GdBCO). They all show common features: a decrease of the Hall coefficient R_H with temperature and a universal law, when plotting $R_H(T)/R_H(T_0)$ versus T/T_0 where T_0 is defined from experimental results. This behaviour is explained by using the well known electronic band structure of a CuO_2 plane, showing saddle points at the energies E_S in the directions $[0, \pm\pi]$ and $[\pm\pi, 0]$. This is well confirmed by photoemission experiments. We remark that in a magnetic field, for energies $E > E_S$ the carrier orbits are hole-like and for $E < E_S$ they are electron-like, giving opposite contributions to R_H . We are able to fit all experimental results for a wide range of hole doping (p_{h0}) ($0.09 < p_{h0} < 0.30$), and to fit the universal curve. For us $k_B T_0$ is simply $E_F - E_S$, where E_F is the Fermi level varying with the doping.

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1. Introduction

Many measurements of the Hall effect in various high T_c cuprates have been published [1–5]. The main results are the following:

(i) at low temperature T , $R_H \approx 1/p_{h0}e$, where p_{h0} is the hole doping, when T increases R_H decreases, and for highly overdoped samples becomes even negative [1];

(ii) these authors are also able to define a temperature T_0 , where R_H changes its temperature behaviour, and such $R_H(T)/R_H(T_0)$ versus T/T_0 is a universal curve for a large doping domain (from $p_{h0} = 0.10$ to 0.27).

We show that we can explain these results by using the band structure for carriers in the CuO_2 planes. In particular, the existence of hole-like and electron-like constant energy curves, which give contributions of opposite sign to the Hall coefficient R_H . The transport properties explore a range of energy $k_B T$ around the Fermi level, when T is increased more and more carriers are on the electron-like orbits, resulting in a decrease of R_H .

^{*} Corresponding author. Tel.: +33-1-4079-4451; fax: +33-1-4079-4425.

E-mail address: julien.bok@espci.fr (J. Bok).

2. Calculation of the Hall coefficient

The constant energy surfaces of carriers in the CuO₂ planes are well described by the following formula:

$$E_{\mathbf{k}} = -2t(\cos K_x a + \cos K_y a) + 4t' \cos k_x a \cos k_y a + E_F - E_S + 4t' \quad (1)$$

where t is the transfer integral between the first nearest neighbours, t' between the second nearest neighbours, a the lattice parameter, \mathbf{k} the wave vector, E_S the energy of the saddle point (Van Hove singularity, VHS) and E_F is the Fermi level, which varies with the doping [6]. These electronic structures have been intensively studied by angular resolved photoemission (ARPES) in BSCCO [7], and more recently by Ino et al. [8] in LSCO, for a wide range of Strontium doping. From ARPES, experimental values for t and t' are obtained. It is very clearly seen [8] that the Fermi level crosses the saddle points, at E_S , (VHS) for a hole doping of $p_{h0} \approx 0.22$. For $E > E_S$ the orbits are hole-like, and for $E < E_S$ they are electron-like.

To compute the Hall coefficient we use the formula obtained by solving the Boltzmann equation. In the limit of low magnetic fields B , perpendicular to the CuO₂ plane, $\mu B \ll 1$, where μ is an average mobility of the carriers, R_H is given by

$$R_H = \frac{\sigma_{xy}}{\sigma_{xx}^2} \frac{1}{B} \quad (2)$$

where σ_{xy} and σ_{xx} are the components of the conductivity tensor. We follow the approach given by Ong [9]:

$$\sigma_{xy} = \int_{E_{\min}}^{E_{\max}} \left(-\frac{\partial f_0}{\partial E} \right) \sigma_{xy}(E) dE \quad (3)$$

where f_0 is the Fermi Dirac distribution function, E_{\min} and E_{\max} are the bottom and the top of the band, and $\sigma_{xy}(E)$ is σ_{xy} computed on a constant energy surface.

