

Linear resistivities in the copper oxides: Fermi-liquid-based approaches

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Mechanisms for a linear temperature-dependent resistivity are discussed in Fermi-liquid-based approaches. For realistic models of the cuprates this behavior arises for temperatures T above the Van Hove energy scale $T^* < 50$ K. This crossover temperature is substantially reduced in magnitude by Coulomb correlations for a wide range of hole concentrations. Calculations of the spectral function α^2F show important \mathbf{q} structure and therefore differences with the "marginal" ansatz. Spin-spin interactions adversely affect the linear resistivity when the system is close to an antiferromagnetic instability. Comparison with NMR calculations indicates that different energy scales are playing a role in resistivity and NMR probes, as observed experimentally.

Whether or not the many transport and magnetic anomalies observed in the metallic copper oxides above T_c are compatible with Fermi-liquid theory is the subject of considerable controversy. Among the most striking features of these metals is the ubiquitous linear resistivity,¹ which is in contrast to a T^2 Fermi-liquid behavior. In support of a Fermi-liquid approach, photoemission experiments have demonstrated² that there exists a Fermi surface (above T_c) which satisfies Luttinger's theorem. In this paper we discuss the origin of the linear resistivity and build on our understanding in the context of other Fermi-liquid systems. Our calculations also focus on the connection between NMR relaxation and the electronic contribution to the resistivity, both of which depend on similar response functions, and both of which experimentally appear to contain different energy scales.

The observation that a linear resistivity can occur within the Fermi-liquid regime is well known in the context of scattering from phonons³ (ph) and localized spin fluctuations (SF), as, for example, in actinide metals.⁴ In these cases the carriers scatter from fluctuations (bosons) external to the charge-carrier system which leads to a linear resistivity at temperatures greater than $\frac{1}{4}$ of the characteristic boson frequency ω_{ph} or ω_{SF} . In addition, scattering between the current carriers is also found to give rise to a linear temperature dependence, above the lowest temperature T^2 regime. Experimental realization of this behavior is found in heavy-fermion metals,⁵ but, presumably, it occurs below the characteristic degeneracy temperature T_{coh} .

A strictly linear resistivity which derives from electronic mechanisms requires (in a Fermi-liquid context) that two criteria be simultaneously satisfied. (1) The T^2 to T "crossover" occurs at temperatures less than T_c . (2) The transport spectral function α^2F must be, at most, weakly dependent on T (as in the case of phonons). Low Fermi-liquid energy scales naturally lead to (1). However, quite frequently, these low electronic energies lead to a breakdown of (2), so that electron-electron scattering is not generally expected to yield linear resistivities over a wide range of T . This is what is observed in the heavy-fermion metals. Similarly in the actinides, where the scattering derives from an electron-boson (spin fluctuation) interaction, α^2F is also too strongly T dependent to yield an ex-

tended linear resistivity. With these Fermi-liquid precedents for the cuprates in mind, it follows that obtaining a linear resistivity over the entire normal-state regime (which may include temperatures as low as 10 K) is a fairly subtle matter.

In the following, it is argued that for the cuprates, an important contribution to the observed linear resistivity ρ arises from a two-dimensional band-structure feature, the Van Hove singularity T^* , whose energy scale is renormalized by Coulomb correlations. Although previous theories⁶ have emphasized the importance of this Van Hove singularity (and/or nesting), one of the main contributions of the present work is to establish that, because of strong Coulomb corrections, T^* is a small energy scale for a wide range of hole concentrations away from half filling. In addition, it is demonstrated that the Van Hove effect is rather unique in that it leads to a relatively temperature-independent transport spectral function α^2F .

Any Fermi-liquid approach to the cuprates must explain why deviations occur, in a wide variety of experiments, from *canonical* Fermi-liquid behavior at the temperatures of the normal state. This suggests that there are electronic energy scales T_{coh} , T^* , and T_{SF} which are comparable to the superconducting transition temperatures. In an "almost localized" Fermi-liquid picture, which we have previously discussed,⁷⁻⁹ a comparison of heavy-fermion and cuprate data suggests⁹ that T_{coh} is roughly 100–300 K in the oxides. As a result, the Cu d electrons are only fully coherent, or itinerant, at low temperatures, $T < T_{\text{coh}}$, and they become progressively more localized as the temperature is raised, just as do the f electrons of the heavy-fermion metals. (In the latter, T_{coh} is generally 2 orders of magnitude smaller.) Full localization is achieved at temperatures T_{loc} , far too high (5000–10000 K) to be observed experimentally, although the counterpart phenomenon is observed in the heavy fermions. For much, if not all, of the temperature regime of the normal state the cuprates are described by a "partially coherent" Fermi liquid.

