NORMAL-STATE C-AXIS RESISTIVITY OF THE HIGH-\(T_c\) CUPRATE SUPERCONDUCTORS

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Abstract

It is shown that a strong intraplanar incoherent scattering can effectively block the interplanar coherent tunneling between the weakly coupled planes of the highly anisotropic but clean (intrinsic) materials such as the optimally doped high-\(T_c\) layered cuprate superconductors. The calculated normal-state C-axis resistivity \(\rho_c(T)\) then follows the metal-like temperature dependence of the ab-plane resistivity \(\rho_{ab}(T)\) at high temperatures. At low enough temperatures, however, \(\rho_c(T)\) exhibits a non-metal like upturn even as \(\rho_{ab}(T)\) remains metallic. Moreover, in the metallic regime, \(\rho_c(T)\) is not limited by the maximum metallic resistivity of Mott-Ioffe-Regel. This correlation between the intrinsic \(\rho_c(T)\) and \(\rho_{ab}(T)\) is observed in the normal state of the high-\(T_c\) stoichiometric cuprates.
1. Introduction.

The normal-state out-of-plane resistivity $\rho_c(T)$ of the high-$T_c$ layered cuprate superconductors\(^1\) has raised a number of questions,\(^2,3\) as yet unresolved, about its temperature dependence, its absolute magnitude, and its dependence on the concentration of carriers, i.e., doping. Thus, while the in-plane resistivity $\rho_{ab}(T)$ is well known to be metallic\(^1\) (i.e., with $TCR \equiv \partial \rho_{ab}/\partial T > 0$, and, in fact, essentially T-linear right from $T_c$ upwards to the highest temperature of measurement) and smaller than the Mott-Ioffe-Regel maximum metallic resistivity $\rho_{max}^M$, the out-of-plane resistivity $\rho_c(T)$ shows a range of behaviour. Thus, it has been variously reported to be non-metallic\(^4−8\) ($TCR < 0$) for underdoped samples; mixed-metallic\(^1,9,10\) (metallic at high temperatures but with a non-metallic upturn at low enough temperatures); and completely metallic\(^5−7,9−14\) for stoichiometric (fully oxygenated) composition showing a T-linear $\rho_c(T)$ from $T_c$ upwards, but with the absolute magnitude of $\rho_c(T) > \rho_{max}^M$ in all cases.

The essential structural feature of weakly coupled layers and the associated large resistive anisotropy with $\rho_c(T)/\rho_{ab}(T) \sim 10^2 − 10^5$, clearly makes the C-axis resistivity highly sensitive to extrinsic details that presumably tend to contaminate its intrinsic behaviour. Thus, it is entirely possible for any measurement of the out-of-plane resistivity to pick up some in-plane component of the resistivity tensor — perhaps externally due to misalignment of the contacts, or internally due to the randomly distributed defects and faults providing shorts between the weakly coupled ab-planes.\(^15\) Such a contamination of the out-of-plane $\rho_c(T)$ by the in-plane $\rho_{ab}(T)$ can make $\rho_c(T)$ track the metallic temperature dependence of $\rho_{ab}(T)$, making the former (
\( \rho_c(T) \) an apparent metal.\(^{15} \) The resistivity data on high quality untwinned single crystals, however, strongly suggests that the out-of-plane resistivity \( \rho_c(T) \) is intrinsically metallic, and in fact T-linear\(^{11,14} \) at least at high temperatures, just as the in-plane \( \rho_{ab}(T) \) is. Its absolute magnitude is, however, much larger. Recently, we had proposed a mechanism that gave precisely such a behaviour. In this mechanism\(^{16} \) the inter-planar tunneling between the weakly coupled metallic planes is cut-off (blocked) by the intra-planar inelastic (incoherent) scattering, leading to \( \rho_c(T) \propto \rho_{ab}(T) \). This physical mechanism has since gained a fair degree of acceptance among the workers in the field,\(^2 \) while some earlier theories, linked closely to the exotic mechanisms for high-\( T_c \) superconductivity in the strongly correlated CuO\(_2\) sheets, have been argued out to be inconsistent with known experimental facts.\(^3 \) Motivated by these developments, we have re-examined the mechanism proposed by us earlier based on simple physical arguments. In doing so we have derived an expression for \( \rho_c(T) \) following the Kubo-Matsubara conductivity formalism applied to a model Hamiltonian incorporating weak interplanar tunneling and strong intraplanar incoherent scattering. Our \( \rho_c(T) \) so derived indeed shows a metallic behaviour with \( \rho_c(T) \propto \rho_{ab}(T) \) in the high temperature limit, thus validating our mechanism proposed earlier. At low enough temperatures, however, we get an additional feature of a resistivity upturn \( (\partial \rho_c/\partial T < 0) \), which is qualitatively consistent with observations as noted above. In the following, we give some details of our derivation, and discuss our results for \( \rho_c(T) \) in the light of some recent findings.

