Model for c-axis resistivity of cuprate superconductors

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On the basis of the structural features and correlation effects that exist in the cuprate systems it has been argued that the Cu $3d_{3z^2-r^2}$ orbitals are reasonably well suited for the transport along the c axis. On the same ground it has also been argued that the band of the out-of-plane states that involves the Cu $3d_{3z^2-r^2}$ orbitals lies higher than the occupied in-plane states by an amount $W(n)$ that decreases with the carrier density (n) so as to vanish beyond a certain critical concentration n_0. Phenomenological arguments are used to obtain expressions for ρ_c within the Boltzmann framework for all n. When $n<n_0$, ρ_c shows a semiconducting behavior for $T<W$ and a metallic behavior for $T>W$. For $n>n_0$ it turns out that ρ_c is metallic for all T. The observed temperature dependence of ρ_c is explained reasonably by the present model for a number of samples of $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{7-y}$, and $Bi_2Sr_{2-x}La_xCuO_y$ with different dopings. The values of $W(n)$ estimated for these samples support one of the main features of our model that this gap $W(n)$ decreases with increasing n. [S0163-1829(98)08909-7]

I. INTRODUCTION

The behavior of the c-direction resistivity $[\rho_c(T)]$ of the high-temperature cuprate superconductors is in general qualitatively different from that of the ab-plane resistivity $[\rho_{ab}(T)]$ of these materials[1–19] The main difference lies in the appearance of a semiconducting behavior in ρ_c $(d\rho_c/dT<0)$ below a certain temperature in the low and optimally doped systems while ρ_{ab} continues to show metallic behavior $(d\rho_{ab}/dT>0)$.[1,4,11,12,14,15] Such a striking difference in T dependence of ρ_c and ρ_{ab} presents a challenging problem. In the literature, a number of attempts have been made to explain this difference in behavior of $\rho_c(T)$ from $\rho_{ab}(T)$.[20–36] The main models that have been proposed by different authors are based on assumptions of Boltzmann theory of three-dimensional anisotropic systems,[20–22] dynamical dephasing,[23] superconducting fluctuations,[24] static and dynamic interlayer disorder,[25] suppression of interlayer tunneling due to in-plane inelastic scattering,[26] resonant valence bond (RVB) approach,[27–29] marginal Fermi liquid (MFL) concept,[30] incoherent hopping between Luttinger liquids,[31,32] tunneling through localized impurity centers,[33] joint effect of in-plane dephasing and c-axis ''barrier'' scattering,[34] coherent motion of polarons,[35] and effect of electron-phonon and strong anharmonic interactions.[36] These assumptions are in general considerably different from each other, and we are still far from the realization of a clear picture of the origin of ρ_c. It appears that some crucial factors that may be central to the c-direction transport in cuprate superconductors are not captured in the existing models. Under such circumstances it is useful to attempt a phenomenological method for the c-axis transport based on our knowledge of the Cu $3d$ and O $2p$ orbitals that are involved in the charge transport.

In the existing theories of c-axis resistivity the main consideration is based on the hybridized Cu $3d_{x^2-y^2}$-O $2p_{x,y}$ orbitals.[20–36] In cuprate systems there are Cu $3d_{3z^2-r^2}$ orbitals also for which the electronic charge distribution is directed for the most part normal to the plane.[37–46] Therefore for transport along the c axis the Cu $3d_{3z^2-r^2}$ orbitals appear to be more suitable than the orbitals Cu $3d_{x^2-y^2}$ and O $2p_{x,y}$ that lie in the ab plane. In order to clarify this point, let r_1 be the quantum-mechanically-averaged extension of the O $2p_{x,y}$ orbital and r_2 that of the Cu $3d_{3z^2-r^2}$ orbital along the nearest apical oxygen orbital O $2p_y$. Then the overlap matrix element between the O $2p_{x,y}$ orbitals of neighboring planes will be phenomenologically proportional to $p_1=e^{-2d/r_1}$ where d is interlayer separation. Similarly the overlap matrix element between the Cu $3d_{3z^2-r^2}$ orbitals of the neighboring planes will be proportional to p_2e^{-2d/r_2}. This means that p_2/p_1 will be $e^{2d/R}$ where $R=r_1r_2/(r_2-r_1)$. Very recently, Nakamura *et al.*[13] have studied the variation of ρ_c with d in the $La_{1.855}Sr_{0.145}CuO_4$ system under hydrostatic pressure upto 7.3 GPa. From their study we find that the hopping parameter along c axis varies like e^{-2d/Λ_n} with $\Lambda_n=0.5$ Å. Since this value of Λ_n is based on experimental observations, Λ_n may be treated as a certain kind of average of r_1 and r_2. When this is so, we may take $r_1<\Lambda_n$, and $r_2>\Lambda_n$. Thus, $r_1<0.5$ Å. Since the Cu $3d_{3z^2-r^2}$ orbital is directed along the c axis, we expect r_2 to be significantly larger than r_1. However, even if r_2 is 10% larger than r_1, $e^{2d/R}>10^2$. This means hopping along the c direction will be negligible via the O $2p_{x,y}$ orbitals as compared to that via the Cu $3d_{3z^2-r^2}$ orbitals. This viewpoint is supported by several experimental observations[43,46] also. Using polarization-dependent L_3-absorption measurements on the $La_{2-x}Sr_xCuO_4$ system, Chen *et al.*[43] have found that the number of doping induced apical O $2p_z$ holes increases with x after $x\approx0.10$. Combining this result with the fact that the O $2p_z$ orbital can hybrid-

ize significantly with the Cu $3d_{3z^2-r^2}$ orbital only,[37] we may say that the Cu $3d_{3z^2-r^2}$ orbitals are involved in the hopping along c axis. A similar conclusion is drawn by Srivastava *et al.*[46] on the basis of the polarization-dependent L_3-absorption measurements on the Tl2212 systems. Under these circumstances, it is plausible to assume that the interplanar motion of electrons in cuprate systems occurs via the Cu $3d_{3z^2-r^2}$ and apical O $2p_z$ orbitals, and that the O $2p_{x,y}$ orbitals take no part in the interplanar hopping process. The aim of the present article is to develop phenomenologically a model on these lines and study its outcome for the c-axis resistivity.

II. FEATURES OF THE IN-PLANE AND OUT-OF-PLANE STATES

A. Elucidation of the essential points using a CuO_2 cluster

In order to see how the in-plane and out-of-plane states arise in a cuprate systems we consider a three-atom cluster CuO_2. One of the atoms of this cluster is a Cu atom having $3d_{x^2-y^2}$ and $3d_{3z^2-r^2}$ orbitals of energies ϵ_{d1} and ϵ_{d2}, respectively. The second atom is an oxygen atom with the orbital $2p_x$ of energy ϵ_{px}. This atom lies in the ab plane at a distance of $a/2$ from the Cu atom where a is the shortest Cu-Cu distance in the plane. The O $2p_x$ orbital hybridizes with the Cu $3d_{x^2-y^2}$ orbitals with t_x as the overlap matrix element. At the same time the O $2p_x$ orbital hybridizes with the Cu $3d_{3z^2-r^2}$ orbital also with t_{xz} as the overlap matrix element. The third atom is also an oxygen atom but it lies along the c axis with the orbital $2p_z$ of energy ϵ_{pz}. This orbital hybridizes with the Cu $3d_{3z^2-r^2}$ orbital with t_z as the overlap matrix element. The Hamiltonian corresponding to this three-atom cluster is

$$\begin{aligned} K=\sum_s\ & [\epsilon_{d1}d_{1s}^\dagger d_{1s}+\epsilon_{d_2}d_{2s}^\dagger d_{2s}+\epsilon_{p_x}p_{xs}^\dagger p_{xs}+\epsilon_{p_z}p_{zs}^\dagger p_{zs} \\ & +t_x(d_{1s}^\dagger p_{xs}+p_{xs}^\dagger d_{1s})+t_z(d_{2s}^\dagger p_{zs}+p_{zs}^\dagger d_{2s}) \\ & +t_{xz}(d_{2s}^\dagger p_{xs}+p_{xs}^\dagger d_{2s})]+U\sum_{i=1,2} n_{i\uparrow}n_{i\downarrow} \\ & +U'\sum_{s,s'} n_{1s}n_{2s'}. \end{aligned} \tag{1}$$

