c-axis Conductivity in the Normal State of Cuprate Superconductors

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The c-axis optical conductivity and dc resistivity are calculated within the t-J model assuming that the interlayer hopping is incoherent. Use is made of numerical results for spectral functions recently obtained with the finite-temperature Lanczos method for finite two-dimensional systems. In the optimally doped regime we find an anomalous relaxation rate $\tau_c^{-1} \propto \omega + \xi_c T$ and $\rho_c(T) \propto \rho_{ab}(T)$, suggesting a common relaxation mechanism for intra- and interlayer transport. At low doping a pseudogap opening in the density of states appears to be responsible for a semimetalliclike behavior of $\rho_c(T)$. [S0031-9007(98)07458-4]

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One of the most striking characteristics of cuprate superconductors is the anisotropy of their structures. The CuO_2 planes common to all high-T_c materials clearly determine most of the normal-state electronic properties which are quite anomalous but at the same time rather universal within the whole family of cuprates. The quantity which most evidently displays the anisotropy of a particular material is the optical conductivity $\sigma(\omega, T)$ and the corresponding dc resistivity $\rho(T)$ [1,2]. The ratio $\zeta(T) = \rho_c/\rho_{ab}$ of the c-axis resistivity ρ_c to the in-plane resistivity ρ_{ab} for temperatures T just above T_c in optimum-doped materials ranges from $\zeta \sim 100$ for $YBa_2Cu_3O_{7-\delta}$ (YBCO), $\zeta \sim 1000$ for $La_{2-x}Sr_xCuO_4$ (LSCO) to $\zeta > 10^5$ in $Bi_2Sr_2CaCu_2O_8$.

In spite of such large quantitative differences there are common qualitative features even in the c-axis transport, in particular, regarding the variation with doping. (a) Optimum-doped YBCO and overdoped LSCO show metalliclike $\rho_c(T) \sim a + bT$ for $T > T_c$. At the same time the optical conductivity $\sigma_c(\omega)$ shows a falloff with ω although far from the usual Fermi-liquid Drude-type behavior. (b) For lower doping the variation is generally semimetalliclike with $d\rho_c/dT < 0$ in the interval $T_c < T < T^*$. The crossover temperature T^* showing up, e.g., as a kink in the in-plane $\rho_{ab}(T)$, in the Hall constant $R_H(T)$, etc. [3], decreases with doping and merges with T_c at the optimum doping. Within the low-doping regime $\sigma_c(\omega)$ is nearly flat in a wide frequency regime for higher T while a pseudogap starts to emerge for $\omega < \omega^*$ for lower $T < T_{\rm pg} < T^*$.

The c-axis conductivity has attracted the attention of theoreticians since the first measurements on cuprates [1]. In spite of open challenging questions of anomalous planar properties, there seems to be an agreement in the conclusion that the c-axis conductivity generally cannot be explained as a coherent interlayer transport [4,5]. The main indication is that the dc σ_c is mostly well below the Mott minimum metallic conductivity [6], with the possible exception of optimum-doped YBCO and overdoped LSCO [1]. In other words, estimates of the mean free path in the c direction appear much shorter than the interlayer distance c_0, i.e., $l_c(T) \ll c_0$, when one assumes the usual Boltzmann approach for metals. The absence of coherent c-axis conduction is a consequence of weak interlayer-hopping matrix element t_c but also of a strong intralayer scattering. Based on the concept of dynamical detuning, Leggett [4] thus derives the condition for the incoherent conduction $t_c \ll 1/\tau_a \sim k_{\rm B}T$ taking the relaxation rate according to anomalous planar $\rho_{ab}(T)$ and $\sigma_{ab}(\omega)$. The incoherent conductivity has been studied in more detail on the example of coupled fermion chains [5] representing Luttinger liquids. Still there have been so far no real attempts to derive more explicitly the c-axis conductivity for models relevant to cuprates.