Alternate proposals for low-energy scales (T_{SF}) in a Fermi-liquid picture assume a proximity to an antiferromagnetic transition.¹⁰ On the basis of considerable experimental evidence for some degree of quasilocization¹¹ of the Cu electrons, and because these "nearly magnetic"

Fermi-liquid approaches are not particularly robust with varying concentration, here it is assumed that the localization instability dominates the physics of the cuprates. Magnetic correlations are, however, generally present in nearly localized models, and will also be considered here.

Our starting point is the three-band Anderson lattice or extended Hubbard Hamiltonian which contains Cu d and oxygen p electrons with strong Coulomb repulsion on the d site. Since the case of large, but finite U is difficult to implement, we take U to be infinite, as is often assumed to be the case. We use the $1/N$ expansion which is one of several equivalent schemes (where N is the d and p electron spin degeneracy) to provide the mean-field equations for deriving the quasiparticle dispersion. This leads to a renormalized quasiparticle band structure (or “one component”) description of the antibonding band and has been previously applied with some success to study the Hall coefficient,⁷ NMR relaxation and neutron-scattering cross section⁸ and the electron-phonon contribution to the resistivity.⁷ It was found in Ref. 7 that the phononic contribution can account for a substantial fraction of the resistivity slope dp/dT for moderate and large hole concentrations, but that as the insulator is approached the experimentally observed increase in slope cannot be explained by electron-phonon scattering alone. This suggests that some electronic or other bosonic mechanism must be invoked. Here we consider the former by calculating the electron lifetime derived from the dynamical susceptibility. This calculation of the temperature dependence of the resistivity is in the same spirit as previous approaches,^{6,12} except that here the effects of very strong Coulomb correlations on the dynamical susceptibility are included.

The quasiparticle lifetime due to electron-electron scattering can be calculated from standard expressions

$$\frac{1}{\tau} = \int_0^{\infty} d\omega N(\epsilon_F) \alpha^2 F(\omega, T) \frac{1}{\sinh(\omega/T)}. \quad (1)$$

Here $\alpha^2 F(\omega, T)$ is the transport spectral function associated with the electron-electron interactions. This function is defined as

$$\alpha^2 F(\omega, T) = \frac{1}{N(\epsilon_F)} \left\langle \left\langle \int \frac{d\mathbf{k}}{2\pi^2} \delta(\omega - \epsilon_{\mathbf{k}}) g^2(\mathbf{p}_F - \mathbf{k}) \times \chi''(\mathbf{p}_F - \mathbf{k}, \omega) \right\rangle \right\rangle_F \quad (2)$$

where $\langle \langle \dots \rangle \rangle_F$ represents the Fermi-surface average over different directions of the Fermi wave vector p_F and χ'' is the imaginary part of the dynamical susceptibility. This susceptibility has been calculated elsewhere,⁸ within a random-phase approximation scheme and found it to be of the form

$$\chi = \chi_0 / [1 - J(\mathbf{q})\chi_0], \quad (3)$$

where $J(\mathbf{q})$ is the quasiparticle spin exchange [evaluated⁸ to order $(1/N)^2$]. Here the susceptibility is to be interpreted as a 2×2 matrix in the (Cu) $3d$ and (O) $2p$ wavefunction space. The \mathbf{q} dependence of $J(\mathbf{q})$ may be roughly approximated by a nearest-neighbor form $J(\mathbf{q}) = J_0 [\cos(q_x a) + \cos(q_y a)]$. Finally, χ_0 is the Lindhard susceptibility associated with the renormalized band

structure. We assume g is a structureless coupling constant and define $N(\epsilon_F)$ as the density of states at the Fermi energy. The whole procedure can be made more precise in the context of a $1/N$ expansion which was developed for the heavy-fermion problem.¹² There it was shown that the $1/N$ formalism leads to an expression similar to that of Eq. (1) and yields, at sufficiently low temperatures, the usual T^2 term in the resistivity. As a first approximation, extension to higher temperature may be viewed as arising entirely from thermal smearing effects which enter through the Fermi functions in χ'' and lead to the $\sinh(\omega/T)$ contribution in Eq. (1). At sufficiently high temperatures, this Fermi-liquid-based scheme must break down and a new formalism introduced to account for the growing incoherence⁹ of the Fermi-liquid state. We estimate that the characteristic upper limit to T is of the order of $4T_{\text{coh}}$.