Here s denotes the electron spin. $d_{1s}^\dagger$ and d_{1s} are creation and annihilation operators of the hole corresponding to the Cu $3d_{x^2-y^2}$ orbital. $d_{2s}^\dagger$ and d_{2s} are creation and annihilation operators of the hole corresponding to the Cu $3d_{3z^2-r^2}$ orbital. $p_{xs}^\dagger$ and p_{xs} are creation and annihilation operators of the hole corresponding to the O $2p_x$ orbital, and $p_{zs}^\dagger$ and p_{zs} are creation and annihilation operators of the hole corresponding to the O $2p_z$ orbital. $n_{is}=d_{is}^\dagger d_{is}$ is the number operator corresponding to the $i=\{x^2-y^2, 3z^2-r^2\}$ orbitals and spin s. U is the on-site Coulomb repulsion when two holes are either in the Cu $3d_{x^2-y^2}$ or in the Cu $3d_{3z^2-r^2}$ orbitals. U' is the Coulomb interaction when one hole is in the Cu $3d_{x^2-y^2}$ orbital, while the other is in the Cu $3d_{3z^2-r^2}$ orbital. $U'=U-U_H$, where U_H is the energy responsible for Hund's rule.

The Hamiltonian of Eq. (1) describes the main features of the basic units of a cuprate system. In this regard it may be noted that we have not considered the O $2p_y$ orbital. While inclusion of this orbital is required for a quantitative understanding of the state, there will be no effect of this simplification on the main features of our model.

With an approximate diagonalization of K in Eq. (1), we obtain two sets of states. The first consists of primarily the hybridized Cu $3d_{x^2-y^2}$-O $2p_x$ and Cu $3d_{3z^2-r^2}$-O $2p_x$ orbitals. We call this set of states ''in-plane'' states. The other set of states described by K comprises the hybridized Cu $3d_{3z^2-r^2}$-O $2p_z$ orbitals. We call this set of states ''out-of-plane'' states. The out-of-plane states are involved in a motion of the hole along the c axis.

Now we present an approximate eigenvalue of K (Eq. 1). For this purpose we employ the Green's function technique. For specificity, we evaluate the Green's function $\langle\langle d_{2\uparrow};d_{2\uparrow}^\dagger\rangle\rangle_\omega$ corresponding to the motion of an $\uparrow$ spin in the $d_{3z^2-r^2}$ state with an energy ω. Without loss of generality we may take $t_{xz}=0$ in Eq. (1). The neglect of the hybridization of the O $2p_x$ and Cu $3d_{3z^2-r^2}$ orbitals in Eq. (1) is not going to affect the essential aspects of our picture. In fact, with $t_{xz}=0$ we are able to obtain the energy levels of the cluster CuO_2 in analytical form. This Green's function will satisfy the equation of motion[47]

$$\omega\langle\langle d_{2\uparrow};d_{2\uparrow}^\dagger\rangle\rangle_\omega=\langle[d_{2\uparrow},d_{2\uparrow}^\dagger]_+\rangle+\langle\langle[d_{2\uparrow},K];d_{2\uparrow}^\dagger\rangle\rangle_\omega. \tag{2}$$

Here $[\cdots,\cdots]$ denotes a commutator, while $[\cdots,\cdots]_+$ denotes an anticommutator. The commutator $[d_{2\uparrow},K]$ is given by

$$[d_{2\uparrow},K]=\epsilon_{d_2}d_{2\uparrow}+t_zp_{z\uparrow}+Un_{2\downarrow}d_{2\uparrow}+U'\sum_{s'=\uparrow,\downarrow} n_{1,s'}d_{2\uparrow}. \tag{3}$$

This shows that we need to consider the Green's functions $\langle\langle p_{z\uparrow};d_{2\uparrow}^\dagger\rangle\rangle_\omega$, $\langle\langle n_{2\downarrow}d_{2\uparrow};\rangle d_{2\uparrow}^\dagger\rangle\rangle_\omega$, and $\langle\langle n_{1,s'}d_{2\uparrow};d_{2\uparrow}^\dagger\rangle\rangle_\omega$ for working out the second term in the right-hand side of Eq. (2).

Following again the method of Zubarev[47] we obtain

$$\omega\langle\langle p_{z\uparrow};d_{2\uparrow}^\dagger\rangle\rangle_\omega=\langle[p_{z\uparrow},d_{2\uparrow}^\dagger]_+\rangle+\langle\langle[p_{z\uparrow},K];d_{2\uparrow}^\dagger\rangle\rangle_\omega, \tag{4}$$

$$\omega\langle\langle n_{2\downarrow}d_{2\uparrow};d_{2\uparrow}^\dagger\rangle\rangle_\omega=\langle[n_{2\downarrow}d_{2\uparrow},d_{2\uparrow}^\dagger]_+\rangle+\langle\langle[n_{2\downarrow}d_{2\uparrow},K];d_{2\uparrow}^\dagger\rangle\rangle_\omega \tag{5}$$

and

$$\omega\langle\langle n_{1,s'}d_{2\uparrow};d_{2\uparrow}^\dagger\rangle\rangle_\omega=\langle[n_{1,s'}d_{2\uparrow},d_{2\uparrow}^\dagger]_+\rangle+\langle\langle[n_{1,s'}d_{2\downarrow},K];d_{2\uparrow}^\dagger\rangle\rangle_\omega. \tag{6}$$

The commutators involved in Eqs. (4)–(6) are given by

$$[p_{z\uparrow},K]=\epsilon_{p_z}p_{z\uparrow}+t_zd_{2\uparrow}, \tag{7}$$

$$[n_{2\downarrow}d_{2\uparrow},K]=\epsilon_{d_2}n_{2\downarrow}d_{2\uparrow}+t_zn_{2\downarrow}p_{z\uparrow}+Un_{2\downarrow}d_{2\uparrow}+U'\sum_{s'} n_{1,s'}n_{2\downarrow}d_{2\uparrow} \tag{8}$$

and

$$[n_{1,s'}d_{2\uparrow},K]=\epsilon_{d_2}n_{1,s'}d_{2\uparrow}+t_z n_{1,s'}p_{z\uparrow}+Un_{1,s'}n_{2\downarrow}d_{2\uparrow}+U'n_{1,s'}(1+n_{1,-s'}d_{2\uparrow}). \quad (9)$$

On the basis of Eqs. (7)–(9) it is seen that the following new Green's functions are required in the right-hand sides of Eqs. (4) to (6): $\langle\langle n_{2\downarrow}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$, $\langle\langle n_{2\downarrow}p_{2\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$, $\langle\langle n_{1\downarrow}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$, and $\langle\langle n_{1\downarrow}d_{2\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$. Out of these we consider equations of motion of only $\langle\langle n_{2\downarrow}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$ and $\langle\langle n_{1\downarrow}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$, while the remaining two are reduced in the form of previously obtained Green's functions by using the mean-field approximation. In fact, we use the following approximations:

$$n_{1,s'}n_{2\downarrow}d_{2\uparrow}\approx\langle n_{1,s'}\rangle n_{2\downarrow}d_{2\uparrow}, \quad (10)$$

$$n_{1\uparrow}n_{1\downarrow}d_{2\uparrow}\approx\langle n_{1\uparrow}\rangle n_{1\downarrow}d_{2\uparrow}. \quad (11)$$

The Green's functions $\langle\langle n_{2\downarrow}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$, and $\langle\langle n_{1,s'}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$ are given by the equations of motion

$$\omega\langle\langle n_{2\downarrow}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}=\langle[n_{2\downarrow}p_{z\uparrow},d^{\dagger}_{2\uparrow}]_{+}\rangle+\langle\langle[n_{2\downarrow}p_{z\uparrow},K];d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega} \quad (12)$$

and

$$\omega\langle\langle n_{1,s'}p_{z\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}=\langle[n_{1,s'}p_{z\uparrow},d^{\dagger}_{2\uparrow}]_{+}\rangle+\langle\langle[n_{1,s'}p_{z\uparrow},K];d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}. \quad (13)$$