In this paper we present the theoretical analysis of $\sigma_c(\omega)$ within the simplest microscopic model incorporating both strong electron correlations in the CuO planes leading to antiferromagnetism in undoped materials, and a weak interlayer coupling. Within each layer we consider the planar t-J model

$$H_l = -t \sum_{\langle ij \rangle s} (c_{ljs}^\dagger c_{lis} + \mathrm{H.c.}) + J \sum_{\langle ij \rangle} (\mathbf{S}_{li} \cdot \mathbf{S}_{lj} - \tfrac{1}{4} n_{li} n_{lj}), \tag{1}$$

where i, j refer to planar sites on a square lattice within the lth layer and $c_{lis}, c_{lis}^\dagger$ represent projected fermion operators forbidding double occupation of sites. As appropriate for cuprates we assume $J = 0.3t$. We allow for the hopping between layers,

$$H = \sum_l H_l - t_c \sum_{lis} (c_{lis}^\dagger c_{l+1is} + \mathrm{H.c.}). \tag{2}$$

The planar t-J model is still a challenge for theoreticians; nevertheless, there is a growing consensus that it contains essential ingredients for an explanation of the anomalous normal-state properties of cuprates, dominated by effects of strong correlations. The lack of reliable analytical methods in the latter regime led to numerous numerical studies [7]. Using the novel finite-temperature Lanczos method (FTLM) [8], it has been shown that several thermodynamic quantities as well as response functions match well the experimental data on cuprates. Most relevant for the present study are the results on the planar conductivity $\sigma_{ab}(\omega)$ [9] and the single-particle spectral functions $A(\mathbf{k},\omega)$ [10].

In the limit of weak interlayer hopping $t_c \ll t$ it is straightforward to evaluate the dynamical c-axis conductivity $\sigma_c(\omega)$ using the linear response theory. Expressing the c-axis current correlation function $\langle j_c(t) j_c \rangle$, with $j_c = e_0 t_c c_0 \sum_{lis} (i c^\dagger_{lis} c_{l+1is} + \text{H.c.})$, in terms of the planar spectral functions $A(\mathbf{k},\omega)$, we arrive at

$$\sigma_c(\omega) = \frac{\sigma_c^0}{\omega} \int d\omega' [f(\omega') - f(\omega' + \omega)] \times \frac{4\pi t^2}{N} \sum_{\mathbf{k}} A(\mathbf{k},\omega') A(\mathbf{k},\omega' + \omega), \quad (3)$$

where $\sigma_c^0 = e_0^2 t_c^2 c_0 / \hbar a_0^2 t^2$ is a characteristic c-axis conductivity scale, N is the number of sites, and $f(\omega) = [1 + \exp(\omega/k_{\mathrm{B}}T)]^{-1}$. The approximation assumes the independent electron propagation in each layer, and is justified for $t_c \ll t$. Note that the interlayer-hopping term, Eq. (2), *conserves* the quasiparticle (QP) momentum $\mathbf{k}$, and in this respect the treatment is analogous to the one of the transverse transport in weakly coupled Luttinger chains [5]. This could be compared with a related problem of interlayer hopping with random matrix elements $(t_c)_{li}$, where only the planar density of states (DOS) $\mathcal{N}(\omega) = 2/N \sum_{\mathbf{k}} A(\mathbf{k}, \omega - \mu)$ enters, with μ denoting the chemical potential. The corresponding expression for the $\mathbf{k}$-nonconserving $\sigma_c^n(\omega)$ is obtained by the replacement

$$\sigma_c^n(\omega) = \frac{\sigma_c^0}{\omega} \int d\omega' [f(\omega') - f(\omega' + \omega)] \times \pi t^2 \mathcal{N}(\mu + \omega') \mathcal{N}(\mu + \omega' + \omega), \quad (4)$$

appearing, e.g., in disordered systems [6], together with a substitution for t_c in the definition of σ_c^0 with some average $\bar{t}_c$. In cuprates both alternatives have a justification, since the disorder introduced by dopands residing between layers modifies the hopping elements. Hence one can expect that the actual conductivity is a linear combination of σ_c and σ_c^n.

