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Model for c-axis transport in high-T_c cuprates

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We present a model for the c-axis resistivity ρ_c in the cuprates which incorporates interplanar disorder. Higher-order perturbative calculations demonstrate that this special disorder stabilizes a low-T metallic state and in the dynamical limit leads to temperature-dependent slopes $d\rho_c/dT$ which are negative (positive) for low (high) hole concentrations. Predictions are presented for correlations which associate a nonlinear planar resistivity with the magnitude of negative $d\rho_c/dT$.

Understanding the nature of c-axis transport in the copper oxides has fundamental consequences for theories of the normal as well as superconducting state.[1] It has been argued that the "semiconductinglike" temperature dependences which are frequently observed indicate a failure of Fermi liquid theory: localization in the c direction alone is inconsistent with the scaling theory of disordered systems. Thus it is claimed that there can be no two-dimensional metallic (i.e., Fermi liquid) state. The situation is made even more complex by the presence of strong Coulomb effects (which underlie the Mott insulating phase) and by the particular nature of the disorder which is predominantly interplanar or "off-diagonal."

In this paper we examine these issues microscopically within the context of a theory, which treats incoherent c-axis conduction as in a highly disordered but nevertheless metallic state. Here the word "incoherent" designates a situation in which there is finite conductivity although the relevant Bloch waves are not defined over several lattice constants.[2–4] Static as well as dynamic interplanar disorder is included and systematic expansions in the (static) scattering matrix element are shown to be fully consistent with a metallic ground state. In this way there is no contradiction with the general concepts of localization theory, which have been raised as objections to a more conventional treatment of the cuprates. However, just as in highly disordered metals a negative resistivity slope $d\rho/dT$ can arise at sufficiently high temperatures T from phonon or other boson assisted hopping processes.

A second and important goal of this paper is to make direct contact with existing experimental trends as well as present experimental tests of our picture. An interesting consequence of our model is the correlation between nonlinearity in ρ_{ab} and the magnitude of the increase with decreasing T of ρ_c. We show here that these effects become more pronounced with decreasing carrier concentration. Elsewhere this deviation from linearity has been associated with "spin gap" effects.[5]

We consider the following model of an anisotropic three-dimensional disordered system.

$$H = \sum_{\mathbf{x},m} \left[W_{\mathbf{x},m}\hat{n}_{\mathbf{x},m} + t_{\parallel} \sum_{i=1,2} \left(c^{\dagger}_{\mathbf{x},m} c_{\mathbf{x}+\mathbf{e}_i,m} + \text{H.c.} \right) + \left((t_{\perp} + V_{\mathbf{x},m}) c^{\dagger}_{\mathbf{x},m} c_{\mathbf{x},m+1} + \text{H.c.} \right) \right] + H_{ab} \quad , \qquad (1)$$

where the $c^{\dagger}$ and c's refer to creation and annihilation operators, m is a plane index, $\mathbf{x}$ is a two-dimensional coordinate within each plane, and W and V are random variables which introduce "diagonal" and "off-diagonal" disorder, respectively. In (1), H_{ab} contains in-plane correlation effects, that in particular give rise to a linear inverse lifetime: $\tau_{ab}^{-1} = \text{Im}\Sigma_{ab} = 2\pi\lambda kT$, where $\lambda \sim 0.2$–0.4, as determined from ac conductivity measurements. This term gives rise to the linear (in temperature) ab resistivity in the case of decoupled planes.

We will be interested in the regime of high anisotropy in which the ratio of the interplane to intraplane hopping matrix elements, $t_{\perp}/t_{\parallel} \ll 1$. We treat Coulomb effects only insofar as they are incorporated into renormalizations of $t_{\parallel}$ and $t_{\perp}$. These renormalizations restrict the hopping so that the closer the system is to the insulating state the smaller are both $t_{\parallel}$ and $t_{\perp}$.