For metals, where $k_B T \ll E_F$, σ_{xy} is usually chosen as $\sigma_{xy} = \sigma_{xy}(E_F)$, computed on the Fermi surface only, this is done by Ong [9]. In our case, $k_B T$ is not small compared to $E_F - E_S$, so when T increases the electron-like orbits as well as the

hole-like orbits are populated. The electron-like orbits give a negative contribution to R_H , so that R_H decreases with temperature. This is our original approach to the problem. To compute R_H , we use the following method: we compute first $\sigma_{xy}(E)$ using the Ong approach. The idea is to draw the \vec{l} curve swept by the vector $\vec{l} = \vec{v}_k \tau_k$ as \vec{k} moves around the constant energy curve (CEC). Then σ_{xy} reduces to

$$\sigma_{xy} = \frac{2e^3}{\hbar^2} A_l B \quad (4)$$

where A_l is the area enclosed by CEC, in the (l_x, l_y) plane. There may be secondary loops in the \vec{l} curve. When the CEC is non-convex, the \vec{l} curve presents several parts where the circulation are opposite (see Ref. [9, Fig. 2]). Then the effective density of carriers that must be taken in computing σ_{xy} is $n'_e = \Gamma n_e$ for the electron-like orbits, with $\Gamma < 1$, and $p'_h = p_h$ for the hole-like orbits, because for the hole-like orbits we can see that the CEC have no non-convex parts. Finally we obtain for the Hall coefficient:

$$R_H = \frac{V}{e} \frac{p_h - b^2 n'_e}{(p_h + b(p_{h0} - p_h))^2} \quad (5)$$

where b is the ratio of the average mobilities of the carriers on the electron- and hole-like orbits. That is the mean value of $\langle \tau/m \rangle$, where τ is the relaxation time and m the effective mass. V is the volume of the unit cell. We adjust the Fermi level so that the total number of carriers p_{h0} remains constant. To compute Γ , we must know the scattering mechanisms and evaluate Γ . Γ was computed by Ong [9] assuming a constant \vec{l} , but this is not valid in our case because \vec{l} is very small near the saddle points (hot spot), both v_k and mainly the relaxation time τ_k are small at this point. So we estimated a much smaller value of Γ , around $\Gamma = 0.2$ for E near E_S and going to $\Gamma = 1$ when E approaches E_{\min} . We choose a function $\Gamma(E)$, varying from $\Gamma(E_S)$ to 1 for $\Gamma(E_{\min})$

$$\Gamma(E) = 1 - \alpha(E - E_{\min})^n$$

$$\alpha = \frac{1 - \Gamma(E_S)}{(E_S - E_{\min})^n}, \quad \text{with } n = 1$$

n'_e , p_h are given by the following formulae:

$$n'_c = \int_{E_{\min}}^{E_S} A_c(E)\Gamma(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \quad (6)$$

$$p_h = \int_{E_S}^{E_{\max}} A_h(E)\Gamma(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \quad (7)$$

$A_c = A_l$ is the area enclosed by the electron-like surfaces for $E < E_S$, $A_h = A_l$ is the area enclosed by the hole-like surfaces for $E > E_S$. E_{\max} is determined in order to only take into account the holes added to the lower half-band. So we obtain for $T = 0$ K the number of free hole carriers p_{h0} for the Hall number $n_H = V/(R_H e) = p_{h0}$. The scattering mechanism being probably the same for the electron and the hole orbits, which are very similar along the (1, 1, 0) direction, then we assume $b = 1$.

3. Results

The results of our calculations and their comparison with the experimental results are given in Figs. 1–4.

When the authors of the experimental results give only the concentration x of doping atoms, and the critical temperature T_c we have to evaluate the actual hole doping p_{h0} using the universal phase diagram of T_c versus hole doping for high T_c superconductors [10].