The commutators involved in Eqs. (12) and (13) are given by

$$[n_{2\downarrow}p_{z\uparrow},K]=\epsilon_{p_z}n_{2\downarrow}p_{z\uparrow}+t_z n_{2\downarrow}d_{2\uparrow} \quad (14)$$

and

$$[n_{1,s'}p_{z\uparrow},K]=\epsilon_{p_z}n_{1,s'}p_{z\uparrow}+t_z n_{1,s'}d_{2\uparrow}. \quad (15)$$

With the approximations given by Eqs. (10) and (11) we now do not require any new Green's functions. Therefore, using Eqs. (2) to (15) it is now possible to obtain an expression of the Green's function $\langle\langle d_{2\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$. This expression will involve various averages of number operators such as $\langle n_{1,s}\rangle$ and $\langle n_{2,s}\rangle$ [cf. Eqs. (10) and (11)]. The magnitudes of these averages of number operators will depend on the number of holes present in the CuO_2 cluster. While it is possible to account for the Coulomb interaction for any given number of holes in a CuO_2 cluster, difficulties will arise when we consider the macroscopic solid of the CuO_2 clusters. So, we divide the role of the Coulomb interaction in two parts. In the first part the Coulomb interaction acts according to the presence of the $\downarrow$ spin hole in the $3d_{x^2-y^2}$ state of the Cu atom. This amounts to consider $\langle n_{1\downarrow}\rangle=1$, $\langle n_{1\uparrow}\rangle=0$, and $\langle n_{2,s}\rangle=1$. The remaining part of the Coulomb interaction will correspond to the Coulomb interaction of the ''doped'' holes only where by ''doped'' holes we mean the holes other than the already present $\downarrow$ spin Cu holes. In this sense K may be written as

$$K=K_0+K'. \quad (16)$$

Here K_0 corresponds to K when $\langle n_{1\downarrow}\rangle=1$, $\langle n_{1\uparrow}\rangle=0$, and $\langle n_{2,s}\rangle=1$, while K' corresponds to the interaction between doped holes only. The expression of $\langle\langle d_{2\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}$ corresponding to K_0 may be obtained from Eqs. (2)–(15). It is

$$\langle\langle d_{2\uparrow};d^{\dagger}_{2\uparrow}\rangle\rangle_{\omega}=\frac{\omega-\epsilon_{p_z}}{(\omega-\omega_{2+})(\omega-\omega_{2-})} \quad (17)$$

where

$$\omega_{2\pm}=\tfrac{1}{2}[(\epsilon_{d_2}+U'+\epsilon_{p_z})\pm\sqrt{(\epsilon_{d_2}+U'-\epsilon_{p_z})^2+4t_z^2}]. \quad (18)$$

It is seen that for $t_z=0$,

$$\omega_{2+}=\epsilon_{d_2}+U' \quad (19)$$

and

$$\omega_{2-}=\epsilon_{p_z}. \quad (20)$$

Using the same approach and approximation we obtain the other Green's functions

$$\langle\langle p_{z\uparrow};p^{\dagger}_{z\uparrow}\rangle\rangle_{\omega}=\frac{(\omega-\epsilon_{p_z})F(\omega,\epsilon_{d_2})+U't_z^2}{\prod_{\alpha=1}^{4}(\omega-\omega_{z\alpha})} \quad (21)$$

and

$$\langle\langle p_{x\uparrow};p^{\dagger}_{x\uparrow}\rangle\rangle_{\omega}=\frac{(\omega-\epsilon_{p_x})L(\omega,\epsilon_{d_1})+Ut_x^2}{\prod_{\alpha=1}^{4}(\omega-\omega_{x\alpha})}. \quad (22)$$

Here

$$F(\omega,\epsilon_{d_2})=(\omega-\epsilon_{p_z})(\omega-\epsilon_{d_2})-t_z^2, \quad (23)$$

$$L(\omega,\epsilon_{d_1})=(\omega-\epsilon_{p_x})(\omega-\epsilon_{d_1})-t_x^2, \quad (24)$$

and $\omega_{z\alpha}$ and $\omega_{x\alpha}$ are roots of

$$F(\omega_{z\alpha},\epsilon_{d_2})=0, \quad (25)$$

$$F(\omega_{z\alpha},\epsilon_{d_2}+U')=0, \quad (26)$$

$$L(\omega_{x\alpha},\epsilon_{d_1})=0 \quad (27)$$

and

$$L(\omega_{x\alpha},\epsilon_{d_2}+U)=0. \quad (28)$$

It may be noted that the roots of Eq. (26) match with $\omega_{2\pm}$. Similarly, the poles of $\langle\langle d_{1\uparrow};d^{\dagger}_{1\uparrow}\rangle\rangle_{\omega}$, say $\omega_{1\pm}$, will be given by Eq. (28). In fact,

$$\omega_{1\pm}=\tfrac{1}{2}[(\epsilon_{d_1}+U+\epsilon_{p_x})\pm\sqrt{(\epsilon_{d_1}+U-\epsilon_{p_x})^2+4t_x^2}]. \quad (29)$$

On the basis of Eqs. (18) and (25)–(29), it is not difficult to conclude that

$$\omega_{z1}=\min\{\omega_{z\alpha}\}=\omega_{2-} \quad (30)$$

TABLE I. Values of the energies ω_{x1} and ω_{z1} for the CuO_2 cluster for $\epsilon_{p_z}-\epsilon_{p_x}=-0.5$, 0.0, and 1.5 eV. Values of the energy difference $E=\omega_{z_1}-\omega_{x_1}$ are also given. In the last column values of $W+2t_\perp$ are given for typical values of $8t_\parallel$ by assuming the square density of states of the ''in-plane'' band.

$\epsilon_{p_z}-\epsilon_{p_x}$ eV	ω_{x1} eV	ω_{z1} eV	E eV	$8t_\parallel$ eV	n_H (per Cu)	E_F eV	$W+2t_\perp$ meV
					0.15	0.45	696
−0.50	1.432	1.078	−0.354	3.0	0.25	0.75	396
					0.35	1.05	96
					0.38	1.14	0.0
					0.20	0.40	744
0.0	1.432	1.576	0.144	2.0	0.22	0.44	704
					0.25	0.50	644
					0.20	0.30	2087
					0.25	0.37	2012
1.5	1.432	3.069	1.637	1.5	0.30	0.45	1937
					0.40	0.60	1787
					0.50	0.75	1637

and

$$\omega_{x1}=\min\{\omega_{x\alpha}\}=\omega_{1-}. \tag{31}$$

For the case when Cu $3d_{x^2-y^2}$ is filled by one hole and Cu $3d_{3z^2-r^2}$ is empty, the energy set of the in-plane states $\{\omega_x\}$, say, involves two states ω_{x1} and ω_{x2} (cf. Fig. 1). The energy set of out-of-plane states, say $\{\omega_z\}$, also involves two states ω_{z1} and ω_{z2}. We arrange ω_{xi}'s and ω_{zi}'s such that $\omega_{x1}=\min\{\omega_{xi}\}$ and $\omega_{z1}=\min\{\omega_{zi}\}$. We define a parameter E (cf. Fig. 1) such that

$$E=\omega_{z1}-\omega_{x1}. \tag{32}$$

We have calculated the values of ω_{x1} and ω_{z1} for the typical values of different parameters.[35,45] In fact, we take $\epsilon_{d_1}=0$, $\epsilon_{d_2}-\epsilon_{d_1}=0.3$ eV, $\epsilon_{p_x}-\epsilon_{d_1}=1.6$ eV, $t_x=1.2$ eV, $t_z=0.4$ eV, $U=10$ eV, and $U'=8$ eV. The results are presented in Table I for $\epsilon_{p_z}-\epsilon_{p_x}=-0.5$, 0.0, and 1.5 eV. These three values of $\epsilon_{p_z}-\epsilon_{p_x}$ correspond relatively to the systems $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{7-y}$, and $Bi_2Sr_2CaCuO_{6+y}$ and Tl_2Ba_2CaCuO. In order to see how it is so, we notice, for example, from the Appendix of Ohta and co-workers[45] that $\epsilon_{p_z}-\epsilon_{p_x}$ is least (and negative) for $La_{2-x}Sr_xCuO_4$, increases for YBa_2CuO_{7-y}, and becomes larger for Bi- and Tl-based systems. The values of E [Eq. (32)] are also given in Table I. It is clear from Table I that E increases with increasing $\epsilon_{p_z}-\epsilon_{p_x}$. In fact for $\epsilon_{p_z}-\epsilon_{p_x}=-0.5$, E is negative. We emphasize that qualitatively the relative features of E will not change with the inclusion of the O $2p_y$ orbitals in K. In fact K will then correspond to the cluster CuO_3.