Our model contains two limiting cases which have been discussed in the literature. In the limit $V = 0$, the c-axis conductivity yields $\rho_{ab} \propto \rho_c$ for both a Bloch wave description ($t_{\perp} > T$) and for the Giaver tunneling or perturbative limit ($t_{\perp} < T$). The opposite case in which $\tau_{ab} \to \infty$, $t_{\perp} = 0$, and $V \neq 0$ has been discussed in Ref. 6 where it is shown within a Boltzmann-Born approximation that static disorder leads to a lifetime in the ab plane whereas it provides the hopping mechanism for transport in the c direction. Thus $\rho_{ab} \propto \rho_c^{-1}$. A combination of these two cases, such as we advocate here, is discussed in Ref. 7, but the full diagrammatic resummation (and therefore a demonstration of self consistency) is not addressed, nor are the detailed experimental consequences explored.

We consider separately the two regimes of static and dynamic off diagonal disorder. In the latter case, $V_{\mathbf{x},m}$ in (1) is replaced by a dynamical bosonic variable $V_2(b_{x,m} + b^{\dagger}_{x,m})$ which may be viewed as phonon or spin fluctuation assisted hopping. In addition the Hamiltonian includes a term that reflects the decoupled dynamics of these bosonic variables. In the static case we consider uncorrelated disorder such that $\langle V_{\mathbf{x},m} \rangle = 0$, and analogously for diagonal disorder $W_{\mathbf{x},m}$. We argue that the static and dynamic limits are qualitatively similar, with the statistical average over impurities being replaced by a thermal average of the boson fluctuations. We characterize the fluctuations by two random functions that obey white-noise Gaussian statistics

$$\langle V_{\mathbf{x}',m'} V_{\mathbf{x},m} \rangle = (V_1^2 + V_2^2)\delta(\mathbf{x}-\mathbf{x}')\delta_{m,m'} , \qquad (2)$$

where V_1^2 are the static and V_2^2 the dynamic contributions, respectively. The latter is given by a temperature-dependent function $I(T)$.

We evaluate the conductivity in the c direction using the Kubo formula

$$\sigma_c(\omega) = \frac{i}{\omega}\int_0^\infty dt\, e^{i(\omega+i0)}\langle[\hat{j}_c(t),\hat{j}_c(0)]\rangle , \qquad (3)$$

with the current operator given by

$$\hat{j}_c = ie\sum_{\mathbf{x},m}\left((t_\perp + V_{\mathbf{x},m})c^\dagger_{\mathbf{x},n}c_{\mathbf{x},n+1} - \text{H.c.}\right) . \qquad (4)$$

In the static case the impurity averaged conductivity in (3) generates two classes of diagrams. One class corresponds to the usual terms that arise in perturbation theory, where the unperturbed one-particle states are eigenstates of momentum $\mathbf{k}$. The presence of off-diagonal disorder with a Gaussian distribution gives rise to a second class of diagrams with "diffusive" vertices. These respective contributions for direct ($t_\perp$) and random (V) hopping are additive in σ_c (after impurity averaging). We find

$$\sigma_c(\omega) = \frac{A(n)}{2}\frac{1}{-i\omega + \frac{1}{\tau'}} + e^2V^2N^2(0) . \qquad (5)$$

Here $A(n)$ is a general prefactor given by $N(0)e^2t_\perp^2$ in the case $t_\perp < T$ and $ne^2t_\perp$ in the oppposite case (where we take the interplane distance as unity). In (5) we have explicitly written the lowest nonvanishing term in the expansion in V^2. This will be justified below by a demonstration that this perturbation theory is stable under localization corrections. In (5) $\frac{1}{\tau'}$ contains lifetime effects that come both from the in-plane (diagonal) impurities (τ_1) as well as off-diagonal disorder (τ_2). It should be noted that vertex corrections coming from the ladder diagrams cancel in τ_1 since diagonal disorder corresponds to structureless point impurities. By contrast τ_2 corresponds to impurities connecting two different planes, thereby giving rise to a $\mathbf{k}$-dependent self energy and therefore a distinction between the one-particle and transport lifetime.