The knowledge of planar $A(\mathbf{k},\omega)$ and $\mathcal{N}(\mu + \omega)$ should thus suffice for the evaluation of $\sigma_c(\omega)$. In cuprates, however, spectral functions are available with sufficient resolution only in the hole part $\omega < 0$ (in principle) via the angle-resolved photoemission [11] and the DOS via the angle-integrated photoemission [12]. Within the t-J model (and the closely related Hubbard model) $A(\mathbf{k},\omega)$ and $\mathcal{N}(\omega)$ have been studied mostly numerically [7], applying the exact diagonalization of small systems [13] and the quantum Monte Carlo method [14]. Results reveal at intermediate doping a large Fermi surface (consistent with the Luttinger theorem) and a quasiparticle dispersion $\epsilon_{\mathbf{k}}$ similar to but reduced in bandwidth relative to the free tight-binding electrons. Only recently, via the FTLM [8], a reliable evaluation of the corresponding self-energy $\Sigma(\mathbf{k},\omega)$ was possible, thus allowing for a study of low-T QP properties. The spectral functions and $\sigma_{ab}(\omega)$ both reveal in this regime the anomalous behavior consistent with the marginal Fermi liquid (MFL) concept [15], i.e., the effective transport relaxation rate as well as the QP damping appear to follow $1/\tau_{ab}(\omega) \propto \Sigma''(\mathbf{k},\omega) \propto |\omega| + \xi_{ab} T$.

In this paper we use numerical results for $A(\mathbf{k},\omega)$ and $\mathcal{N}(\omega)$, as obtained using FTLM on systems with $N = 16, 18, 20$ sites for various hole dopings $c_h = N_h/N$. Spectral functions are available for the whole range of N_h for $N = 16$, $N_h \leq 2$ for $N = 18$, and $N_h \leq 1$ for $N = 20$ [8,10]. One should keep in mind the restriction that FTLM results become dominated by finite-size effects for $T < T_{fs}$. T_{fs} is clearly size and doping dependent. The lowest T can be reached in the intermediate regime $c_h \sim 0.2$ where $T_{fs} \sim 0.1t$, while T_{fs} increases for both lower and higher doping. To make contact with experiments, we note that $t \sim 0.4$ eV, i.e., our numerical results apply to $T \gtrsim 450$ K, while for lower T they can give some qualitative indications.

To set the frame for further discussion let us first present in Fig. 1 the DOS $\mathcal{N}(\mu + \omega)$ for the two lowest nonzero doping levels $c_h = 1/20$ and $c_h = 2/18$ for several $T \leq J$. The DOS at larger doping $c_h \gtrsim 0.15$ (not shown here) [10] is T-independent and featureless at $\omega \sim 0$, as expected for a Fermi liquid away from van Hove singularities. At low doping the DOS in Fig. 1 is also structurelesss for $T > J$, but here this reflects the incoherent character of QP due to large damping. Upon lowering T a gradual transfer of weight in the underdoped samples from above μ to $\omega < 0$ is observed, leading to

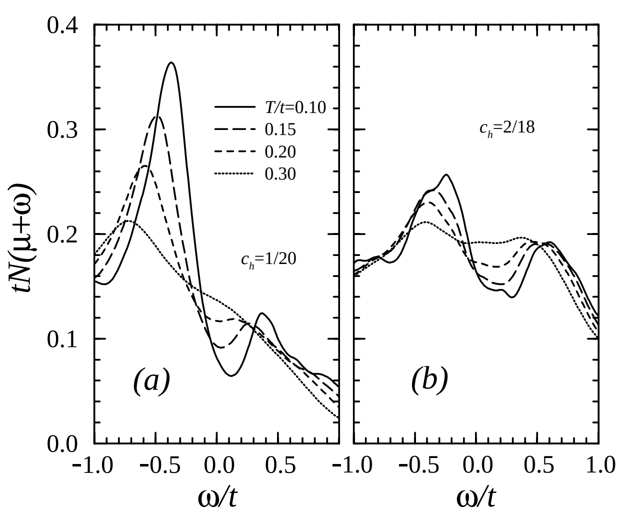

FIG. 1. The DOS $\mathcal{N}(\mu + \omega)$ at various $T \leq J$ for hole concentrations: (a) $c_h = 1/20$ and (b) $c_h = 2/18$.