The various energy scales which govern the behavior of $\alpha^2 F$ are illustrated by studying the density of states of the renormalized band structure. Plotted in Fig. 1 is the density of states for the antibonding band for a hole concentration of $x=0.28$ (which might be viewed as corresponding to fully oxygenated $\text{YBa}_2\text{Cu}_3\text{O}_7$) with the parameters $\epsilon_p - \epsilon_d^0 = 4.0$ eV and with hybridization $V_{dp} = 1.6$ eV and oxygen-oxygen transfer matrix elements $t_{pp} = 0.4$ eV. The results for a smaller concentration of $x=0.16$ are shown in the inset. These parameter choices are derived from estimates based on the band structure of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The temperature T_{coh} corresponds to about a quarter of the splitting between the Fermi energy and nearest band edge and is roughly 150 and 300 K for the lower and upper concentrations, respectively. The figures emphasize the small energy separation between the Fermi (vertical line) and the Van Hove energies. The temperature T^* , which is about $\frac{1}{4}$ of this energy splitting, corresponds to 10 K for the lower and 50 K for the higher concentration. This “pinning” of the Van Hove singularity energy around the Fermi level results from the strong Coulomb repulsion at the copper sites. The importance of this Van Hove energy scale has also been addressed in the context of spectroscopic and magnetic properties.¹³

A family of curves for $\alpha^2 F(\omega, T)$ is shown in Fig. 2(a) as a function of ω and for various exchange energies J_0/J_c and for $x=0.28$ with $T \sim 0$. Here J_c is the critical value of J_0 needed to produce an antiferromagnetic instability.

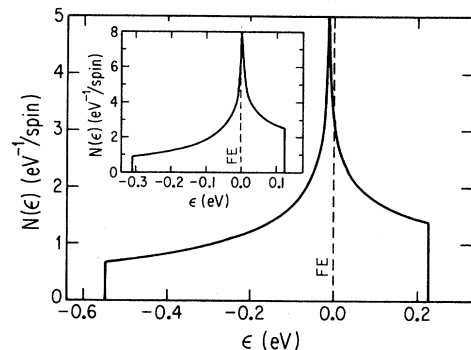


FIG. 1. Density of states as a function of energy for $x=28\%$ and (inset) $x=16\%$. Here FE refers to the Fermi energy.

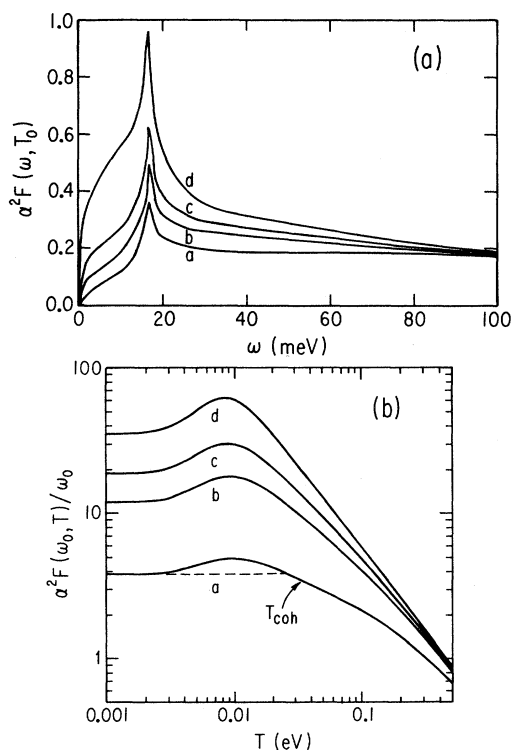


FIG. 2. (a) Frequency dependence of $\alpha^2 F(\omega, T_0 \sim 0)$ for $x=0.28$ and various J_0/J_c equals *a*, 0; *b*, 0.7; *c*, 0.85; *d*, 0.98. (b) Temperature dependence of $\alpha^2 F(\omega_0 \sim 0, T)/\omega_0$ for $x=0.28$ and the same J_0/J_c as in Fig. 2(a).

