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# Two-band model for anisotropic Hall effect in high-$T_c$ Y-Ba-Cu-O

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Recent experimental measurements show that for the magnetic field parallel to the $c$ axis and the current in the $a$-$b$ planes, the inverse Hall coefficient $1/R_H$ is $p$ type and linearly temperature dependent; and for the magnetic field in the $a$-$b$ plane, the Hall coefficient is $n$ type and nearly independent of temperature. In this paper, we analyze various possibilities to cause this unusual temperature behavior of $R_H$. A two-band model with an exterior carrier source is proposed to explain the temperature dependences of both the resistivity and Hall number. The connection between this simple model and the high-$T_c$ oxide Y-Ba-Cu-O is discussed.

There has been much interest in the remarkable electronic behavior of the newly discovered high-$T_c$ oxides.[1,2] While much of the theoretical work on high-$T_c$ superconductivity has concentrated on various novel mechanisms causing such a high $T_c$, the normal-state transport properties that reveal much about the anomalous electron behavior of the oxide superconductors are still puzzling and mysterious. Understanding the normal-state electronic behavior may be a necessary step in understanding the novel mechanism for high-$T_c$ superconductivity.

The main features of the normal-state transport in the high-$T_c$ oxides are the strong anisotropies and unusual temperature dependences of some transport coefficients including the resistivity, Hall tensor, and thermoelectric power. Recent experimental measurements of a single crystal of $YBa_2Cu_3O_{7-x}$ as well as ceramic samples show that (1) the in-plane resistivity $\rho_{ab}$ (parallel to the Cu-O plane) is nearly linearly temperature dependent from $T_c$ up to room temperature,[3-5] (2) the out-plane resistivity $\rho_c$ (perpendicular to the Cu-O plane) is at least ten times larger[5] than that of the in-plane direction, and its data can be fit to the formula $\rho_c = aT + b/T$ (Refs. 6-8), (3) the Hall coefficient $R_H$, for the magnetic field parallel to $c$, and the current in the $a$-$b$ planes, is $p$ type and $1/R_H$ is linearly $T$ dependent,[8,9] and (4) the Hall constant, with a magnetic field applied parallel to the $a$-$b$ planes, is $n$ type and nearly independent of temperature.[5]

There have been several theoretical discussions on the linearly $T$-dependent behavior in terms of the traditional electron-phonon scattering mechanism[10-13] or the elastic scattering between the charged bosons (holons) and neutral spinons[6] in the two-dimensional resonating-valence-bond (RVB) picture. Quantitative estimations[6,12,13] for the magnitude of $\rho_{ab}$ have also been given. On the other hand, there are only a few theoretical works on the $c$-axis conductivity $\sigma_c$. Anderson and Zou[6] suggested that $\sigma_c$ with linear temperature dependence is due to the tunneling of holons between the Cu-O planes. Recently, we[14] obtained the same $T$ dependence of $\sigma_c$ based upon the hopping mechanism of charged carriers between the $a$-$b$ planes with emission or absorption of phonons. So far the temperature dependence of the Hall coefficient of Y-Ba-Cu-O has no reasonable explanation even though the signs of the Hall effect are consistent with the band-structure calculation of Allen, Pickett, and Krakauer.[12] Particularly, how to understand the $T$ dependences of both the resistivity and Hall coefficient in terms of a unified physical picture is still an open question. In this paper we first analyze the difficulties of some present theoretical models in accounting for these unusual normal-state transport phenomena, and then propose a possible two-band model for the two-dimensional Cu-O planes with an exterior carrier source to interpret the behaviors of the resistivities and the Hall coefficients along both the $a$-$b$ and $c$ directions.

## I. SINGLE-BAND MODEL

In a single parabolic band picture the conductivity $\sigma$ and Hall constant $R_H$ satisfy the following formulas:

$$\sigma = ne\mu = ne^2\tau/m , \tag{1}$$

and

$$R_H = 1/nec , \tag{2}$$

where $n$ is the charged carrier (electron or hole) density, $e$ is the carrier charge, and $c$ is the speed of light. $\mu = e\tau/m$ is the mobility of the carriers, $m$ is the carrier effective mass, and $1/\tau$ is the carrier scattering rate. In almost all works calculating $\rho_{ab}$ of high-$T_c$ oxides based upon a two-dimensional single-band model for holes in the Cu-O plane, the nearly linear $T$ dependence of $\rho_{ab}$ is obtained by assuming $n$ to be a constant and deducing the approximate relation that $1/\tau \propto T$ from the electron-phonon interaction[10-13] or holon-spinon scattering.[6] On the other hand, the measurement[8] of the Hall constant for a single-crystal Y-Ba-Cu-O shows that for the magnetic field parallel to the $c$ axis, and the current in the $a$-$b$ plane, $R_H$ is inversely proportional to temperature and the charge carriers are holes with $R_H > 0$. The extremely unusual behavior of $R_H$ implies that the carrier density of Y-Ba-Cu-O would increase linearly with temperature. Therefore, starting from a single parabolic band picture, there exists a dilemma on the $T$ dependences of the carrier density $n$ from either $\rho_{ab} \propto T$ or $R_H \propto 1/T$, the former indicating that $n$ is $T$ independent with $1/\tau \propto T$ and the latter implying that $n \propto T$. In Refs. 11 and 12, it is pointed out that

 

for a high-$T_c$ oxide compound with complex band structure the free-electron formulas (1) and (2) no longer hold, and instead a variational solution of the Boltzmann transport equations is applied to analyze the anisotropic transport. However, the calculated result for $R_H$ in Ref. 12 is still $T$ independent and cannot be used to explain the experimental data of $R_H \propto 1/T$. From Eqs. (1) and (2), the unique solution satisfying both $R_H \propto 1/T$ and $\rho_{ab} \propto T$ is that $n \propto T$ and $1/\tau = \alpha T + \beta T^2$ with $\alpha$ and $\beta$ related to the constant term of $\rho_{ab}$ and the slope $d\rho_{ab}/dT$, respectively. Such an expression for $1/\tau$ can be obtained by assuming that $1/\tau = 1/\tau_{e\text{-ph}} + 1/\tau_{e\text{-}e}$, where the electron-phonon scattering rate $1/\tau_{e\text{-ph}}$ has been shown[12,13] to be a nearly linearly $T$ dependent from $T_c$ up to room temperature, and the carrier-carrier scattering ($U$ process) rate $1/\tau_{e\text{-}e}$ is well known to be proportional to $T^2$ at low temperature.[15] So the relation $1/\tau = \alpha T + \beta T^2$ seems to be a reasonable approximation although the coefficient $\beta$ is expected to be small.[15] At the same time, the other assumption, $n \propto T$, is difficult to understand. One may assume that there exist some localized states from which electrons can transfer to the carrier band so that the carrier density can change with temperature. However, it is still difficult to explain the linearly $T$-dependent behavior of the carrier density. Furthermore, the Hall coefficient obtained experimentally[5] for the magnetic field perpendicular to the $c$ axis yields the charged carriers as electrons ($R_H < 0$). The understanding of these phenomena is the main difficulty associated with a two-dimensional single-hole band model.

## II. TWO-BAND MODEL

For a two-band (parabolic) model with both electrons and holes as charged carriers in the Cu-O planes, the in-plane conductivity and Hall coefficient (the magnetic field parallel to $c$ and the current in the $a$-$b$ planes) can be shown to have the following forms:

$$\sigma = pe\mu_p + ne\mu_n , \tag{3}$$

$$R_H = \frac{p\mu_p^2 - n\mu_n^2}{ec(p\mu_p + n\mu_n)^2} , \tag{4}$$

where $p$ and $n$ are the densities of holes and electrons, respectively, and $\mu_p$ and $\mu_n$ are the corresponding mobilities in the $a$-$b$ plane. It seems that there are four independent variables: $p$, $n$, $\mu_p$, and $\mu_n$ in Eqs. (3) and (4), and the solution which satisfies both $\sigma \propto 1/T$ and $R_H \propto 1/T$ has many choices. However, the existence of some physically constrained conditions makes it very difficult to find a physically reasonable solution. Very recently an interesting solution has been suggested by Davidson *et al.*[16] Two very special conditions are assumed under the two-band model: (i) $p = n$ for all temperature, and $p$ (or $n$) is independent of $T$; (ii) $\mu_{p,n} = C(1 \pm D/T)/T$, i.e., the hole and electron mobilities have exactly the same value to order $1/T$, but opposite sign in the next order term $1/T^2$. These assumptions lead to $\sigma = 2neC/T$ and $R_H ec = 2D/nT$. Here we wish to check if this solution can be physically derived. First, the conservation condition of the electron number in a two-band system will give the relation $p - n = \text{const}$. Assumption (i) satisfies this relation if the constant is taken to be zero. Second, let us examine if assumption (ii) is reasonable. When the electron-hole scattering is not considered, the mobilities of electrons and holes usually have the similar $1/T$ dependences due to electron- (hole-) phonon interaction even though their magnitudes can be different due to the disparity of the effective masses of electrons and holes, or $\tau_{e\text{-ph}}$ and $\tau_{h\text{-ph}}$. The origin of the $1/T^2(-1/T^2)$ dependent term in $\mu_p$ ($\mu_n$) is rather difficult to understand. It may come from the electron-hole interaction. Kukkonen and Maldague[17] have studied the effect of the electron-hole scattering on the electrical resistivity of a simple degenerate semimetal. From their calculation with the assumption $\tau_{e\text{-ph}} = \tau_{h\text{-ph}}$, the following expressions for $\mu_p$ and $\mu_n$ are obtained:

$$\mu_p = \frac{e}{pm_h + nm_e}\left[\frac{n(1+m_e/m_h)}{1/\tau_{e\text{-ph}} + 1/\tau_{e\text{-}h}} + (p-n)\tau_{e\text{-ph}}\right] , \tag{5}$$

$$\mu_n = \frac{e}{pm_h + nm_e}\left[\frac{p(1+m_h/m_e)}{1/\tau_{e\text{-ph}} + 1/\tau_{e\text{-}h}} - (p-n)\tau_{e\text{-ph}}\right] , \tag{6}$$

where $1/\tau_{e\text{-}h}$ is the electron-hole scattering rate and is $T^2$ dependent at low temperatures, and $1/\tau_{e\text{-ph}}$ is the electron-phonon or hole-phonon scattering rate. The resistivity for two types of carriers with $\tau_{e\text{-ph}} \neq \tau_{h\text{-ph}}$ has also been studied,[18] but its expression is rather lengthy and will not be presented here. It is easily seen from Eqs. (5) and (6) that if $p = n$ as in Ref. 16 one will get the similar temperature dependences for $\mu_p$ and $\mu_n$. Even in the case of $p \neq n$ and $\tau_{e\text{-ph}} \neq \tau_{h\text{-ph}}$, one still cannot obtain the required $T$ dependences of $\mu_p$ and $\mu_n$ suggested by authors in Ref. 16. Therefore, the assumption (ii) for $\mu_{p,n}$ seem to be artificial, and its physical origin has not been identified. In the following a different model to explain the transport properties in high-$T_c$ Y-Ba-Cu-O will be proposed and discussed.

## III. TWO-BAND WITH EXTERIOR CARRIER SOURCE

We consider a system composed of two parabolic bands, as shown by Fig. 1, and many localized electron states near the Fermi level $E_F$. The electrons and holes in the two bands are the carriers contributing to the conductance and Hall effect. The electrons on the localized energy levels, which make no direct contribution to the transport, can transfer to carrier bands with increasing temperature.

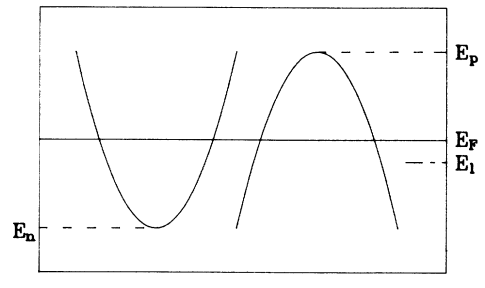


FIG. 1. Two-band model with localized energy levels.

In the present case, Eqs. (3) and (4) remain valid if the original conservation condition of electrons, $n-p=$const, is replaced by $n-p+n_1=$const with $n_1$ the density of the localized electrons.

The electron density for a two-dimensional parabolic band can be calculated by

$$n=(2/d)\sum_{\mathbf{k}} f[(\epsilon_{\mathbf{k}}-E_F)/T]$$

with $d$ the lattice parameter along the $c$ axis ($d=11.7$ Å) for Y-Ba-Cu-O, $\mathbf{k}$ the wave vector, $\epsilon_k=k^2/2m_n$, and $f(x)$ the usual Fermi function. For a two-dimensional case under consideration, the sum over $\mathbf{k}$ in the above formula is easily performed and the result is

$$n=(Tm_e/\pi d)\ln(1+e^{(E_F-E_n)/T}), \tag{7}$$

where $E_n$ is the energy at the bottom of the electron band. Similarly, the hole density for the other two-dimensional parabolic band is

$$p=(Tm_h/\pi d)\ln(1+e^{(E_p-E_F)/T}), \tag{8}$$

where $E_P$ is the energy at the top of the hole band. The density of the localized states is

$$n_1=2N_1 f[(E_1-E_F)/T], \tag{9}$$

where $E_1$ and $N_1$ are, respectively, the energy level and density of the localized states. The Fermi energy $E_F$ in Eqs. (7)–(9) is temperature dependent, and it will be determined by the relation $n-p+n_1=$const. In order to get the expected $T$ dependence of the Hall coefficient, the constant on the right-hand side of the above equation is taken to be $N_1$, from which we get