the formation of a pseudogap at $\omega \sim 0$. The deepening is more pronounced for lowest dopings, e.g., $c_h = 1/20$ in Fig. 1(a), where the pseudogap energy scale is well below t and appears to be $\Delta_{\rm pg} \sim J$, reflecting the onset of the short-range antiferromagnetic order. The above development of the DOS as well as the behavior of SF and corresponding (anomalous) self-energies should determine the behavior of optical conductivity $\sigma_c(\omega)$. In Fig. 2 we show $\sigma_c(\omega)$ for two dopings $c_h = 3/16$ and $c_h = 1/20$ for $T \le J$, as calculated from Eq. (3). At intermediate doping $c_h = 3/16$ $\sigma_c(\omega)$ in Fig. 2 exhibits a central peak, sharpening at lower T. This can be explained with the properties of $A(\mathbf{k},\omega)$ in this regime, consistent with a large Fermi surface and a QP dispersion $\epsilon_{\mathbf{k}}$ corresponding to a tight-binding band. The QP damping is, however, large and MFL-like $\Sigma''(\mathbf{k},\omega) \propto |\omega| + \xi_{ab}T$, but only weakly $\mathbf{k}$-dependent. Inserting the latter into Eq. (3) it is easy to see that the resulting $\sigma_c(\omega)$ also follows the MFL behavior; i.e., one can represent it in the generalized Drude form with an effective relaxation rate $1/\tau_c \propto |\omega| + \xi_c T$. The vanishing rate for $\omega, T \to 0$ is clearly the consequence of the $\mathbf{k}$ conservation in the interlayer hopping. On the other hand, Eq. (4) would yield a qualitatively different result, i.e., an almost flat and T-independent $\sigma_c^n(\omega)$ due to the structureless DOS $\mathcal{N}(\omega)$ for $\omega \sim 0$.

The corresponding results for low-doping $c_h = 1/20$ are also shown in Fig. 2. In contrast, we find rather weakly ω- and T-dependent $\sigma_c(\omega)$, both for the $\mathbf{k}$-conserved and the $\mathbf{k}$-nonconserved approximation. Quantitative agreement of both approaches indicates that in this regime we are dealing with a strongly reduced effective dispersion $\epsilon_{\mathbf{k}} \propto J$ but still large QP damping, hence weakly $\mathbf{k}$-dependent $A(\mathbf{k},\omega) \sim \mathcal{N}(\mu + \omega)$, at least for $T > T_{fs}$. It seems puzzling how rather constant $\sigma_c^n(\omega)$ in Fig. 2 for $c_h = 1/20$ can be compatible with a well pronounced pseudogap at $\omega \sim 0$ in the DOS (see Fig. 1) at low $T < T^*$. These facts are, however, reconciled by observing that the Fermi functions in Eqs. (3) and (4) have an effective width $\sim 4T$, hence down to reachable T_{fs} they smear out both the QP dispersion as well as the $\Delta_{\rm pg}$. Nevertheless, there is some signature of a pseudogap opening on a scale $\omega \sim J$ in $\sigma_c(\omega)$ for lowest T, in qualitative agreement with experimental data [16].

In Fig. 3 we present the dc resistivity $\rho_c(T) = 1/\sigma_c(\omega = 0, T)$ for a wider range of c_h. In the regime of intermediate and even higher doping $c_h \ge 3/16$ $\rho_c(T)$ is metalliclike for all T. In particular, from the previous arguments relating the c-axis transport to the MFL-like planar relaxation one expects that $\rho_c(T) \propto T$ for $T < J$. From Fig. 3 we realize that the latter behavior is really restricted to $T < 0.2t$. It should be stressed again that in this regime weak interlayer disorder as implied by Eq. (3) is *essential* for the resulting linear-in-T behavior of $\rho_c(T)$, whereas $\rho_c(T)$ in the case of $\mathbf{k}$-nonconserving interlayer hopping yields an almost T-independent $\rho_c(T)$.