The pronounced peak at 16 meV for $J_0=0$ is associated with the Van Hove singularity. The effect of nonzero J_0 is to increase the peak height and lower the frequency to T_{SF} . It is important to stress that in either case our results for $\alpha^2 F$ do *not* coincide with the polarizability of the “marginal ansatz.”¹⁴ A comparison of the ω dependence of $\text{Im}\chi_0$, by contrast, shows that for wave vectors \mathbf{q} along the zone diagonal, the marginal ansatz works rather well for $T > T_{coh}$. However, when the appropriate “on-shell,” \mathbf{q} -weighted function is evaluated as $\alpha^2 F$, a peak appears at T^* and this agreement is invalidated. Thus our calculations of this spectral function underline the importance of q structure in $\text{Im}\chi$. The high-frequency, nearly constant, contribution to $\alpha^2 F$ eventually cuts off at the full band edge which corresponds to 3000 and 6000 K for the smaller and larger x , respectively.

While the characteristic frequency structure in $\alpha^2 F$ occurs at the Van Hove energy, its temperature dependence appears to depend primarily on T_{coh} and only weakly (logarithmically) on T^* , for $J_0=0$. This is best illustrated by Fig. 2(b) in which is plotted $\alpha^2 F(\omega_0, T)/\omega_0$, for $\omega_0 \rightarrow 0$, as a function of temperature. When $J_0=0$ (curve *a*) $\alpha^2 F$ is relatively constant in temperature (with only fine structure associated with the Van Hove point) until the temperature is large enough so that the effective d -band edge becomes evident. The effects of nonzero J_0 are shown in curves *b-d*. Here it is clear that the temperature variations become more dramatic, presumably varying as T/T_{SF} , rather than logarithmically, as J_0 increases towards J_c .

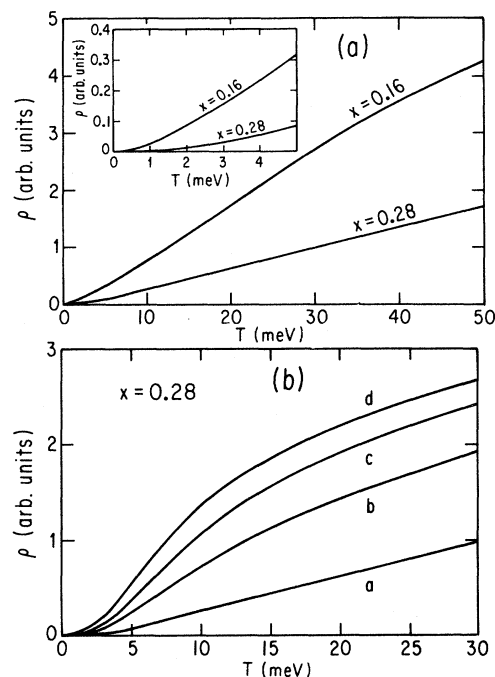


FIG. 3. (a) Temperature dependence of resistivity for $x=0.16$ and $x=0.28$ and $J_0=0$. The inset gives an expanded view of low-temperature behavior. (b) The temperature dependence of resistivity for $x=0.28$ and the same J_0/J_c , as shown in Fig. 2(a).

The resulting temperature dependent resistivities are shown in Fig. 3(a) for $x=0.16$ and 0.28 with $J_0=0$ and Fig. 3(b) for nonzero J_0 . The inset plots the low-temperature, mainly T^2 regime which is below the appropriate superconducting transition temperature and so should not be observable experimentally. The linear regime persists over a wider range of T and the measured trend in the concentration dependence of the slope is consistent with that deduced from our calculations of the lifetimes. At high hole concentrations, as in “overdoped” samples, it is predicted that the Fermi-liquid T^2 regime will become increasingly apparent. The mechanism which yields this linearity is formally similar to that which leads to linear phonon resistivities above $\omega_{ph}/4$. It reflects the saturation of scattering modes, in this case those associated with the lowest energy, Van Hove, scale T^* which dominates $\alpha^2 F$ and therefore ρ . As in the phonon case, the T dependence of ρ above T^* is controlled by the effective number of electrons T/ε_F which are involved in the scattering. While the present theory is not valid at temperatures above $\sim 3-4T_{coh}$, if it is extended without modification, it will lead to departures from linearity and eventual saturation in the resistivity due to saturation of the number of electrons involved in the scattering. This high-temperature regime generally occurs in, for example, actinide metals⁴ in association with a Curie-Weiss $1/T$ dependent dc susceptibility, which is not seen in the cuprates.

