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Single-band model of normal-state transport properties of high-T_c copper oxides

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In order to account for linear temperature dependences of the in-plane resistivity and Hall carrier density observed in $YBa_2Cu_3O_{7-y}$ and other high-T_c oxides, we have proposed a single-band model consisting of both extended states and localized ones, separated by a mobility edge. The scattering of the extended holes, which carry the current, by the localized electrons is assumed to be the dominant transport mechanism.

The normal-state properties of Cu-O superconductors are as perplexing as their high transition temperatures. There are two striking anomalies in the "normal" transport properties. One is the linear temperature dependence of the normal-state resistivity ρ in all families of the high-T_c copper oxides, the other is the increase in the reciprocal Hall coefficient $1/R_H$ with temperature, and in particular, the relation $1/R_H=\beta T$ found in the metallic normal phase of the $YBa_2Cu_3O_{7-y}$ (hereafter referred to as Y-Ba-Cu-O) systems. Quite a few types of transport mechanisms have been proposed to account for both linear relations: $\rho\propto T$ and $1/R_H=\beta T$ observed in Y-Ba-Cu-O, but neither one to date can be considered generally accepted.

The remarkable linear ρ-vs-T behavior has been found over a large temperature range. It was reported[1] that in ceramic samples of Y-Ba-Cu-O there is a linear law $\rho\propto T$ from T_c (=90 K) to 600 K, above which a deviation from linearity is due only to the loss of oxygen. The transport-anisotropy measurements[2] on single crystals of Y-Ba-Cu-O show that the linearly T-dependent resistivity ρ_{ab} occurs in the a-b planes (basal Cu-O planes). This linear resistivity easily brings to mind the conventional electron-phonon interaction of metallic conduction.[3-6] According to the Bloch-Grüneisen (BG) treatment of electron-phonon scattering, a linear temperature law for the resistivity holds above a characteristic temperature T^*, and the nearly-linear regime can extend down to $T^*/4$. For a conventional metal with a high density of electrons, T^* is equal to the Debye temperature Θ_D. But if the density of carriers is low enough or the Fermi wave vector k_F is sufficiently small compared to the reciprocal-lattice vector, which is the case for Y-Ba-Cu-O and other high-T_c oxides,[3] $T^*=2p_Fs/k_B$ (p_F denoting the Fermi momentum and s the speed of sound) can be substantially smaller than Θ_D. It was shown[6] that the observed linear ρ-vs-T behavior for Y-Ba-Cu-O with $T_c=90$ K is consistent with a fit to BG theory using $T^*=200$ K. However, the higher T_c and the lower T^* would make it difficult to observe the nonlinear behavior predicted by BG theory of electron-phonon scattering.

Very recently, the resistivities of single crystals of $Bi_{2+x}Sr_{2-y}CuO_{6\pm\delta}$, with $T_c=6.5$–8.5 K, have been measured.[7] The striking behavior is that the in-plane resistivity ρ_{ab} varies linearly with temperature from just above T_c ($\cong 7$ K) to 700 K. This result, that the linear T dependence remains still unchanged as the temperature decreases down to 7 K, seems to be unfavorable to the electron-phonon mechanism. Although a BG fit for $T^*=35$ K can describe the experimental data well,[7] it is very difficult to explain such a small value of T^* in terms of electron-phonon scattering. Several non-phonon transport mechanisms have predicted $\rho_{ab}\propto T$, including the resonating-valence-bond (RVB) model,[8,9] the quantum-percolation model,[10] and the marginal-Fermi-liquid model.[11]

In the RVB theory, the T dependence of ρ_{ab} arises from holon-spinon scattering. One point of view is that the scattering of the holons, which carry the current, by the spinons would lead to a linear T dependence,[8] while another viewpoint is that the lowest-order process for holon-spinon scattering should give $\rho_{ab}\propto T^{3/2}$.[12] It was reported[11] that the marginal-Fermi-liquid model, which is based upon a single hypothesis, can explain a series of anomalies in the normal state, except for the temperature behavior of $R_H(T)$. However, this model is phenomenological, and lacks a clear microscopic interpretation.

On the other hand, the linear temperature behavior of the Hall carrier density n_H (defined as $1/R_He$) of Y-Ba-Cu-O, has been observed in ceramic samples,[13] thin films,[14] and single crystals.[15] Experimental measurements[16-18] on other high-T_c oxides, including Bi- and Tl-based compounds, and $La_{2-x}Sr_xCuO_4$, show that n_H increases with temperature in a manner similar to that observed in the Y-Ba-Cu-O systems. Furthermore, it has been reported[19] that for each separate compound, the T dependence of n_H is suppressed whenever T_c is reduced by chemical doping, indicating a distinct correlation between the characteristic n_H-vs-T profile and high-T_c behavior. Thus, the T dependence of n_H, together with the ubiquitous linear ρ_{ab}-vs-T behavior, should be regarded as properties intrinsic to the high-T_c copper oxides.