For the lowest $c_h = 2/18$ and $c_h = 1/20$, ρ_c and ρ_c^n yield the same qualitative behavior, $\rho_c^n(T)$ being systematically higher. While $\rho_c(T)$ is increasing for $T > J, t$ as generally expected for incoherent transport, the relevant question is its behavior for $T < J$. In Fig. 3 we notice that in this regime $d\rho_c/dT \sim 0$, signaling the onset of a nonmetalliclike behavior in agreement with experimental results for cuprates in the underdoped region [17].

When we comment on the relation of our results with measurements on cuprates, the most natural application is to LSCO having the simplest layered structure among cuprates. The presence of several nonequidistant layers per unit cell, and possibly chains as well, in other materials complicate the interpretation of the c-axis transport considerably. In Fig. 4 we present the resistivity ratio $\zeta(T) = \rho_c/\rho_{ab}$ as a function of T for different doping levels, where results for ρ_{ab} are taken from previous

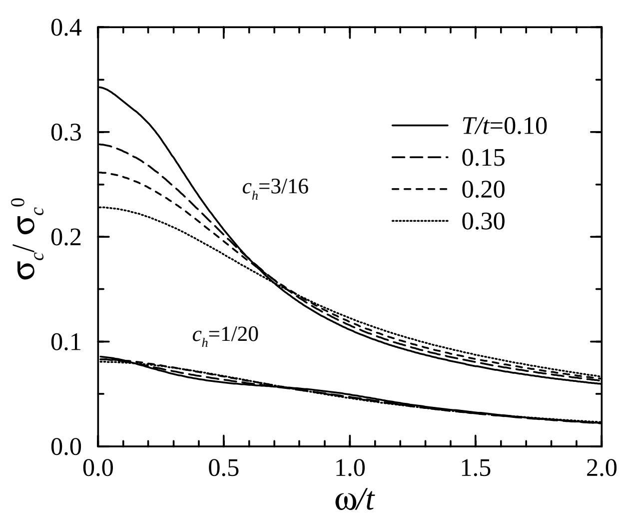

FIG. 2. $\sigma_c(\omega)$ at several T for dopings: $c_h = 3/16$ and $c_h = 1/20$.

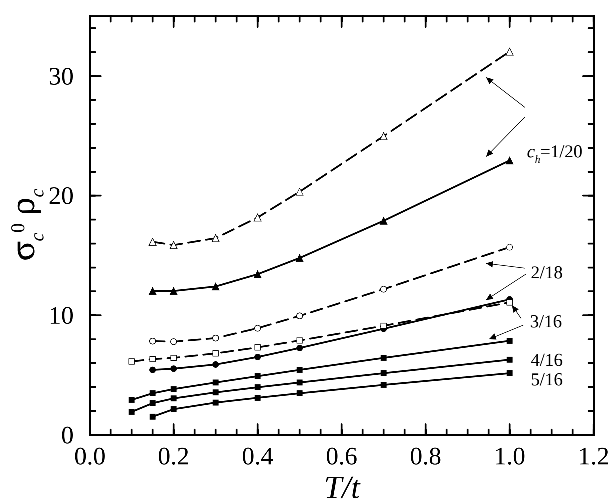

FIG. 3. $\rho_c(T)$ vs T for various c_h. Solid and dashed lines represent results within the $\mathbf{k}$-conserving and $\mathbf{k}$-nonconserving approximations, respectively.

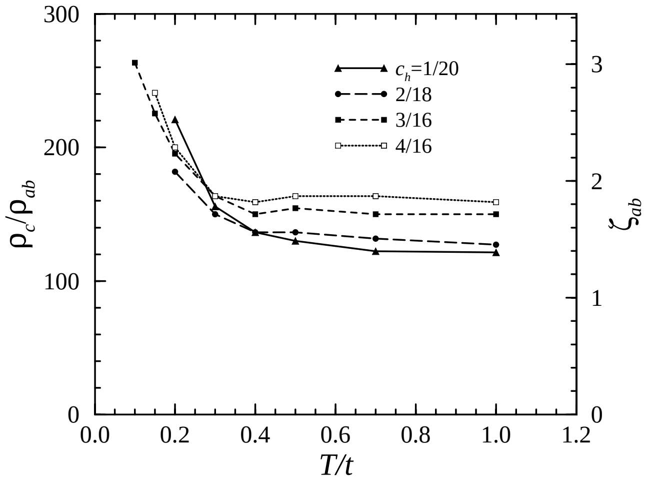

FIG. 4. ρ_c/ρ_{ab} vs T for various c_h (left scale) and $\zeta_{ab}(T) = \rho_{ab}^{\rm dec}/\rho_{ab}$ (right scale).