B. Occurrence of gap between in-plane and out-of-plane states in the solid system

When the CuO_3 units are combined to form the cuprate solid system, the states ω_{x1}, ω_{y1}, and ω_{z1} will be replaced by the bands $\{\epsilon_{\mathbf{k}};\mathbf{k}=(k_x,k_y)\}$ and $\{\epsilon_{k_z}\}$, respectively. This is shown schematically in Fig. 1. While the former is the band originating from the ''in-plane'' states, the latter is the band arising out of the ''out-of-plane'' states. In the tight binding model, the width of these bands will be $8t_\parallel$ and $4t_\perp$ respectively. Here $t_\parallel(t_\perp)$ describes overlap matrix elements between the neighboring CuO_3 cluster in the $ab(c)$ direction. In the present treatment we treat these parameters phenomenologically (cf. Table I). In the tight-binding scheme the in-plane and out-of-plane bands are approximately described by

$$\epsilon_{\mathbf{k}}=-2t_\parallel(\cos k_x a+\cos k_y a) \tag{33}$$

and

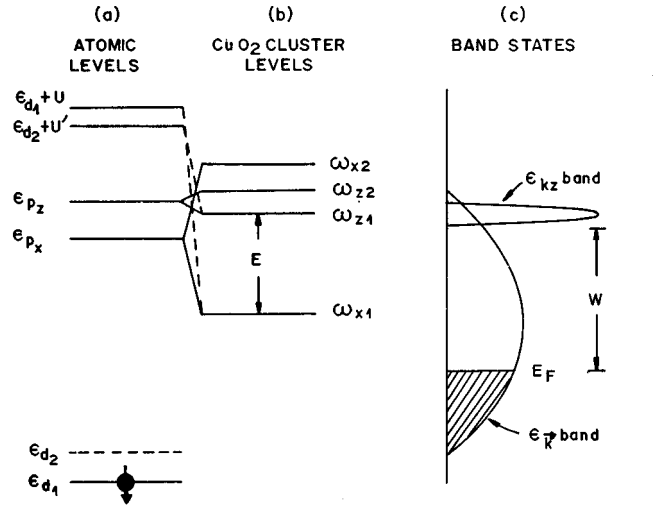

FIG. 1. Schematic plot of electronic structure of a spin up hole for the case when there is a spin down hole in the Cu $3d_{x^2-y^2}$ orbitals. (a) Atomic levels are shown. The Cu $3d_{3z^2-r^2}$ level is shown by a dashed line to signify that due to the presence of a spin down in the Cu $3d_{x^2-y^2}$ orbital, the Cu $3d_{3z^2-r^2}$ orbital of energy ϵ_{d_2} will be vacant. (b) Formation of cluster states of Cu O_2 corresponding to the O $2p_x$, O $2p_y$ atomic levels are shown. Dashed lines signify the admixture of the Cu $3d_{x^2-y^2}$ or Cu $3d_{3z^2-r^2}$ orbitals. (c) Formation of in-plane and out-of-plane band states are shown. W is the gap defined in Eq. (35).

$$\epsilon_{k_z} = -2t_\perp \cos k_z c + E. \tag{34}$$

In the CuO_3 cluster the states $\epsilon_{\mathbf{k}}$ and ϵ_{k_z} become independent of $\mathbf{k}$ and k_z and according to Eq. (32) differ by E. E appears in Eq. (34) to satisfy this requirement. For a given number of holes in the solid the general situation, which Eqs. (33) and (34) represent, will be that the band of in-plane states will be filled upto the Fermi energy E_F, and the bottom of the band of out-of-plane states will be above by the gap

$$W = E - 2t_\perp + 4t_\parallel - E_F. \tag{35}$$

Fig. 1(c) illustrates this situation. Here E_F is measured from the bottom of the ''in-plane'' band.

Since E_F depends on the number of band holes n, W will be a function of the hole doping (cf. Fig. 1). Since E_F increases with n, $W(n)$ will decrease with increasing n. It may be noted that W is already a function of $\epsilon_{p_x} - \epsilon_{p_z}$ through E (cf. above). For an illustrative purpose we have calculated values of $W + 2t_\perp$ for $\epsilon_{p_z} - \epsilon_{p_x} = -0.5$, 0.0, and 1.5 eV. It is clear from the Table I (for $t_\perp = 0$ that there is a high chance for W to vanish for the $\epsilon_{p_z} - \epsilon_{p_x} = -0.5$ case for $n > \approx 0.38$. For $t_\perp > 0$, W will vanish even for smaller n. We emphasize that $t_\perp$ is a parameter of relatively much smaller value than $t_\parallel$. For $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_7$, and $Bi_2Sr_2CaCu_2O_8$ systems $t_\perp$ is typically 5, 40, and 0.1 meV, respectively.[34] As pointed out above, this case corresponds to the $La_{1.85}Sr_{0.15}CuO_4$ system. In this system trend of vanishing W is indeed observed in measured ρ_c for $n = 0.3$ (see Table II). On the other hand, there is no chance for W to vanish in the $\epsilon_{p_z} - \epsilon_{p_x} = 0$ case even upto $n = 0.5$ for $t_\perp < 0.05$ eV. As mentioned above, these values of parameters $\epsilon_{p_z} - \epsilon_{p_x}$ and $t_\perp$ correspond relatively to $YBa_2Cu_3O_7$. In this system measured ρ_c does not show any signature of vanishing W (see Table II). We may therefore say that our model with a doping dependent energy gap W is supported by measured experimental data on ρ_c for the cuprate superconductors.

We emphasize that the energy gap $W(n)$ is physically different from the gap that occurs in semiconductors where the energy gap is the energy separation between the top of the occupied valence band and bottom of the empty conduction band. The other difference is that here $W(n)$ is n-independent, contrary to the n-independent gap in the semiconductors. An idea of the semiconductorlike gap for the c-direction transport has been proposed by Ong[48] and Yan and co-workers.[49] The recent model of Abrikosov based on the resonant impurity levels also involves a gap for the c-direction transport.[33] For the case of the $YBa_2Cu_3O_{7-y}$ system considered by Abrikosov, the impurities are the O atoms of the CuO chain. Since the O atoms control the carrier density also, the gap involved in the Abrikosov's approach is indirectly related with the carrier concentration. The concept of gap is also involved in the theory of Alexandrov and co-workers.[35] In the work of these authors the gap is due to the dissociation of a bipolaron into two polarons.

TABLE II. Values of n and $W(n)$ for various cuprate superconductors. The values of n for the YBCO samples of Takenaka *et al.* (Ref. 6) are estimated according to the method given by Fukuzumi *et al.* (Ref. 48), by using the interpolation method. Values of $W(n)$ for $La_{2-x}Sr_xCuO_y$ ($x = 0.12$ and $x = 0.20$) and $Bi_2Sr_{2-x}La_xCuO_4$ ($x = 0.2$ and 0.3) are based on the ρ_c data for $T > 50$ K and $T > 75$ K, respectively. The value of n for $HgBa_2Ca_2Cu_3O_8$ is at $T = 150$ K.