Owing to the difficulty in explaining the Hall effect in terms of a simple single-band model,[20] various two-band models have been proposed to account for the n_H-vs-T be-

havior.[20,21] These models, however, often depend upon certain special band structures or need some particular compensation conditions. The lack of universal applicability to all high-T_c systems is a principle weakness of two-band models.

In this paper we propose a single-band model with a mobility edge to account for both linear dependences: $\rho_{ab} \propto T$ and $n_H = \beta T$. Our model includes two basic assumptions. One is that the single band contains both extended states and localized ones, separated by the mobility edge; the other is that the scattering, by localized electrons, of the extended holes, which carry the current, is the dominant transport mechanism. Transport measurements on single crystals and oriented films of Y-Ba-Cu-O, as well as other high-T_c oxides, have shown that there exists a metal-insulator transition with decreasing carrier density by chemically doping[19] or by changing oxygen content.[22] Measurements of the Pauli susceptibility and the electrical conductivity for Y-Ba-Cu-O with substitution of Ni, Fe, and Zn for Cu indicate that the Fermi energy shifts towards the mobility edge with an increasing degree of substitution.[23] These experimental results undoubtedly support the first assumption in the present model. On the other hand, it is generally accepted that in the high-T_c systems strong Coulomb interaction between carriers would play an important role in both the normal and superconducting states. The scattering between the extended carriers (holes), however, does not contribute to the resistivity when the carrier density is small enough so that umklapp scattering can be neglected, which is the case for Y-Ba-Cu-O as well as other high-T_c oxides. So, it is undoubtedly logical to consider the hole–localized-electron scattering as the dominant transport mechanism.

In the single-band model under consideration the charge carriers are the holes on the extended states, and the hole density p is just equal to the Hall carrier density n_H. For a two-dimensional hole band with a quadratic dispersion relation, the number of holes per unit volume is[20]

$$p = n_H = (m_h k_B T/\pi\hbar^2 c)\ln\{1+\exp[(E_c-\mu)/k_B T]\}\,, \quad (1)$$

where m_h is the effective mass of the extended holes, c is the lattice parameter along the c axis, E_c is the mobility edge, and the chemical potential μ is temperature dependent. On the other hand, the localized-electron density n_l can be calculated by $n_l = \int_{E>E_c} dE N(E) f(E)$, where $f(E) = 1/\{\exp[(E-\mu)/k_B T]+1\}$ is the usual Fermi function, and $N(E)$ is the localized-electron density of states. Assuming that $N(E) = N(E_c)$ is a constant, we obtain

$$n_l = k_B T N(E_c)\ln\{1+\exp[(\mu-E_c)/k_B T]\}\,. \quad (2)$$

The total number of electrons which occupy both the extended states below E_c and the localized states above E_c is a constant, independent of temperature. The conservation condition requires

$$n_l(T) - p(T) = n_l(T=0) - p(T=0) \quad (3)$$

for all temperatures. This equation is used in determining the chemical potential $\mu(T)$.

Measurements on high-quality samples of Y-Ba-Cu-O have shown that the linear n_H-vs-T data have an extrapolated intercept that approaches the origin at $T=0$, indicating $p = n_H = \beta T$. In order to make Eq. (1) satisfy the relation $p = \beta T$, the factor $(E_c-\mu)/k_B T$, which appears on the right-hand side of (1), should be taken to be a fixed constant γ, i.e.,

$$\mu = E_c - \gamma k_B T\,, \quad (4)$$

from which it is easily seen that the chemical potential varies linearly with T and approaches the mobility edge at $T=0$. In the ground state of the system, due to $\mu(T=0) = E_c$, all extended states are filled by electrons and all localized states are empty, i.e., $p(0) = n_l(0) = 0$. So, at finite temperatures, the conservation condition (3) reduces to $p(T) = n_l(T)$. On combining it with (1) and (2),

$$(m_h/\pi\hbar^2 c)\ln(1+e^{\gamma}) = N(E_c)\ln(1+e^{-\gamma})\,, \quad (5)$$

which is the equation determining the value of γ. Making use of Eqs. (1) and (4), we can obtain

$$n_H = \beta T \quad (6)$$

with the slope as $\beta = (m_h k_B/\pi\hbar^2 c)\ln(1+e^{\gamma})$. This result is suitable for the case of a stoichiometric Y-Ba-Cu-O system.