The limit $t_\perp = 0$ is particularly interesting. In this case the c-axis contribution is given by

$$\sigma_c(\omega) = e^2V^2N^2(0) , \qquad (6)$$

where $N(0)$ is the two-dimensional density of states at the Fermi level. While this is in some sense an extreme and possibly unphysical, special case, it appears also to give rise to a metallic behavior. The frequency independence of (6), which arises as a direct consequence of the diffusive vertices, has been obtained elsewhere.[6,8,9]

For the a-b conduction we get the usual Drude behavior

$$\sigma_{ab}(\omega) = \frac{nt_\parallel^2e^2}{2}\frac{1}{-i\omega+\frac{1}{\tau}} , \qquad (7)$$

with $\frac{1}{\tau}$ including the effects of both diagonal and off-diagonal disorder. Furthermore, if $V^2 \gg W^2$, then the lifetime effects of plane waves in the a-b direction are dominated by the off-diagonal couplings, $\frac{1}{\tau} \sim V^2N(0)$, and

$$\sigma_{ab} \sim \tau , \quad \sigma_c \sim \frac{1}{\tau} , \qquad (8)$$

as was obtained previously[6] at the perturbative level.

A focus of the present paper is to explore higher-order corrections to determine if the metallic behavior contained in Eqs. (5) and (7) , as well as the special case (6), is stable. Indeed the regime $V^2 \gg t_\perp^2$ is in some sense strongly disordered. Within the framework of Anderson localization it could be argued that in this case there is no conduction in the c direction. It would then follow that the conduction processes in the ab plane should be treated as two dimensional and thus disorder within the plane would lead to an insulating planar state as well. However, our detailed numerical and analytical calculations, which evaluate the ladder and maximally crossed diagrams, demonstrate that Eq. (5) is qualitatively robust, so that there is nonzero c-axis conduction even when localization corrections are included.[10] Other work which has addressed the different temperature dependences of the conductivities assuming an Anderson insulator with very anisotropic localization lengths can be found in Ref. 11. Our results are a consequence of the delocalizing nature of off-diagonal disorder. These conclusions are consistent with earlier studies which showed that the effects of off-diagonal disorder V on the mobility edge compete with diagonal disorder.[12] More specifically the bandwidth of extended states is an increasing function of V.

We turn next to dynamical disorder. The effect of the dynamic term on σ_{ab} is to add to the inverse lifetime a contribution proportional to V_2^2; therefore its effect is superimposed on that of the *in-plane* boson which gives rise to the linear ab resistivity. This is a consequence of Matthiesen's rule which applies to these processes in the ab plane.

By contrast, along the c axis the interplanar dynamical contribution V_2^2 increases σ_c with increasing T, which reflects the increasing amplitude of the tunneling matrix element. This contribution from the diffusive vertex opposes the temperature-dependent effects arising from the in-plane boson which (via $t_\perp$) lead to a decrease in the conductivity (as temperature increases). This latter effect which is associated with the interplanar lifetime can be viewed as thermal dephasing. From these considerations and Eqs. (7) and (5) it is straightforward to show that the zero frequency conductivities in the c-axis and ab plane directions are of the general form[13]

$$\sigma_c = bI(T) + c + \frac{1}{b'T+c'}, \qquad (9a)$$

$$\sigma_{ab} = \frac{1}{a+dT+d'I(T)}, \qquad (9b)$$

where c' and c derive from the static impurity contributions (diagonal and off-diagonal, respectively), $c' \sim t_\perp^{-2}$, and the high-temperature amplitude of the thermal fluctuations of V_2, $I(T) \sim T$.

The different temperature dependences appearing in Eqs. (9) are consequences of the breakdown of Matthiesen's rule resulting from the diffusive vertex. This behavior, which is similar to that of Ref. 7 can be contrasted with that obtained by Anderson and Zhou[15] and (for different reasons) by Littlewood and Varma,[16] who find $\rho_c = AT + B/T$. In these other theories the c-axis conduction is nonmetallic in the ground state so that ρ_c is infinite. Furthermore, the system becomes a poor conductor again at sufficiently high temperatures.