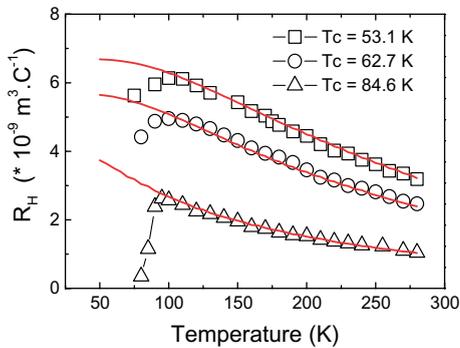


Fig. 1. Symbols: experimental $R_H(T)$ given by Matthey et al. [4] in $\text{GdBa}_2\text{Cu}_3\text{O}_{7-\delta}$. Full lines: theoretical fits. Theoretical hole doping level $p_{h0} = 0.10, 0.12$ and 0.16 for the experimental $T_c = 53.1, 62.7$ and 84.6 K, respectively. The calculations are made with: $t = 0.18$ eV, $t' = 0.04328$ eV, $2t'/t = 0.48$, $\Gamma(E_S) = 0.2$.

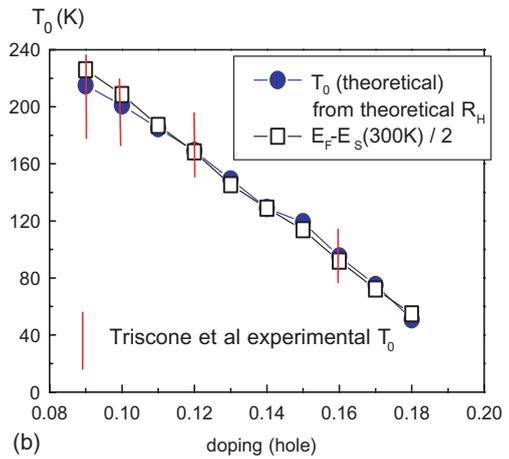
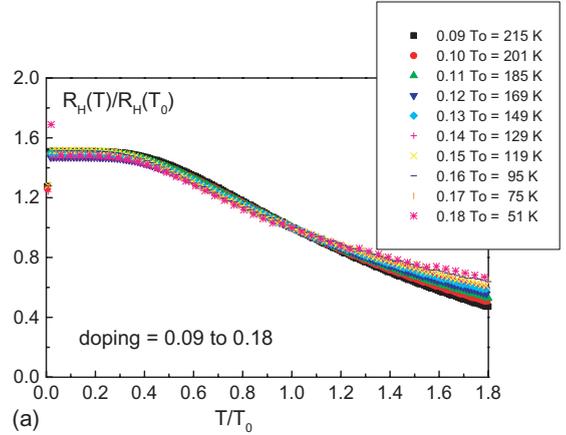


Fig. 2. (a) Universal law $R_H(T)/R_H(T_0)$ versus T/T_0 for various hole doping levels, from 0.09 to 0.18. (b) Calculated T_0 , $2k_B T_0 = E_F - E_S$, compared with the experimental T_0 given by Matthey et al. [4].

For the theoretical results of Figs. 1–3 we use the following parameters: $t = 0.18$ eV, $t' = 0.04328$ eV, $2t'/t = 0.48$, $\Gamma(E_S) = 0.2$. These values of t and t' mean that the shape of the Fermi surfaces changes when we cross the critical doping $p_{h0} \approx 0.22$. This is also seen in the photoemission curves reported by Ino et al. [8].

In Fig. 2, we can see the representation of the universal law $R_H(T)/R_H(T_0)$ versus T/T_0 , where T_0 is defined experimentally by the fact that R_H becomes almost constant above this temperature [1–4]. In our model this temperature is given by $2k_B T_0 = E_F - E_S$, this shows that this universal behaviour is due to the 2D band structure, in