The effects of including antiferromagnetic spin fluctuations in the resistivity are illustrated in Fig. 3(b) for $x=0.28$ and various J_0/J_c . In our previous analysis of NMR data we were led to conclude that J_0/J_c was of the

order of 0.6 to 0.7. For larger J_0/J_c , the T dependence of $\alpha^2 F$ is now more profound at low T so that the resistivity is no longer strictly linear. This “over-shooting” behavior has also been demonstrated elsewhere.⁶ Here we find that the \mathbf{q} dependence of $J(\mathbf{q})$ helps to partially counteract these effects due to cancellations.

It might be expected that the NMR spin-induced relaxation rate (at the Cu site) and the resistivity behavior in the cuprates are related, since both properties are based on the same dynamical response function. Experimentally, the two measurements are found to reflect different energy scales since the resistivity does not show structure where the Cu NMR begins to saturate. In addition, theoretically there are differences. As can be seen from Eqs. (1) and (2), the resistivity involves a summation over all frequency modes weighted by an “on-shell” δ function as well as a statistical factor $1/\sinh(\omega/T)$. On the other hand, $1/T_1$ probes only one frequency ω_0 , the nuclear Zeeman energy which is smaller than any electronic energy scale:

$$1/T_1 = \langle \langle A(\mathbf{q})^2 \chi''(\mathbf{q}, \omega_0) \rangle \rangle_{\mathbf{q}} / (\omega_0/T). \quad (4)$$

If the \mathbf{q} dependence of the Cu form factor $A(\mathbf{q})$ is relatively unimportant (as is generally agreed), then the T dependence of $1/T_1 T$ is reflected in the plot of Fig. 2(b).¹⁵ Thus our NMR calculations⁸ found that the dominant NMR energy scale is T_{coh} , renormalized slightly by spin fluctuations. This explains why the characteristic NMR energy scale is¹⁶ roughly 100–200 K. However, due to the integrability of the logarithmic divergence, T^* is only weakly manifested in the temperature dependence of $1/T_1$ and enters by gently “interrupting” the Korringa (linear in T) behavior. The resulting T dependence can be probed experimentally only in low or zero T_c systems, where the low Van Hove temperature is unobscured by

the superconductivity. Indeed, weak structure is found in nonsuperconducting, but metallic cuprates.¹⁶

Further support for the difference of NMR and resistivity energy scales comes from heavy-fermion systems. Here the canonical T^2 resistivity is found at temperatures below T_ρ , which is usually considerably smaller than T_{coh} , as measured in NMR experiments.⁸ Furthermore, the upper limit of the linear regime appears to scale with T_ρ , rather than T_{coh} as found here. Proximity to instabilities, as well as electronic fine structure, may lead to low-energy scales within the Fermi-liquid regime of heavy-fermion metals. It is likely that these differ from the two-dimensional (2D) Van Hove singularity, in that the T dependence in $\alpha^2 F$ associated with these low-energy scales is more profound, just as was found for the “soft” spin fluctuations in Fig. 3(b). This leads to a much narrower regime of linearity in ρ than in the present 2D case, as seems to be observed experimentally.

In conclusion, we have demonstrated that linear temperature-dependent resistivities are not incompatible with Fermi-liquid-based approaches. The 2D Van Hove singularity leads to a low crossover temperature T^* which separates the canonical T^2 from linear regimes. Because of the weak T dependence in $\alpha^2 F$, this 2D effect is rather unique in leading to a low T^* without restricting the range of the linear resistivity. For the cuprates we have argued that T^* is sufficiently low so that the superconducting state obscures the Landau T^2 regime. The observation of a T^2 resistivity in slightly overdoped samples with suppressed T_c reinforces our conclusions.

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