FTLM studies [9]. In the saturation regime $T \gtrsim J$ we set $\zeta \sim 150$ as obtained from experimental data for LSCO, e.g., by Nakamura and Uchida [17] and Kao *et al.* [18] from which we can estimate t_c. Taking the standard value for $c_0/a_0 = 3.5$ in LSCO [1] we get $t_c \sim 0.03t$, or $t_c \sim 12$ meV.

A distinctive feature is that $\zeta(T)$ is almost independent of c_h and T, but for the lowest $T < J$ presented. This indicates that planar resistivity and c-axis resistivity are related, at least for $T > T_{fs}$, pointing to a common current relaxation mechanism in all directions. In fact, if we calculate within the same decoupling scheme the planar conductivity $\sigma_{ab}^{\rm dec}(\omega)$ and the related $\rho_{ab}^{\rm dec}(T)$, the actual $\sigma_{ab}(\omega)$ is reproduced remarkably well, as can be concluded from $\zeta_{ab}(T) = \rho_{ab}^{\rm dec}/\rho_{ab}$ in Fig. 4. For $T \sim J$ we detect the onset of a different behavior, although the ratio is less affected than $\rho_{ab}(T)$ and $\rho_c(T)$ separately. It is, however, indicative that the increase of $\zeta(T)$ is most pronounced for lowest c_h. Our results for $\zeta(T)$ are in a remarkable qualitative agreement with experimental data [18].

In conclusion, let us briefly summarize our main results on the c-axis conductivity. In our analysis $\sigma_c(\omega, T)$ is obtained from (numerically) known SF and DOS for the planar *t-J* model supplemented with a small (doping independent) interlayer hopping t_c leading to the incoherent c-axis transport. A qualitative agreement with experiments in LSCO, e.g., for the anisotropy $\zeta(T)$, gives support to such a minimum model. Our results also confirm the general experimental observation that $\rho_c(T)$ changes from a metallic one to a semimetallic one $d\rho_c(T)/dT \lesssim 0$ by decreasing doping. It should be noted, however, that in the overdoped regime LSCO already shows indications of an enhanced coherentlike c-axis transport which is beyond our analysis assuming $t_c \ll t$.

Let us finally point to open questions, mainly related to the onset of a pseudogap in $\sigma_c(\omega)$ and even semiconductorlike $d\rho_c(T)/dT \ll 0$ as found experimentally in underdoped cuprates [2]. In our analysis the indication for such a development comes from a pseudogap in the DOS, which at low doping starts to emerge for $T < T^* \lesssim J$, and is compatible with recent photoemission experiments [12]. Clearly, this phenomenon is related to the onset of short-range antiferromagnetic spin correlations, persisting up to the optimum doping. It is also evident from our results that this does not lead directly to a well pronounced pseudogap in $\sigma_c(\omega)$ at the same T. Eventually this can happen only for $T < T_{\rm pg} < T^*$, which in our systems is hardly reachable due to $T_{fs} \sim 0.2t$ at low doping. One simple explanation can be given in terms of the Fermi-function broadening $\sim 4T$. Another source of suppression of the pseudogap in calculated $\sigma_c(\omega)$ is the shift of the photoemission leading edge towards μ (see Fig. 1), thus compensating in part for the deepening of the pseudogap in the DOS at lowest T. This results in a much weaker doping dependence of ρ_c down to $T \sim T_{fs}$, not inconsistent with experimental data [17] which show semiconductorlike upturn only at lower T. Still it remains the subject of future studies to clarify whether the small pseudogap scale in underdoped cuprates is directly related to the T^* scale or is of different origin.

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