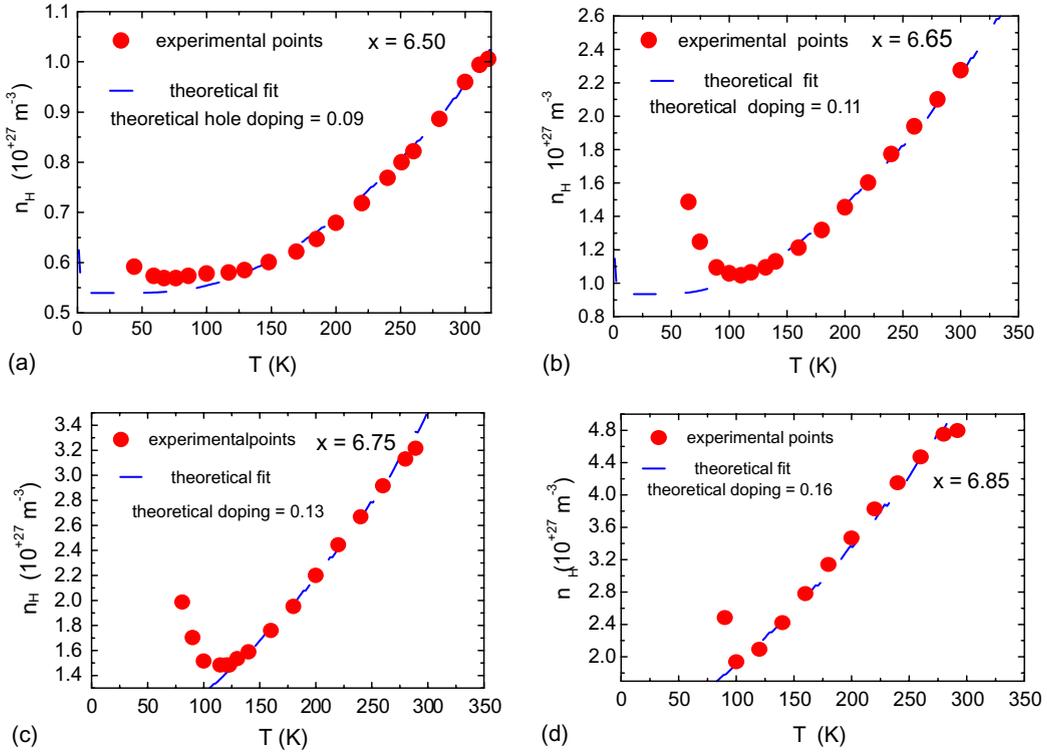


Fig. 3. Filled circles: experimental $n_H(T) = V/(R_H e)$ given by Wuyts et al. [2] in $\text{YBa}_2\text{Cu}_3\text{O}_x$. Dashed lines: theoretical fits. (a) $x = 6.50$, theoretical hole level = 0.09; (b) $x = 6.65$, theoretical hole level = 0.11; (c) $x = 6.75$, theoretical hole level = 0.13; (d) $x = 6.85$, theoretical hole level = 0.16. The calculations are made with: $t = 0.18$ eV, $t' = 0.04328$ eV, $2t'/t = 0.48$, $\Gamma(E_S) = 0.2$, then we obtain the same universal law as in Fig. 2a, expressed in $n_H(T)/n_H(T_0)$.

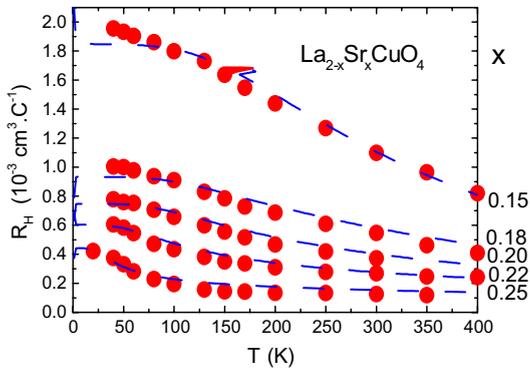


Fig. 4. Filled circles: experimental $R_H(T)$ given by Hwang et al. [1], in polycrystalline $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, for $x = 0.15, 0.18, 0.20, 0.22, 0.25$. Dashed lines: theoretical fits, the theoretical hole levels as the same as the experimental. The calculations are made with: $t = 0.23$ eV, $t' = 0.06$ eV, $2t'/t = 0.52$, $\Gamma(E_S) = 0.1$.

which the shift $E_F - E_S$ is connected to the hole doping. This is very natural in our approach, because the factor $(E_F - E_S)/k_B T$ enters the Fermi-Dirac distribution.