For off-stoichiometry samples with oxygen deficiency or substitution for Cu, the carrier density decreases when either the number of oxygen vacancies or the degree of substitution increases. This decrease implies that $\mu(0)$ increases and goes away from the mobility edge [$\mu(0) > E_c$], so that $p(0) = 0$ and $n_l(0) = N(E_c)[\mu(0) - E_c]$ at $T=0$. In this case the conservation condition (3) becomes

$$k_B T(m_h/\pi\hbar^2 c)\ln(1+e^{\gamma}) = k_B T N(E_c)\ln(1+e^{-\gamma}) - n_l(0)\,, \quad (7)$$

where $\gamma = \{[E_c-\mu(0)]/k_B T\}$ is temperature dependent. From (1) and (7) we have calculated γ and n_H as functions of temperature for several values of $n_l(0)$. The calculated result for the T dependence of n_H is shown in Fig. 1, in which curve A is for $n_l(0) = 0$ [$\mu(0) = E_c$] and curves B–E are for the systems with successively higher value of $n_l(0)$. We see that as n_H decreases with increasing values of $\mu(0)$ or $n_l(0)$, the slope dn_H/dT also decreases. This behavior is consistent qualitatively with the experimental data of Co-doped samples of Y-Ba-Cu-O,[19] as well as single-crystal $Bi_2Sr_2CaCu_2O_{8-x}$ with variable oxygen content.[22]

After considering the $n_H = \beta T$ relation, we now turn our attention to the scattering of the extended holes by the localized electrons to account for the linear $\rho \propto T$ behavior. The resistivity due to the hole-electron scattering can be calculated either from the Boltzmann equation using a variational approach, or from the balance equation or memory-function approach. Following the analysis described in Ref. 12, easily modified for extended holes scattering off localized electrons, we obtain the expression

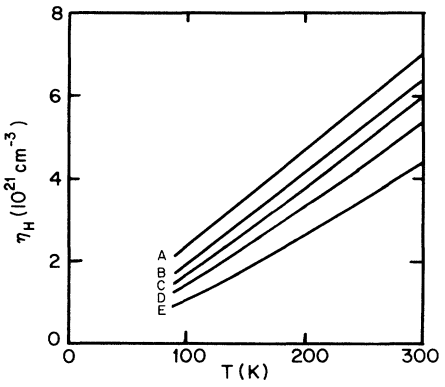

FIG. 1. Temperature dependence of the Hall carrier density n_H calculated from (1) and (7) with $m_h=5m_e$ and $N(E_c)\pi c/m_h=10^3$. Curves A, B, C, D, and E refer to $n_l(0)=0$, 4.5×10^{21}, 9.0×10^{21}, 1.8×10^{22}, and 4.5×10^{22} cm^{-3}, respectively.

for the resistivity as

$$\rho_{ab}=\frac{-\hbar^2t^2}{2ce^2p^2k_BT}\int_0^\infty d\omega\bar{n}_+(\omega)\bar{n}_+(-\omega)\times\int_0^\infty q^3dq\chi_-^h(\mathbf{q},\omega)\chi_-^l(\omega)\,, \quad (8)$$

where t is the matrix element for the hole-electron scattering, taken to be independent of momentum and energy. $\bar{n}_+(\omega)=1/[\exp(\hbar\omega/k_BT)-1]$ is the Bose function at zero chemical potential. $\chi_-^h(q,\omega)$ is the two-dimensional Fermi polarizability for the extended holes,

$$\chi_-^h(\mathbf{q},\omega)=\int\frac{d\mathbf{k}^2}{(2\pi)^2}[f(\epsilon_{\mathbf{k}+\mathbf{q}})-f(\epsilon_{\mathbf{k}})]\times\delta(\hbar\omega+\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})\,, \quad (9)$$

and $\chi_-^l(\omega)$ is the Fermi polarizability for the localized electrons,

$$\chi_-^l(\omega)=\sum_{E,E'>E_c}[f(E)-f(E')]\delta(\hbar\omega+E-E')\,. \quad (10)$$