Distinguishing between the two viewpoints and in particular between a metallic or nonmetallic behavior of ρ_c as $T \to 0$ is to some extent academic, since this regime is cut off by the superconducting transition. The present approach is however compatible with a Fermi liquid based viewpoint, whereas those of Refs. 15 and 16 are not. Furthermore it is predicted here that ρ_c may either increase or decrease with T at high T depending on the degree of disorder and the magnitude of the hole concentration (which sets the scale for $t_\perp$). In Refs. 15 and 16, ρ_c ultimately increases with T.

The parameters in the model are hole concentration x dependent; Coulomb renormalizations imply that the parallel and perpendicular hopping matrix elements progressively increase with x. This explains why in the overdoped regime of La-Sr-Cu-O, (where the off-diagonal disorder also increases), σ_c begins to approach σ_{ab}. More generally, since the effects of hole doping (x) are mainly interplanar, it is reasonable to assume that the interplanar disorder (V) decreases faster with decreasing x than the intraplanar disorder (W). As a consequence, the residual resistivities $\rho_c(0)$, $\rho_{ab}(0)$ and their ratio $\rho_c(0)/\rho_{ab}(0)$ also increase with decreasing x, as is observed experimentally.

Our remaining conclusions may be stated in a more quantitative fashion by distinguishing between various regimes of the parameter space. As an illustration of the associated temperature dependences, in Figs. 1(a) and (b), we plot the ab and c-axis resistivities (normalized to the residual resistivity) as a function of T in terms of the characteristic energy scale for the boson assisted hopping T^*. The highest energy c-axis phonons correspond to a Debye temperature $\omega_D = 80 - 100$ meV. For simplicity we take a Bloch-Gruneisen form for the spectral function $I(T)$. Thus a linear contribution will appear in $I(T)$ for $T > T^* = \omega_D/4$ which is approximately $200 - 250$ K.

We consider three extreme cases: (i) $V_2^2 \gg t_\perp^2$. We associate this limit with the underdoped regime for Y-Ba-Cu-O and La-Sr-Cu-O compounds. Here ρ_c decreases with increasing temperature, while ρ_{ab} is roughly linear with T, with deviations from linearity associated with the degree of downturn in ρ_c. This corresponds to the short- and long-dashed curves of Fig. 1. (ii) $V_2^2 \ll t_\perp^2$. We associate this limit with optimally doped Y-Ba-Cu-O and, in general, overdoped systems such as in the La-Sr-Cu-O family. In this case ρ_{ab} and ρ_c both have a similar T dependence, as shown by the solid lines in Fig. 1. (iii)

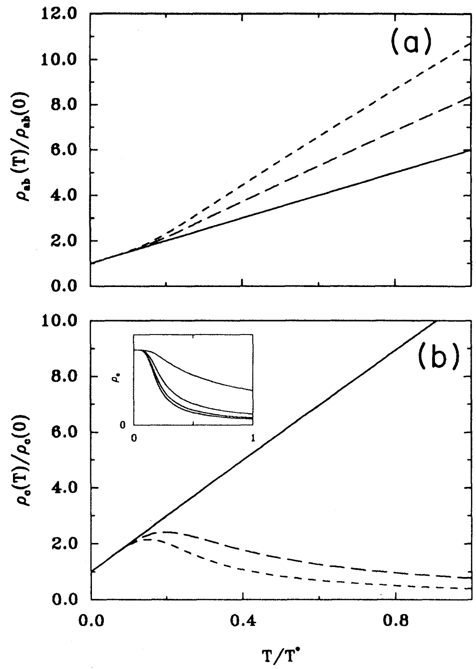

FIG. 1. Resistivity as a function of temperature both in-plane (a) and in the c direction (b). The three curves correspond to increasing values of $V_2/t_\perp$ (amplitude of dynamic off-diagonal disorder): 0 (solid), 1 (dashed) and 2 (short dashed). The inset corresponds to $t_\perp = 0$ and different values of $V_2/t_\parallel$.