Systems	Reference	n(Holes/CuO_2)	$W(n)$ (meV)
$La_{1.90}Sr_{0.10}CuO_4$	3	0.10	12.5
$La_{1.88}Sr_{0.12}CuO_4$	3	0.12	8.33
$La_{1.85}Sr_{0.15}CuO_4$	3	0.15	5.50
$La_{1.80}Sr_{0.20}CuO_4$	3	0.20	2.28
$YBa_2Cu_3O_{6.68}$	6	0.145	17.2
$YBa_2Cu_3O_{6.78}$	6	0.18	12.0
$YBa_2Cu_8O_{6.88}$	6	0.21	7.5
$YBa_2Cu_3O_{6.93}$	6	0.24	5.75
$Bi_2Sr_{1.7}La_{0.3}CuO_y$	12	n_1	7.58
$Bi_2Sr_{1.8}La_{0.2}CuO_y$	12	$n_2 (> n_1)$	4.06
$Bi_2Sr_{1.95}La_{0.05}CuO_y$	12	$n_3 (> n_2)$	2.05
$Bi_2Sr_{1.95}La_{0.05}CuO_y$ (sample *A*)	16	-	3.36
$Bi_2Sr_{1.95}La_{0.05}CuO_y$ (sample *B*)	16	-	3.02
$Bi_2Sr_{1.95}La_{0.05}CuO_y$ (sample *C*)	16	-	4.27
$HgBa_2Ca_2Cu_3O_8$ (sample *A*)	18	0.13	20.5

C. Model Hamiltonian for the cuprate system

In order to describe resistivity of the system we consider the CuO_2 layer and the one-dimensional chain passing through the Cu atoms along the c axis. The chain is supposed to make up of the Cu $3d_{3z^2-r^2}$ and O $2p_z$ atoms. There may be other atoms also on this chain. The specification of such atoms is not important for the present model. In fact, the parameter $t_\perp$ involves the effects of such atoms in a phenomenological manner. According to Eq. (16) we have divided the Coulomb interaction in two parts. The part corresponding to K_0 defines the band states $\epsilon_{\mathbf{k}}$ and ϵ_{k_z} [Eqs. (33) and (44)]. Let the momentum $\mathbf{k}$ and k_z be collectively denoted by γ. Then, according to Eq. (16) the second part of the Coulomb interaction will correspond to the holes of the states γ. The Hamiltonian which describes this situation may be written as

$$H = \sum_{\gamma,s} \epsilon_\gamma c^\dagger_{\gamma,s} c_{\gamma,s} + \sum_{\gamma\gamma'\gamma''\gamma'''} V(\gamma - \gamma'') c^\dagger_{\gamma'',\uparrow} c^\dagger_{\gamma''',\downarrow} c_{\gamma',\downarrow} c_{\gamma,\uparrow}. \tag{36}$$

Here $c^\dagger_{\mathbf{k},s}$ and $c_{\mathbf{k},s}$ correspond to the creation and annihilation operators of a hole in the ''in-plane'' band, while $c^\dagger_{k_z,s}$ and $c_{k_z,s}$ correspond to the creation and annihilation operators of a hole in the ''out-of-plane'' band. $V(\gamma - \gamma'')$ denotes the Coulomb interaction for the momentum transfer $\gamma - \gamma'$ between the holes described by the $|\gamma s\rangle$ states. (We emphasize that the effect of the Coulomb interaction due to the Cu holes is taken in constructing the $|\gamma s\rangle$ states.) Let $\phi_{\gamma s}(\mathbf{r}_i)$ denote

the cluster wave function corresponding to the momentum γ, spin s, and position $\mathbf{r}_i$ of a hole. Then $V(\gamma-\gamma'')$ may be written as

$$V(\gamma-\gamma'')=\delta_{\gamma+\gamma',\gamma''+\gamma'''}\int \phi^*_{\gamma'',s}(\mathbf{r}_i)\phi^*_{\gamma''',s}(\mathbf{r}_j) \times V(\mathbf{r}_i-\mathbf{r}_j)\phi_{\gamma',s}(\mathbf{r}_j)\phi_{\gamma,s}(\mathbf{r}_i)d\mathbf{r}_i d\mathbf{r}_j, \quad (37)$$

where

$$V(\mathbf{r}_i-\mathbf{r}_j)=\frac{e^2\ \exp(-\kappa|\mathbf{r}_i-\mathbf{r}_j|)}{\epsilon(\infty)|\mathbf{r}_i-\mathbf{r}_j|}. \quad (38)$$

Here, $\mathbf{r}_i$ and $\mathbf{r}_j$ are the coordinates of the two interacting holes, κ is inverse screening length due to the hole-hole interaction, and $\epsilon(\infty)$ is the dielectric constant at optical frequency due to the lattice ions.

Because of the gap W, the band of out-of-plane states will start to get filled only when the band of in-plane states is filled up to the bottom of the band of out-of-plane states. Let n_0 denote the maximum hole density for which the upper band will remain unoccupied. Then, for $n<n_0$ the motion of holes along the c axis will be governed by the existence of a finite gap W.

Because of the gap W there will be no hole motion along c direction at the temperature $T=0$. For $T>0$, a number of holes proportional to $e^{-W(n)/K_BT}$ will be excited to the out-of-plane bands. Here K_B is the Boltzmann constant. Phenomenologically, the number of holes excited to the out-of-plane states may be written as

$$n_c=n_z e^{-W(n)/k_BT} \quad (n<n_0). \quad (39)$$

In order to specify the parameter n_z we proceed as follows. We emphasize that in our model the motion of holes along c direction depends upon the occupancy of the Cu $3d_{3z^2-r^2}$ orbitals. In fact, we have already mentioned in the beginning of this article that practically the O $2p_{x,y}$ holes will not take part in the motion along c direction. As is clear from Eq. (1) the Cu $3d_{3z^2-r^2}$ orbital hybridizes with the O $2p_x$ orbital also. The resulting states will be along the ab plane. From such hybridized states we may estimate the number of holes present on the average in the Cu $3d_{3z^2-r^2}$ orbital corresponding to the planar motion [i.e., for $t_z=0$ in Eq. (1)]. Since, the thermally activated motion along c axis will depend on these holes, we specify n_z by

$$n_z=\sum_s \langle d^\dagger_{1s}d_{2s}\rangle_{t_z=0}. \quad (40)$$

The value of n_z has been calculated by Zotos and co-workers[40] for a Cu_2O_3 chain along x axis (cf. Table I of Ref. 40).

It may be noted that the Cu $3d_{3z^2-r^2}$ orbital hybridizes with the O $2p_z$ orbital also. The states resulting in this manner have already been considered to form the band of out-of-plane states [cf. Eqs. (18) and (34)]. For $n>n_0$, the holes will be divided in two parts: those which move along ab plane, and those which move along c direction. Let n_{ab} and n_c denote the number of holes corresponding to the ab plane and c direction, respectively. Then,

$$n_{ab}+n_c=n. \quad (41)$$

This relation will be applicable to the $n<n_0$ case also with the value of n_c given by Eq. (39). In fact, for $n<n_0$, n_c will be T-dependent, while for $n\geqslant n_0$ n_c will be T-independent. Whether a hole moves in the ab-plane or along the c direction, its lifetime, say τ, will be same. In order to see how it happens, let τ_{ab} and τ_c denote the hole lifetime along the ab and c direction, respectively. For specificity, let $\tau_c<\tau_{ab}$. Then, if a hole of c direction comes at a copper atom with lifetime τ_c, it finds that it can raise its lifetime (lower the scattering rate) by changing its direction to the ab plane. Thus $\tau_c<\tau_{ab}$ affects the hole distribution between the ab plane and c direction. But the hole distribution has already been fixed in the sense of the Hamiltonian K_0 (Eq. (16)). This will force $\tau_c=\tau_{ab}$. This means that in our model hole will have the same lifetime irrespective of its direction of motion. This is in fact, the case in other models also.[24,34] The extra T dependence along c direction that arises in such models is due to, for example, the combining of holons and spinons along the c direction.[24,34]

III. RESISTIVITY

In the overdoped regime where the Coulomb interaction is screened and where the antiferromagnetic background of the Cu ions has lost its significance, the scattering rate will be given by the Fermi liquid picture. So the hole scattering rate will be given by

$$\frac{\hbar}{\tau}=AT^2 \quad (\text{overdoped regime}). \quad (42)$$

Here A is a parameter independent of temperature. $\hbar$ is the reduced Plank's constant.

When carrier concentration n is reduced from the overdoped limit for a certain range of n, a situation will arise where Coulomb interaction becomes poorly screened and where the magnetic interaction due to the Cu ions (with each Cu having one down spin hole) cannot be ignored. It has been shown in the literature by a number of workers that under such circumstances the scattering rate is enhanced and is given by[28–30]

$$\frac{\hbar}{\tau}=BT \quad (\text{intermediate doping}). \quad (43)$$

Here B is of order of 1.