The two-dimensional Fermi polarizability $\chi_-^h(q,\omega)$ has been calculated and its explicit expression can be found in Ref. 5. For $[E_c-\mu(T)]\gg k_BT$ and $\omega\ll v_Fq$, the Fermi polarizability has the following approximate expression:

$$\chi_-^h(q,\omega)\cong(m_h\omega/\pi^2\hbar^2qv_F)\Theta(k_F-q)\,, \quad (11)$$

where $v_F=\hbar k_F/m_h$ is the Fermi velocity of the hole gas, and $\Theta(x)$ is the unit step function. At the same time, in the case when $[E_c-\mu(T)]\gg k_BT$, $f(E)$ for $E>E_c$ can be approximated by the classical Boltzmann distribution function so that

$$\chi_-^l(\omega)\cong N(E_c)n_l(T)[1-\exp(-\hbar\omega/k_BT)]\,. \quad (12)$$

Substituting (11) and (12) into (8), and taking into account that

$$\hbar^2\int_0^\infty d\omega\,\omega\bar{n}_+(\omega)=\pi^2k_B^2T^2/6\,,$$

and

$$\int_0^\infty dq(q^2/v_F)\Theta(k_F-q)=m_hk_F^2/3\hbar\cong2\pi cm_hp(T)/3\hbar\,, \quad (13)$$

we finally obtain the expression for the resistivity as

$$\rho_{ab}=\alpha Tn_l(T)/p(T) \quad (14)$$

with $\alpha=\pi k_Bt^2m_h^2N(E_c)/(18e^2\hbar^3)$ as a constant. For the stoichiometric Y-Ba-Cu-O system, as discussed above, $n_l(T)=p(T)$, so that from (14) the resistivity is given by $\rho_{ab}=\alpha T$. This purely linear temperature dependence, arising from hole-electron scattering, can extend down to any low temperature so long as the condition $\gamma\gg1$ is satisfied. For the off-stoichiometry system the situation is a bit different. Since $n_l(T)=p(T)+n_l(0)$, as given by (7), the expression (14) for the resistivity becomes

$$\rho_{ab}=\alpha T+\alpha n_l(0)[T/p(T)]\,. \quad (15)$$

It is notable that besides the linear term αT, ρ_{ab} in (15) also contains a term proportional to $T/p(T)$. For small values of $n_l(0)$, $n_H(T)$ (curve B in Fig. 1) is still linearly T dependent. So $T/p(T)$ is independent of temperature, and ρ_{ab} is equal to αT plus a constant term, this constant being proportional to $n_l(0)$. As is shown in Fig. 1, $n_H(T)$ [or $p(T)$] deviates gradually from linearity with the continuous increase of $n_l(0)$. When fitting $n_H(T)\propto T^\delta$ to curves C-E in Fig. 1, we find that $\delta\cong1$ at higher temperatures and $\delta>1$ at lower temperatures, and the lower the temperature, the more obviously δ deviates from unity. It then follows that $T/p(T)$, proportional to $T^{1-\delta}$, will increase with decreasing temperature, and the second term on the right-hand side of (15) will provide insulating (or semiconductive) temperature behavior for ρ_{ab}, particularly at low temperatures. Furthermore, as $n_l(0)/p(T)\gg1$, the semiconductive behavior will dominate $\rho_{ab}(T)$.

Making use of the previous calculated results for $\gamma(T)$ and $n_H(T)$, from (15) we have evaluated ρ_{ab} as a function of temperature for several values of $n_l(0)$; this is shown in Fig. 2. We see that there is a transition from metallic-to-insulating behavior with increasing values of $n_l(0)$ or $\mu(0)$. It is interesting to notice from Figs. 1 and 2 that as the system is driven through the metal-"insulator" transition, n_H decreases but continues to have nearly linear T dependence. This behavior has been reported by Briceno

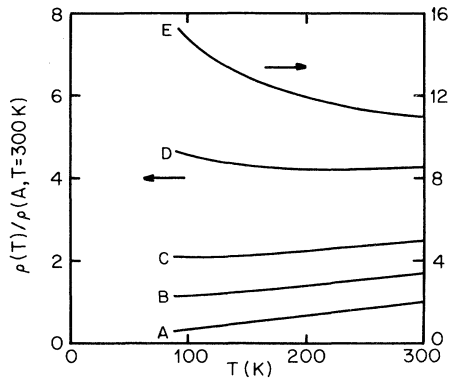

FIG. 2. Temperature dependence of the resistivity at $T=300$ K and $n_l(0)=0$ calculated from (15), together with (1) and (7), for several values of $n_l(0)$. All parameters are the same as those in Fig. 1.

and Zettl[22] on single-crystal $Bi_2Sr_2CaCu_2O_{8-x}$ with different oxygen content. The agreement with experimental data indicates the success of the present model in explaining unusual normal-state transport properties of the high-T_c copper oxides. It is expected that the hole-electron interaction may also be correlated with the mechanism for superconductive pairing.

In summary, we have proposed a single-band model consisting of both extended and localized states to account for $n_H = \beta T$ and $\rho_{ab} = \alpha T$ observed in Y-Ba-Cu-O and other high-T_c oxides. The change of $\rho_{ab}(T)$ from metallic-to-insulating behavior can also be explained in terms of the present model.

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