$$p-n=N_1\tanh[(E_F-E_1)/T], \tag{10}$$

with $E_F-E_1>0$. This choice of the constant implies the assumption that the charge compensation condition $p=n$ for $T\to\infty$, while in Ref. 16 it is assumed that $p=n$ for all temperatures. By using Eqs. (7), (8), and (10), $n$, $p$, and $E_F$ can be determined self-consistently. To see clearly the temperature behaviors of $n$, $p$, and $E_F$, we make some approximations in the following. First, we consider $E_1$ to be close to the Fermi level so that

$$\tanh[(E_F-E_1)/T]\simeq(E_F-E_1)/T$$

when $E_F-E_1<T$ in the range from $T_c$ up to room temperature. Second, we consider that both the degenerate conditions $E_p-E_F\gg T$ and $E_F-E_n\gg T$ are satisfied. So Eqs. (7) and (8) can approximately reduce to

$$\begin{aligned} n&=(m_e/\pi d)(E_F-E_n),\\ p&=(m_h/\pi d)(E_p-E_F). \end{aligned} \tag{11}$$

Under these approximations we obtain the solutions

$$p+n=[m_hE_p-m_eE_n+(m_e-m_h)E_F]/\pi, \tag{12}$$

$$p-n=N_1\left[\frac{E_F(\infty)-E_1}{T^*}\right]\left[\frac{1}{1+T/T^*}\right], \tag{13}$$

$$E_F=E_F(\infty)-\Delta E_F(T), \tag{14}$$

with

$$E_F(\infty)=(m_hE_p+m_eE_n)/(m_h+m_e), \tag{15}$$

$$\Delta E_F(T)=\frac{E_F(\infty)-E_1}{1+T/T^*}, \tag{16}$$

and

$$T^*=\pi dN_1/(m_e+m_h), \tag{17}$$

where $E_F(\infty)$ is the constant term of $E_F$, and $\Delta E_F(T)$ given by (16) depends on the temperature. It is easily seen that $p+n$ is almost a constant independent of temperature, while $p-n$ is sensitive to temperature.

Here we wish to connect the present simple model with the high-$T_c$ oxide compounds Y-Ba-Cu-O. Band-structure calculations[19–21] for Y-Ba-Cu-O indicate the essentially two-dimensional nature of the electron dynamics. The present two-band model may be extracted from the complex band structure for $YBa_2Cu_3O_7$ calculated by Herman, Kasowski, and Hsu,[19] in which an electron valley near point $\Gamma$ and a hole valley near point $M$ can be found. The localized states of electrons may be assumed to come from oxygen vacancies in the Cu-O chain planes of Y-Ba-Cu-O. The oxygen vacancy carries an effective charge $2|e|$ and thus should be able to trap two electrons at low temperature [see Eq. (9)].

In the following we wish to study the $T$ dependences of both $\rho_{ab}$ and $R_H$ of Y-Ba-Cu-O using such a two-band model with an exterior carrier source. However, in order to obtain the expected behaviors of $\rho_{ab}$ and $R_H$, it is necessary to make a further assumption $\mu_p\simeq\mu_n$. From Eqs. (3) and (11), we find the in-plane conductivity

$$\sigma_{ab}=(p+n)e\mu_p. \tag{18}$$

Since from $T_c$ to room temperature the nearly linear $T$ dependence of $\mu_p$ has been shown[12,13] and $p+n$ is almost independent of temperature as discussed above, $\rho_{ab}(=1/\sigma_{ab})$ obtained from Eq. (18) has linear $T$ dependence, which is in agreement with the experimental data of Y-Ba-Cu-O. It is interesting to notice from Eq. (18) that the temperature slope of $\rho_{ab}(=1/\sigma_{ab})$ due to electron-phonon scattering is almost independent of $N_1$ if the variation of $N_1$ is small and does not change the band structure. The measured resistivity is the sum of the phonon-induced $\rho_{ab}$ and the impurity-induced resistivity $\rho_i$. The latter is $T$ independent but increases with the increase of the oxygen deficiencies. These deductions seem to be supported by the experimental data[22] of $\rho_{ab}$ of Y-Ba-Cu-O, in which for several values of oxygen content (more than 6.7 but less than 7), the slopes of $\rho_{ab}$ are almost identical to each other but the extrapolated values at $T=0$ increase upon decreasing the oxygen content or creating more oxygen vacancies.