While going from the overdoped regime to the intermediate regime the screening length κ^{-1} and the appearance of magnetic interaction of antiferromagnetic origin vary gradually. We therefore believe that for a general carrier doping n, the hole scattering rate will be given by

$$\frac{\hbar}{\tau}=CT^m \quad (1\leqslant m\leqslant 2). \quad (44)$$

Here m varies from 2 to 1 gradually as we go from the overdoped regime to the intermediate doped regime. In fact, this fact can be deduced from the analysis of the resistivity data of systems of varying carrier density.[17,50]

Having discussed the hole density and hole lifetime along the ab plane and c direction, we now turn to specify the

resistivity. We use the Boltzmann equation. It has been shown by Liu and Xing[21] that formally the results of the Boltzmann equations are similar to the models based on the incoherent motion along the c axis. In using the Boltzmann equation we need hole mass along the ab plane and c direction. In terms of band energy $\epsilon_{\mathbf{k}}$ [Eq. (32)] the ab-plane effective mass of a hole is given by

$$m_{ab}^{*}=\hbar^{2}\Big/\frac{\partial^{2}\epsilon_{\mathbf{k}}}{\partial k_{x}\partial k_{y}}. \tag{45}$$

Similarly, the effective mass along the c direction is given on the basis of band energy ϵ_{k_z} [Eq. (34)]. That is,

$$m_{c}^{*}=\hbar^{2}\Big/\frac{\partial^{2}\epsilon_{\mathbf{k}}}{\partial k_{z}^{2}}. \tag{46}$$

With mass $m_{ab}^{*}(m_{c}^{*})$, carrier density $n_{ab}(n_c)$ and lifetime τ, the resistivity along the ab plane and (c direction) is given by

$$\rho_i=\frac{m_i^{*}}{n_i e^{2}\tau}, \tag{47}$$

where, $i=ab,c$.

We discuss Eq. (47) for two cases. The first correspond to the situation where the hole density is such that $n_c=0$ for $T=0$. Let n_0 denote this initial hole density. The other case corresponds to the case where $n>n_0$ or $n_c>0$ for $T=0$. In both of these cases $n_{ab}>0$ and is independent of T.

A. Case I: $n<n_0$

In this case only the in-plane band will be partially filled (upto E_F). The out-of-plane band will be above the gap $W(n)$. The magnitude of n_c will be given by Eq. (39). When this is so, according to Eq. (41) n_{ab} also acquires a T dependence in this case. Consequently, Eq. (47) leads to

$$\frac{\rho_c}{\rho_{ab}}=\frac{m_c^{*}n}{m_{ab}^{*}n_z}\left(e^{W/K_BT}-\frac{n_z}{n}\right). \tag{48}$$

This shows that for low T, $\rho_c/\rho_{ab}\approx e^{W/K_BT}$. That is, ρ_c/ρ_{ab} diverges at $T=0$.

We emphasize that Eq. (48) shows that the ab-plane resistivity ρ_{ab} is affected due to the c-direction electronic motion (parameterized by n_z/n). In order to assess the effect of n_z/n, we consider the estimation of n_z/n on the basis of the work of Zotos and co-workers.[40] In fact, we can calculate n_z from our model also. But, in our model the Cu-O cluster has less number of atoms so that the values of n_z obtained by Zotos and co-workers will be more realistic. We notice from Table I of Zotos and co-workers that for the total number $n_{\text{total}}=2$ of the holes in the Cu_2O_3 chain the occupancy of Cu $3d_{x^2-y^2}$ orbital per Cu atom is 0.67, and not 1. Because of this, we define the average number of doped holes n as the sum of the occupancies of the O $2p$ and Cu $3d_{3z^2-r^2}$ orbitals per Cu. Then, since the occupancy of the Cu $3d_{3z^2-r^2}$ orbital per Cu is n_z, the occupancy of the O $2p$ orbital per Cu will be $n-n_z$. In Fig. 2 we plot n_z/n obtained in this manner against n_{total}. It is clear from this figure that for low n_{total} (i.e., for $n_{\text{total}}\sim 2$), n_z/n is significantly smaller than 1. The ratio n_z/n will be further smaller if we treat the realistic Cu_2O_7 cluster in place of Cu_2O_3. This is because as the number of O atoms in the cluster increases, the probability of the average occupancy of the O $2p$ orbital per Cu atom will also increase. Because of this and because of the fact that $e^{W/K_BT}>1$, we neglect the factor of n_z/n in the bracket of Eq. (48). We may thus use the result that

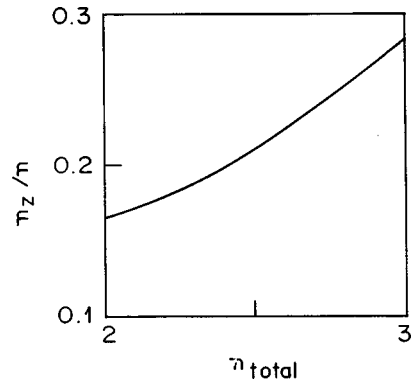

FIG. 2. Plot of n_z/n vs n_{total} (total number of holes in the Cu_2O_3 chain) on the basis of the calculations of Zotos and co-workers (Ref. 40).

$$\frac{\rho_c}{\rho_{ab}}\propto e^{W(n)/K_BT}. \tag{49}$$

This equation resembles formally with that of Alexandrov and co-workers.[35] However, as mentioned above the origin of W and Δ of Alexandrov *et al.* are completely different.

The main result is that ρ_c shows a semiconducting behavior ($d\rho_c/dT<0$) below a certain temperature with a crossover to the metallic behavior ($d\rho_c/dT>0$) at higher temperatures. A large number of samples of the $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{7-y}$, and other cuprate systems show this behavior.[1–19] The most important difference of the present model from that of others that also explain this crossover[25,27–35] lies in the form of the T dependence of $\rho_c(T)$. According to Eq. (47), for the case of $n<n_0$, the T dependence of $\rho_c(T)$ is governed by the factor $T^m(e^{W/k_BT}-n_z/n)$. On the other hand, in the RVB theory and MFL theory, the T dependence of $\rho_c(T)$ is given by $\rho_c(T)=BT+C/T$ for all n (Refs. 28–30). In the model of Rojo and Levin[25] $\rho_c(T)$ varies like $a+bT+(c+dT)^{-1}$ where a, b, c, and d are T-independent parameters. In the model of Zha and co-workers[34] the T dependence of $\rho_c(T)$ is hidden in the density of states $N(0)$, while in Abrikosov's model[33] the T-dependent resistivity is of the type $T[\cosh(E/k_BT)+\cosh(\epsilon/k_BT)]/\sinh(\epsilon/k_BT)$ and arises due to resonant impurity levels. Here $E-\epsilon$ and $E+\epsilon$ characterize the lower and upper limits of the resonant (impurity) levels.[33] E does not depend on the carrier density, rather it depends on disorder. In the present case, the gap $W(n)$ is dependent on the carrier density and has nothing to do with disorder. In the model of Alexandrov and co-workers[35] the T dependence of ρ_c is governed by $\rho_{ab}e^{-\Delta/K_BT}$ where Δ is the bipolaron binding energy.