2. Theoretical.

First note that the C-axis transport, except possibly for the overdoped
cuprates, is known to be incoherent, e.g., \( \omega_{pc} \tau_{ab} \ll 1 \), where \( \omega_{pc} \) is the C-axis plasma frequency and \( 1/\tau_{ab} \) is the intraplanar inelastic scattering rate.\(^2\)\(^,\)\(^17\) Thus, the successive interplanar tunneling amplitudes are phase-uncorrelated. It is, therefore, sufficient to consider simply a bilayer (AB) coupled weakly by a tunneling matrix element \((-t_c)\). In real systems the individual layer (A or B) can by itself represent a single \( \text{CuO}_2 \) sheet as in LSCO, or also a group of strongly coupled \( \text{CuO}_2 \) sheets, as in YBCO, BSCCO and other multilayered cuprates, separated by the spacer oxide layers. Also, we will consider only the clean limit as suggested by the smallness of the zero-temperature intercept\(^11\) \( \rho_{ab}(T \to 0) \), and also assume that the inter-planar tunneling conserves the wavevector parallel to the a-plane. Then the model Hamiltonian (in obvious notation) is

\[
H = H_a + H_b + H_{ab} + H_{aa} + H_{bb}, \tag{1}
\]

with

\[
H_a = \sum_{k\sigma} \epsilon_k a_{k\sigma}^\dagger a_{k\sigma},
\]

\[
H_b = \sum_{k\sigma} \epsilon_k b_{k\sigma}^\dagger b_{k\sigma},
\]

\[
H_{ab} = -t_c \sum_{k\sigma} (a_{k\sigma}^\dagger b_{k\sigma} + b_{k\sigma}^\dagger a_{k\sigma})
\]

In the following we will drop the spin index \( \sigma \). Here \( H_{aa} \) and \( H_{bb} \) represent the inelastic intra-planar electron-electron scattering characteristic of the strongly correlated two-dimensional \( \text{CuO}_2 \) sheets. In the present analysis, however, these terms shall enter only implicitly and summarily through the imaginary part of the associated retarded electron self-energy chosen so as to be consistent with the known T-linear in-plane resistivity \( \rho_{ab}(T) \).\(^18\) Our
problem then is to calculate the out-of-plane resistivity $\rho_c(T)$, given the above $\rho_{ab}(T)$ as an input. It is really this connection between $\rho_c(T)$ and $\rho_{ab}(T)$ that is being addressed here.

Now, for the inter-planar current operator, we have

$$j_c = -ie t_c \sum_k (a_k^+ b_k - b_k^+ a_k).$$

(2)

The Kubo conductivity in the dc limit is then given by \((\hbar = 1)^{19}\)

$$\sigma = -\left(\frac{c}{L^2}\right) \omega \lim_{\omega \rightarrow 0} \frac{Im\Pi_{ret}(\omega)}{\omega},$$

(3)

where $c =$ bilayer separation (the C-axis lattice constant), $L^2 =$ area of the layer, and the retarded correlation

$$\Pi_{ret}(\omega) = \lim \Pi(i\omega_\nu)$$

(4)

$$i\omega_\nu \rightarrow \omega + i\delta \text{ (analytic continuation)}$$

with $\Pi(i\omega_\nu)$, the current-current correlation given by

$$\Pi(i\omega_\nu) = 2e^2 t_c^2 \sum_k \frac{1}{\beta} G_a(k, i\omega_n) G_b(k, i\omega_n + i\omega_\nu)$$

(5)

with

$$\omega_\nu = \frac{2\pi \nu}{\beta}, \text{ the Bosonic Matsubara frequency},$$

$$\omega_n = \frac{(2n+1)\pi}{\beta}, \text{ the Fermionic Matsubara frequency}.$$

Here $G_a$ and $G_b$ are the temperature Green functions for the layers A and B, respectively, in the presence of inter-planar tunneling. For identical layers, as in the present case, we have $G_a = G_b = G$, say.

In the high temperature limit, i.e., for $\hbar/\tau_{ab} \gg |t_c|$, we can evaluate $G$ in the presence of interplanar tunneling in terms of $G_o$, the corresponding
temperature Green function in the absence of tunneling, from the Dyson equation

\[ G_a = G_{oa} + G_{oa} t_c G_{bt_c} G_{oa}, \]  

(6)
giving

\[ G_a = G_b \equiv G = \frac{G_o}{1 - t_c^2 G_o^2}. \]  

(7)

In writing Eqn. (6) we have used the approximation that for \( \hbar/\tau_{ab} \gg |t_c| \) one can neglect the vertex correction arising from the interplanar tunneling \( t_c \).

Now, the intra-planar thermal Green function \( G_o(k, i\omega_n) \) corresponds to an isolated layer (i.e., with \( t_c = 0 \)) and has the general form

\[ G_o(k, i\omega_n) = \frac{1}{i\omega_n - \epsilon_k - \Sigma(k, i\omega_n)}. \]  

(8)

Substituting from Eqns. (8) and (7) into Eq. (5), we get

\[ \Pi(i\omega_\nu) = 2e^2 t_c^2 \sum_{k,n} G_{o\eta}(k, i\omega_n)G_{o\xi}(k, i\omega_n + i\omega_\nu) \]  

(9)

Here \( \pm \) refers to \( G_o \) in Eq. (8) with \( \epsilon_k \) replaced by \( \epsilon_k \pm |t_c| \).