On the other hand, with a symmetry of the mobilities, $\mu_p\simeq\mu_n$, the Hall coefficient in Eq. (4) reduces to the following form:

$$R_H=\frac{p-n}{(p+n)^2}[1+4pn(1-\mu_n/\mu_p)/(p^2-n^2)]. \tag{19}$$

Substituting (11), (13), and (15) into (19) and neglecting the second term on the right-hand side of the above for-

mula, we obtain the expression for the Hall number ($n_H = 1/R_H ec$) as

$$n_H = n_H(0)(1 + T/T^*) , \tag{20}$$

with

$$n_H(0) = \pi(p+n)^2/\{(m_e+m_h)[E_F(\infty) - E_1]\} . \tag{21}$$

The sign of $n_H(0)$ depends on the position of the localized level $E_1$ relative to $E_F(\infty)$. It is positive when the localized energy levels are below $E_F(\infty)$. Equation (20) gives the linear temperature dependence of $n_H$ for the magnetic field parallel to $c$ and the current in the $a$-$b$ planes. This result is in qualitative agreement with the recent experimental data of both single-crystal[8] and ceramic[9] samples of Y-Ba-Cu-O. It is easily seen from Eqs. (17) and (20) that the slope $dn_H/dT$ is inversely proportional to $N_1$, but this is valid only when the second term on the right-hand side of Eq. (19) can be neglected. This deduction indicates that the larger the number of the oxygen defects ($\propto N_1$), the smaller the slope $dn_H/dT$. It is also qualitatively consistent with the experimental data of Ref. 9 in which the slope $dn_H/dT$ decreases upon increasing the number of oxygen vacancies or decreasing oxygen vapor pressure.

Here we wish to give some rough estimations for $n_H$, $n$, and $p$. If we choose $E_p - E_n \simeq 2000$ K, $[E_F(\infty) - E_1]/T^* \simeq 0.5$, $N_1 = 2\times10^{21}$ cm$^{-3}$, and $m_e \simeq m_h \simeq 5m_0$ with $m_0$ the free-electron mass, we obtain from Eqs. (12), (13), and (17) that $T^* \simeq 650$ K, $p+n = 3\times10^{21}$ cm$^{-3}$, $p-n \simeq 0.87\times10^{21}$ cm$^{-3}$ for $T = 100$ K and $p-n \simeq 0.68\times10^{21}$ cm$^{-3}$ for $T = 300$ K. It follows that $n_H$ increases linearly from $1\times10^{22}$ cm$^{-3}$ at $T_c$ to $1.3\times10^{22}$ cm$^{-3}$ at room temperature. These Hall numbers can be compared with the experimental data of recent Hall coefficient measurements.[9]

For the magnetic field parallel to the $a$ axis in the $a$-$b$ plane and the current in the $b$-$c$ planes, Eqs. (4) and (18) are no longer valid due to the anisotropic mobilities of electrons and holes. For such a case we have derived the expression for $R_H$ as

$$R_H = \frac{p\mu_p\mu_{pc} - n\mu_n\mu_{nc}}{(p\mu_p + n\mu_n)(p\mu_{pc} + n\mu_{nc})}\frac{1}{ec} , \tag{22}$$

where $\mu_p$ and $\mu_n$ are the in-plane mobilities of holes and electrons, respectively. $\mu_{pc}$ and $\mu_{nc}$ are corresponding out-plane mobilities, and they have the similar linear $T$ dependences which can be obtained by the phonon-assisted tunneling process.[14] Under the same approximation $\mu_p \simeq \mu_n$ we obtain

$$R_H = \frac{p\mu_{pc} - n\mu_{nc}}{(p+n)(p\mu_{pc} + n\mu_{nc})}\frac{1}{ec} . \tag{23}$$

In Ref. 14 we have proposed that the conductivity parallel to $c$ axis originates from the phonon-assisted tunneling process of electrons or holes. In general, the hopping rates of electrons and holes are different. If we assume $\mu_{nc} > \mu_{pc}$, $R_H$ will be negative and will slowly vary with temperature, and $n_H$ will be almost a constant, that is, larger than $p+n$. The measured Hall constant, with a magnetic field applied parallel to the $a$-$b$ plane, is $n$ type and nearly independent of temperature.[5] This experimental result can be explained in terms of the present theoretical model by assuming a larger out-plane mobility for electrons and a smaller one for holes.

In summary, we have shown that a two-band model for the Cu-O planes with an exterior carrier source can be used to explain the temperature dependences of both $\rho_{ab}$ and the anisotropic $R_H$ in the high-$T_c$ Y-Ba-Cu-O compound as long as two assumptions are made: (i) $\mu_p \simeq \mu_n$ and $\mu_{pc} < \mu_{nc}$; (ii) the charge compensation condition $p = n$ for $T \to \infty$.

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