B. Case II: $n > n_0$

In this case the out-of-plane band will also be filled up partially so that n_c will be T-independent. Thus as a result of Eq. (41), n_{ab} will also be T-independent. Consequently, Eq. (42) will lead to

$$\rho_c \propto \rho_{ab} . \tag{50}$$

Many overdoped samples of the cuprates show this behavior.[2,3,15,50] Many other workers have also arrived at a behavior of ρ_c given by Eq. (50) (Refs. 21, 26, 34, and 35). However, in the present case Eq. (50) is valid only for the case where $n > n_0$. They way we have introduced the gap W makes it clear that the situation of $n > n_0$ or of $W = 0$ requires $(\epsilon_{p_z} - \epsilon_{p_x})$ to be negative. As has been already mentioned this condition is satisfied only by the La-Sr-Cu-O-based cuprate systems (cf. Appendix of Ohta and co-workers). In fact, in other families of cuprate systems $\epsilon_{p_z} - \epsilon_{p_x}$ is positive. So, the case of $W = 0$ may not be realized in these systems. On the basis of the measured ρ_c of various cuprate systems, it turns out that among others the $x = 0.3$ sample of $La_{2-x}Sr_xCuO_4$ (Ref. 3) and the $x = 0.22$ sample of $La_{2-x}Sr_xCuO_4$ (Boebinger *et al.*, Ref. 51) correspond to $W = 0$. In fact according to Fig. 3 of Nakamura and Uchida[3] $\rho_c \propto \rho_{ab}$ for $x = 0.3$ sample. As far as the $x = 0.22$ sample of Boebinger *et al.*[51] is concerned, we have estimated the T dependence of ρ_c and ρ_{ab} assuming ρ_c, $\rho_{ab} \propto T^m$. It is found that $m = 1.4$ for ρ_{ab}, while $m = 1.3$ for ρ_c. This means that the value of m differs only by 8% for ρ_c and ρ_{ab}. This is not a significant difference and it may be concluded that for the $La_{2-x}Sr_xCuO_4$ sample of Boebinger *et al.* with $x = 0.22$, Eq. (50) is applicable.

The c-direction resistivity of the sample $Tl_2Ba_2CaCu_2O_8$ single crystal measured by Duan *et al.*[52] is also metallic down to T_c. It is clear from Fig. 1 of Duan *et al.* that $\rho_c \propto \rho_{ab} \propto T$ for $T > \sim 200$ K. Between T_c and 200 K the resistivities ρ_{ab} and ρ_c show fluctuation effects that may be considered a source of deviation of ρ_{ab} and ρ_c from the linear T behavior. We thus conclude that for the $Tl_2Ba_2CaCu_2O_8$ sample of Duan *et al.*, also $\rho_c \propto \rho_{ab}$ within the fluctuation effects.

The fact that this result is obtained primarily on the basis of the values of $\epsilon_{p_z} - \epsilon_{p_x}$ shows that the main points of the present model is able to explain the essential feature of the cuprate systems.

IV. EXTRACTION OF $W(n)$ FROM RESISTIVITY DATA

In order to illustrate the importance of the present model of $\rho_c(T)$ we consider the experimental observations made by different groups on the samples of the $La_{2-x}Sr_xCuO_4$ (LSCO), $YBa_2Cu_3O_{7-y}$ (YBCO), $Bi_2Sr_{2-x}La_xCuO_y$ (BSLCO) and $HgBa_2Ca_2Cu_3O_8$ (HBCCO) systems. In Figs. 3, 4, 5, and 6 we plot the experimental values[3,6,12,16] of $\ln[\rho_c(T)/\rho_{ab}(T)]$ vs T^{-1} for the LSCO, YBCO, and BSLCO samples.

In order to estimate the values of $W(n)$ from these plots we have used Eq. (49), since the term n_z/n turns out to be negligible against the exponential factor. The values of the energy gap $W(n)$ obtained from the plots of Figs. 3–6 by using Eq. (49) are presented in Table II. The values of $W(n)$ for the sample a of HBCCO of Carrington *et al.*[18] is also presented in Table II. The $\ln(\rho_c/\rho_{ab})$ vs T^{-1} plots for this sample is almost linear. From Figs. 3–6 it is clear that the exponential increase of $\rho_c(T)/\rho_{ab}(T)$ fits well in the case of most of the samples considered here (cf. Table II). Discrepancy is, however, encountered in the case of the $La_{2-x}Sr_xCuO_4$ ($x = 0.12$ and 0.2) (Ref. 3) and $Bi_2Sr_{2-x}La_xCuO_y$ ($x = 0.2$ and 0.3) samples[12] towards low T (less than 50 K and 75 K, respectively). For the LSCO samples ($x = 0.12$ and 0.2) the deviation of $\ln[\rho_c(T)/\rho_{ab}(T)]$ vs T^{-1} in Fig. 3 may be attributed to structural changes at low T. Such a change is indeed seen in the resistivity curves of these samples (cf. Fig. 2 of Ref. 3). For $Bi_2Sr_{2-x}La_xCuO_y$ samples the root of this discrepancy may be attributed to the T dependence of $\rho_{ab}(T)$. According to Eqs. (44) and (47), $\rho_{ab}(T)$ increases monotonically with T. On the other hand, according to Fig. 4 of Wang *et al.*[12] $\rho_{ab}(T)$ starts to change its behavior below about 75 K for $x = 0.2$ and 0.3 samples. If, instead of Fig. 4 of Wang *et al.*,[12] we use extrapolated linearly varying values of $\rho_{ab}(T)$ for $T < 75$ K also, we find

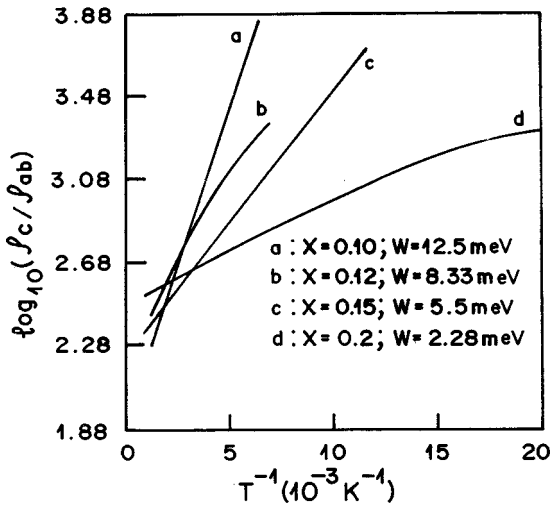

FIG. 3. Plot of $\ln(\rho_c/\rho_{ab})$ vs T^{-1} for the observed data of $La_{2-x}Sr_xCuO_4$ for different values of x taken from Nakamura and Uchida (Ref. 3).

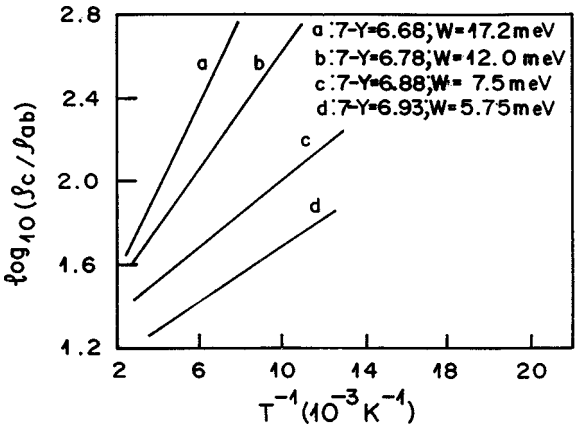

FIG. 4. Plot of $\ln(\rho_c/\rho_{ab})$ vs T^{-1} for the observed data of $YBa_2Cu_3O_{7-y}$ for different values of $(7-y)$ taken from Takenaka *et al.* (Ref. 6).

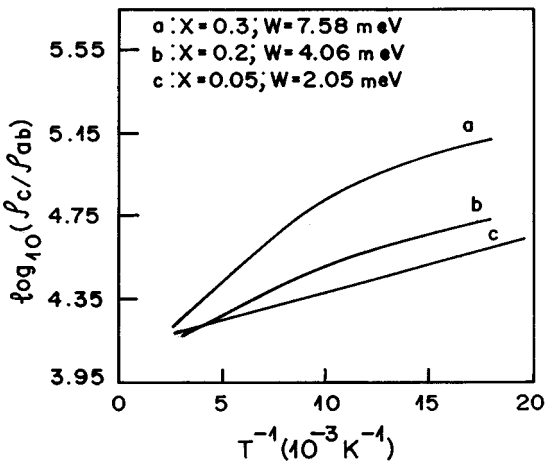

FIG. 5. Plot of $\ln(\rho_c/\rho_{ab})$ vs T^{-1} for the observed data of $Bi_2Sr_{2-x}La_xCuO_y$ for different values of x taken from Wang *et al.* (Ref. 12).

excellent agreement with the observed T dependence of ρ_c/ρ_{ab} with the values of $W(n)$ presented in Table II. This suggests that the T-dependent effect of disorder is a reasonable source of the discrepancy in the $\ln[\rho_c/\rho_{ab}]$ vs T^{-1} plots for $x=0.2$ and 0.3 of the $Bi_2Sr_{2-x}La_xCuO_y$ samples (Fig. 5).