Now we impose our condition of T-linearity of \( \rho_{ab}(T) \) as input at the level of \( G_o(k, i\omega_n) \) namely, that the self-energy of the corresponding retarded Green function must have an imaginary part \( \Delta(T) \) (at the Fermi level) \( = -Im \sum_{ret} \propto T \). With this input Eq. (9) together with Eq. (3) gives, after the usual frequency summation and analytic continuation, a simple expression for the dc conductivity

\[ \sigma = \frac{1}{2} \left( \frac{e^2}{\hbar c} \right) (c^2 \nu) \frac{|t_c|^2}{\Delta(T)} \frac{1}{1 + \left( t_c/\Delta(T) \right)^2}. \]  

(10)

Here we have introduced the two-dimensional density of states \( \nu \), assumed constant. Also, \( \hbar \) has been re-instated. This is our main result.
Eq. (10) it is readily seen that in the high-temperature limit, \( \Delta(T) \gg |t_c| \), \( \sigma \propto 1/(\Delta(T)) \), or equivalently, the C-axis resistivity \( \rho_c(T) \propto \Delta(T) \propto T \), confirming the T-linearity of \( \rho_c(T) \) at high temperatures. It is also clear that this mechanism giving incoherent transport along the c-axis does not involve the usual \( k_F\ell \)-parameter characteristic of metallic transport. Hence, \( \rho_c(T) \) is not subject to \( \rho_{\text{max}}^M \).

Next, we consider the low-temperature limit, \( \hbar/\tau_c < |t_c| \). Now, we must diagonalize the tunneling Hamiltonian \( H_t \equiv H_a + H_b + H_{ab} \) first, and then use the T-linearity of \( \rho_{ab}(T) \) as an input at the level of the layer-diagonal Green function. We have

\[
H_t = \sum_k (\epsilon_k - |t_c|)\alpha^\dagger_k \alpha_k + \sum_k (\epsilon_k + |t_c|)\beta^\dagger_k \beta_k,
\]

where \( \alpha_k = (a_k + b_k)/\sqrt{2} \), \( \beta_k = (a_k - b_k)/\sqrt{2} \). The inter-planar current operator

\[
\hat{J} = i e t_c \sum_k (\alpha^\dagger_k \beta_k - \beta^\dagger_k \alpha_k).
\]

Repeating the earlier steps with this current operator, we now get

\[
\sigma = \frac{1}{2} \frac{(e^2)(c^2\nu)}{\hbar^2} \frac{\Delta(T)t_c^2}{t_c^2 + \Delta^2(T)}
\]

Thus, at low enough temperatures we get an upturn for \( \rho_c \) because \( \Delta(T) \propto T \). This upturn has been noticed as discussed earlier. It must be emphasized here that this upturn is a consequence of our assumption of conservation of wavevector parallel to the planes in the tunneling process. This leads to a hybridization gap that suppresses the overlap of the spectral functions corresponding to \( G_{o+} \) and \( G_{o-} \).
3. Discussion.

We would now like to comment on a recent attempt to explain away the metallicitiy of $\rho_c(T)$ as a thermal expansion effect. Based on a recent study of the pressure dependence of $\rho_c(T)$ and the lattice constant ‘c’ in $La_{2-x}Sr_xCuO_4$, it has been argued that the observed metallicity (i.e., TCR > 0) merely reflects a thermal expansion effect, i.e.,

$$TCR \equiv (\partial \rho_c/\partial T)_P = (\partial \rho_c/\partial P)_T (\partial c/\partial P)_T^{-1} (\partial c/\partial T)_P,$$

and, therefore, the observed metallicity is only apparent. While some such expansion effect cannot be ruled out, we find the argument somewhat flawed for the following reason. The thermal expansion $< \delta c >$ of the lattice parameter ‘c’, or more precisely $< \delta B >$ of the width ‘B’ of the potential barrier for the rate-determining tunneling, is a mean-anharmonic effect that, of course, tends to diminish the tunneling rate. There is, however, also a thermal fluctuation about this mean-value which is of comparable magnitude, if not larger. Now, inasmuch as the tunneling time is expected to be much shorter than the typical lattice vibrational time period, we must average the instantaneous tunneling rate over the anharmonic fluctuations of $\delta B$. As the tunneling rate depends exponentially on $\delta B$, overall it is expected to produce an enhancement of the tunneling rate with increasing temperature, and hence a negative, rather than positive TCR.

Finally, a remark on the recent attempts to explain the resistivity upturn in terms of pre-existing real-space pairs (Bosonic) as precursor to their condensation at $T_c$. Such a system of charged Bosons in the normal state is, however, expected to exhibit large, universal diamagnetism which is not reported.
In conclusion, the present microscopic-treatment of the C-axis resistivity supports the mechanism proposed by us earlier, namely that the strong intra-planar incoherent scattering cuts-off the interplanar tunneling, and thus correlates $\rho_c(T)$ with $\rho_{ab}(T)$. 
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