We see that the agreement of our fits with the experiments are excellent. There is a small discrepancy between the values of our theoretical R_H and the experimental values. We think that this is due to the inhomogeneities in the material and to the way to carry out the R_H measurements. This can may be explained by the evaluation of the experimental volume V . We use in our calculation the unit cell volumes:

$$V_{\text{LSCO}} \cong 189 \times 10^{-30} \text{ m}^3 \quad \text{for LSCO}$$

and

$$V_{\text{YBCO}} \cong 174 \times 10^{-30} \text{ m}^3 \quad \text{for YBCO}$$

The experimental value of R_H is determined by the geometrical aspect of the sample (the thickness in particular). This value is evaluated assuming that the current flow is homogeneous throughout the sample, this is not always true. We find a discrepancy between 1.5 and 2 in the case of YBCO [2] and GdBCO [4], a larger discrepancy is found in the case of LSCO [1]. In this later case, the authors find different R_H results for the same doping, with various compounds (single crystals and thin films).

Anyway, adjusting our values for R_H , at low temperature, we can fit many experimental results, for the three different compounds. We also use a rigid band model, where the bandwidth does not change with the doping. This is not exactly the case as shown in the photoemission experiments [8], but the effect is small and does not change our conclusions.

From overdoped to lightly underdoped samples the upturns (in n_H) or downturns (in R_H), at low temperature, in the experimental curves are due to the occurrence of the superconductivity transition.

4. Theoretical results and discussion

We use a theoretical band structure closed to the observed experimental one, but not in the fine details. We take a rigid band structure not varying with the doping, but we know that this variation occurs. Here we make our study with the ratio of transfer integrals of transfer closed to $2t'/t = 0.48$ in order to obtain this special doping $p_{h0} \approx 0.22$ when $E_F = E_S$ as in our previous studies, leading to convincing results [6].

In Figs. 1–4, we give the best fits with the parameters that we need for this. The value of Γ maybe is too big because with our choice of t and t' the curvatures of the CEC are not so pronounced as in reality.

But the aim of this paper is to demonstrate that the temperature dependence of the Hall coefficient is due to the effect of the distribution of the hole carriers in the electron-like energy levels and in the hole-like energy levels with increasing temperature. The results of our model do not change

appreciably if we change slightly our set of parameters.

Γ itself could change with the doping when the band structure varies. Near the optimum hole doped and overdoped systems Γ could decrease due to bigger curvatures of the CEC. In Fig. 5, we show the effect of the decreasing of Γ for a slightly overdoped system. This accounts for the behaviour of $R_H(T)$ in the optimum and slightly overdoped samples, where $R_H(T)$ is very flat and its value is very low closed to zero, and even can goes under zero at low or high temperature [1–3,5]. Theoretically this is due to the proximity of E_F and E_S .

As the curvatures of the orbits increase, Γ goes from positive to negative value. This leads to very low (even negative) values to higher positive values at low T , for $R_H(T)$ in the optimum and overdoped samples.

In Fig. 6, we show the theoretical $R_H(T)$ curves for a set of doping, using the same fit parameters as in Fig. 5, letting $\Gamma(E_S) = 0$. We can see that the general behaviour of $R_H(T)$ is kept.