$V_2 = 0$, $V_1^2 \gg t_\perp^2$. In this regime static off-diagonal impurities dominate the c-axis transport. ρ_{ab} is linear and ρ_c is roughly temperature and frequency independent as in Ref. 6. This limit appears to correspond to La-Sr-Cu-O at and slightly below optimal stoichiometry. In considering other cuprates, it appears that the one layer thallium compounds exhibit the canonical behavior of optimal to overdoped systems as in (ii). By contrast members of the Bi-Sr-Ca-Cu-O family may not fit into our physical picture. There the anisotropy is so high that the c axis is

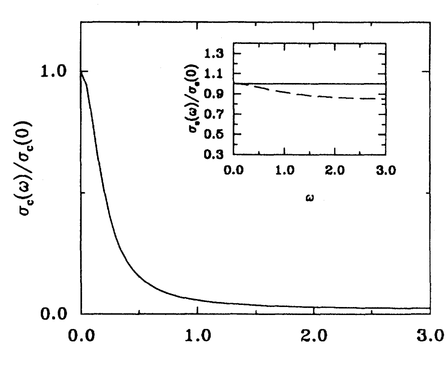

FIG. 2. Optical conductivity in the c direction as a function of frequency for $(t_\perp/V)^2 = 10$ and $t_\perp = 1$. The inset corresponds to $t_\perp = 0$ (solid line) and $(t_\perp/V)^2 = 1$ (dashed line).

possibly insulating at $T = 0$. This insulating behavior is unlikely to arise from anisotropic localization[17] or possibly from a tunneling barrier picture.[18] In the inset of Fig. 1(b) are shown results for the special case $t_\perp = 0$ which may be viewed as representative of extremely anisotropic, but nevertheless metallic behavior. Here the resistivity decreases monotonically and at high $T > T^*$ behaves roughly as $1/T$.

The frequency dependence of the c-axis conductivity is plotted in Fig. 2. As seen in (5), this has a Drude contribution with constant background. In the temperature regime where ρ_c has a negative slope, the background term will outweigh that of the Drude term, as indicated in the inset. The overall result is that for underdoped cuprates (where the residual conductivity is very small), σ_c is essentially frequency independent, and the Drude contribution will not be detectable. By contrast in the overdoped regime, the behavior will be dominated by a Drude frequency dependence shown in the main portion of the figure. These results appear to be consistent with the general experimental trend[1] that when $d\rho_c/dT$ is positive (negative) Drude behavior will (will not) be observed.

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[1] For a review of experiments see Y. Iye, in *Physical Properties of High T_c Superconductors*, edited by D. M. Ginsberg (World Scientific, Singapore, 1992).

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[8] Recent numerical calculations by A. G. Rojo and J. Miller (unpublished) lend support to this, at first sight, surprising conclusion that the metallic state is stable under higher-order corrections.

[9] The f-sum rule is nevertheless satisfied since there is necessarily a frequency cutoff above which $\sigma_c = 0$.

[10] We have proven that (6) is the first term in a convergent expansion in powers of V^2. The first term shown corresponds to a diffusive tunneling between two adjacent layers. The higher-order terms can be written in the form $\sigma_c' = V^4 \left[2\pi N(E_F)\right]^3 \tilde{\tau}$, where $\tilde{\tau}$ depends both on V and W (diagonal disorder). This last expression is of infinite order (through $\tilde{\tau}$) in the sense that it includes hops between layers which are far apart.

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[13] In Eq. (9) we have omitted vertex corrections and therefore we obtain from V_2 an equivalent contribution to the lifetime in the c direction and inverse lifetime for the ab direction. In analogy with the electron phonon problem, if this correction were added we expect a low-temperature difference between $I(T)$ in σ_c and σ_{ab} (see also Ref. 14).

[14] For phonons, we expect $I(T) \sim T^5$ in (9a) and $I(T) \sim T^3$ in (9b). This difference arises because the vertex correction arising from c-axis phonons alone vanishes for ab conduction.

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