Study of the $Bi_2Sr_{2-x}La_xCuO_y$ system has also been made by Ando *et al.*[16] These authors have considered three

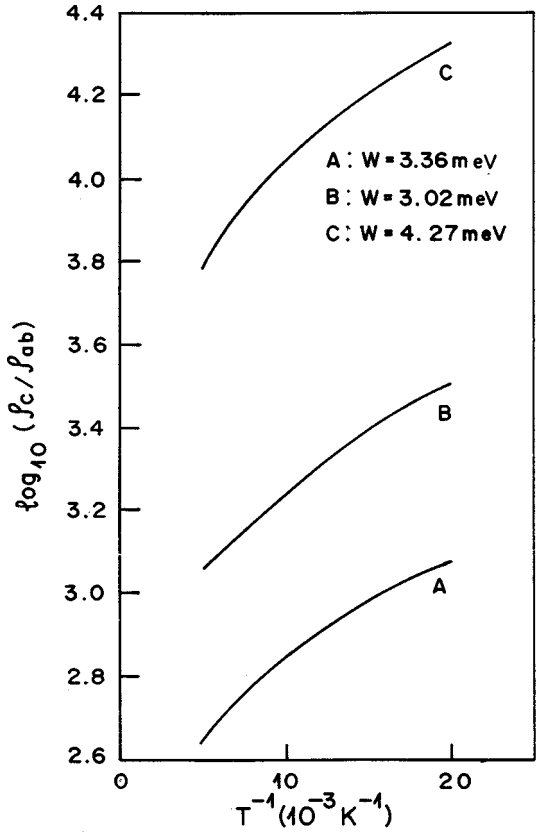

FIG. 6. Plot of $\ln(\rho_c/\rho_{ab})$ vs T^{-1} for the observed data of the samples A, B, and C of $Bi_2Sr_{1.95}La_{0.05}CuO_y$ taken from Ando *et al.* (Ref. 16). Samples A, B, and C marked in the plots correspond to different amounts of disorder.

samples of this system for $x=0.05$. The three samples are marked by A, B, and C. These samples were chosen such that the superconducting transition temperature T_c is expected to be nearly same in all the three samples. The samples differ from each other in the amount of the disorder. From Fig. 1(a) of Ando *et al.* it may be seen that sample B has practically linear-T behavior of $\rho_{ab}(T)$ above T_c. Because of this, we may say that the T-dependent effect of disorder that may be, for example, due to weak localization is least in the case of sample B. On the basis of the above arguments we therefore expect the $\ln(\rho_c/\rho_{ab})$ vs T^{-1} plot for sample B to be relatively more linear than for samples A and C. In order to see whether it is so or not, we have plotted $\ln(\rho_c/\rho_{ab})$ vs T^{-1} for the experimental data of Ando *et al.* for all the three samples. The values of $W(n)$ are presented in Table II. The plots are shown in Fig. 6 wherefrom it is quite clear that the $\ln(\rho_c/\rho_{ab})$ vs T^{-1} plot of sample B is indeed relatively more linear than that of samples A and C. This gives support to our point that the deviation of the $\ln(\rho_c/\rho_{ab})$ vs T^{-1} plot from a linear behavior is due to (T-dependent) effects of the disorder. This means that in a pure cuprate system our model is a reasonable model of the transport along the c axis.

From Table II it is clear that the correlation-induced gap $W(n)$ decreases with increasing n. This trend agrees well in general with the trend expected on the basis of Sec. II. For the $La_{2-x}Sr_xCuO_4$ system we may examine the variation of $W(n)$ with n more specifically. According to Chen *et al.*,[43] the gap between the in-plane and out-of-plane states is less then 30 meV. The values presented in Table II fall in this range. Chen *et al.*[43] also find that the relative occupancy of the Cu $3d_{3z^2-r^2}$ states remains fixed and negligibly small for $x \lesssim 0.15$. Furthermore, for the LSCO system the density of states at Fermi level, $N(0)$, increases with n.[53,54] This signifies that with increasing n the increase of $E_F(n)$ will become slow.[55] In light of Eq. (35), this implies that with increasing x the increase of $W(n)$ will become slow. This is indeed what we observe from Table II. This provides yet another support in favor of the basic assumption that the Cu $3d_{3z^2-r^2}$ orbitals are important for the transport along the c axis.

Yet another feature of the variation of $W(n)$ is evident from the HBCCO samples of Carrington *et al.*[18] These authors have considered six samples of this system. All of these samples appear to correspond to the same carrier density n. This is clear from the fact that ρ_{ab} is same for all the samples (cf. Fig. 1 of Ref. 18). The variation of $W(n)$ for different samples of HBCCO may then be due to the variation of the phenomenological parameter $t_\perp$. In fact, if $t_\perp$ increases when going from sample ''a'' to sample ''f'' of the HBCCO system, according to Eq. (35) W will decrease.

V. CONCLUSIONS

In this paper we have made an attempt to analyze the role of the Cu $3d_{3z^2-r^2}$ orbitals in the context of the transport along c axis in the high-T_c cuprates. These orbitals are extended along the c axis and the Cu ions are relatively much nearer to the apical oxygen ions as compared to the in-plane O atoms. A relatively larger extension of the Cu $3d_{3z^2-r^2}$ orbitals along the c axis than that of the hybridized Cu

$3d_{x^2-y^2}-\mathrm{O}\ 2p_{x,y}$ orbitals, led us to the hypothesis that the transport along c axis will be controlled by the Cu $3d_{3z-r^2}$ orbitals, and the hybridized in-plane orbitals O $2p_{x,y}$-Cu $3d_{x^2-r^2}$ make a relatively negligible contribution to ρ_c. We have examined the behavior of ρ_c on the basis of phenomenological expressions.

The expressions of ρ_c presented here provide us with quite satisfactory results. At low carrier density, we have a situation where the Fermi level lies below the out-of-plane states by an energy $W(n)$. Consequently, the resistivity will show a semiconducting behavior corresponding to activation energy $W(n)$. However, this semiconducting behavior will last only up to $T^* \approx W(n)$. Here T^* is the crossover temperature. The correlation-induced finite lifetime of carrier holes τ_{ab} will force ρ_c to show metallic behavior for large $T > W(n)$. This ''crossover'' in $\rho_c(T)$ from insulating to metallic behavior, occurs while $\rho_{ab}(T)$ remains metallic for all T. This is what is observed in most of the samples of the cuprate systems.

For overdoped systems, the Fermi level may pass through the energy level of the out-of-plane states. The $La_{2-x}Sr_xCuO_4$ sample of Nakamura and Uchida[3] for $x = 0.3$ appears to correspond to this case. In this case $\rho_c(T)$ turns out to be always metallic. This amounts to a crossover to metallic behavior for the whole temperature range when the carrier density exceeds a critical value n_0 (i.e., $n > n_0$).

Although the present model is a phenomenological one, it is weaved around the essential features of the cuprate systems. The coherent interpretation of experiments on three different systems for different doping give credence to the model. This phenomenological model may serve as a pointer in search of a microscopic theory of transport along the c axis of the normal state of cuprate superconductors.

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[54] We consider the density of states at Fermi level, $N(0)$ to be independent of T due to the following reasons. The way Zha *et al.* (Ref. 34) have used the Knight-shift data for extracting the density of states $N(0)$ makes it clear that this (latter) quantity involves effects of the correlations that exist in the cuprate systems. In the present model the correlation effects are accounted for in terms of the gap $W(n)$. Thus, if we take $N(0)$ similar to that of Zha *et al.*, we will be considering the correlation effects twice. In order to avoid such an inconsistency we consider $N(0)$ to be T-independent.

[55] This feature is also evident for low hole density from the observed electronic band structure of the doped holes in cuprate system. See, e.g., E. Dagotto *et al.*, Phys. Rev. Lett. **74**, 310 (1995); A. A. Abrikosov *et al.*, Physica C **214**, 73 (1993).