For very underdoped samples, near the metal–insulator transition our approach is no longer valid. We propose an explanation for the downturns observed in $R_H(T)$ [3,5] based on the localization of the carriers above an energy E_{loc} , due to

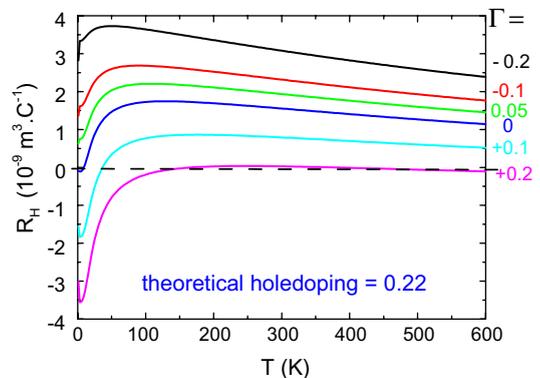


Fig. 5. Theoretical curves of $R_H(T)$ showing the effect of Γ with, from the top to the bottom, the values: $-0.2, -0.1, -0.05, 0, +0.1, +0.2$. The calculations are made with: $t = 0.23$ eV, $t' = 0.0553$ eV, $2t'/t = 0.48$, $V_{YBCO} \cong 174 \times 10^{-30}$ m³, for a theoretical hole doping = 0.22.

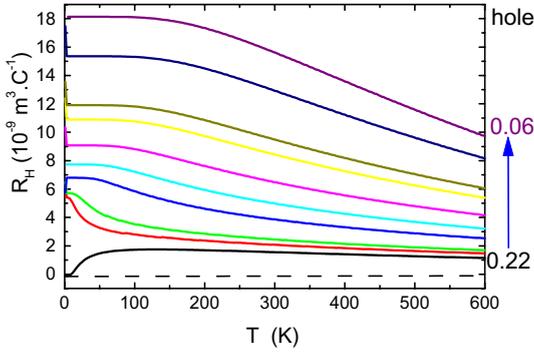


Fig. 6. Theoretical curves of $R_H(T)$ with the same fit parameters of Fig. 5 and with $\Gamma(E_S) = 0$. From the bottom to the top the hole dopings are the following: 0.22, 0.20, 0.19, 0.16, 0.14, 0.12, 0.10, 0.09, 0.07, 0.06.

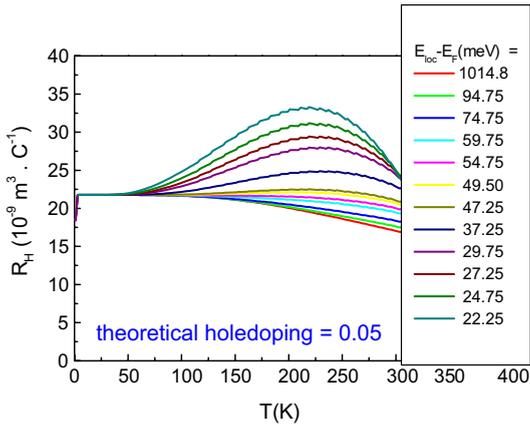


Fig. 7. A localization level (E_{loc}) is introduced in the model to take into account the proximity of the metal–insulator transition is very underdoped sample. The calculation are made for a hole doping of 0.05, with: $t = 0.18$ eV, $t' = 0.04328$ eV, $2t'/t = 0.48$, $\Gamma(E_S) = 0$, $V_{YBCO} \cong 174 \times 10^{-30}$ m³.

the proximity of the metal–insulator transition (see Fig. 7).

From the bottom to the top of the Fig. 7 $E_{loc} - E_F$ varies from the infinity, that means no localization, to +22 meV, effective localization. We see that a strong maximum appears when the localization increases. This is due to the loss of

localized particles, Which do not contribute to transport.

5. Conclusion

In conclusion we find that the electronic structure of CuO_2 planes, with hole-like and electron-like orbits can explain the values of R_H for the high T_c cuprates in the normal state and its temperature behaviour, this conclusion is reinforced by the fact that we obtain a representation of the experimental universal law $R_H(T)/R_H(T_0)$ versus T/T_0 .

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