

High-frequency behavior of the infrared conductivity of cuprates

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We analyze recent infrared conductivity data in the normal state of the cuprates. We find that the high-frequency behavior, which has been suggested as evidence for quantum-critical scaling, is generally characteristic of electrons interacting with a broad spectrum of bosons. From explicit calculations, we find a frequency exponent for the modulus of the conductivity, and a phase angle, in good agreement with experiment. The data indicate an upper cutoff of the boson spectrum of the order of 300 meV. This implies that the bosons are of electronic origin rather than phonons.

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Infrared conductivity has proven to be a powerful probe of the electronic degrees of freedom of the cuprates.¹ It has the advantage of being bulk sensitive, and yields useful information over a wide range of energies. Of particular interest is a generalized Drude analysis of the data, which provides information on the optical analog of the fermion self-energy.^{2,3} Most data indicate a linear frequency dependence of the imaginary part of the optical self-energy (i.e., $1/\tau$) up to very high energies. Such behavior is characteristic of a marginal Fermi liquid.⁴ In some data,⁵ this trend persists up to the plasma frequency (1 eV).

Recently, van der Marel and collaborators⁶ have obtained a somewhat different behavior at high frequencies for $1/\tau$, showing a tendency to saturate⁷ above 0.5 eV. They have also found that in a wide frequency range (125–900 meV), both real (σ_1) and imaginary (σ_2) parts of the optical conductivity are described by the same power law (ω^α) with an exponent -0.65 [and an associated phase angle $\phi = \tan^{-1}(\sigma_2/\sigma_1)$ of 60°]. The same behavior was observed earlier by El Azrak *et al.*,⁵ and its theoretical implications discussed extensively by Anderson.⁸ The exponent and phase angle in this frequency range are roughly temperature independent, and have been suggested to be indicative of quantum-critical scaling.⁶

In this paper, we analyze the frequency-dependent optical data using a model based on electrons interacting with a broad spectrum of bosons. We find that the essential results mentioned above are captured by this analysis, indicating that the observed behavior is generic for interacting electrons. We show that the power-law behavior of the conductivity σ is not indicative of quantum-critical scaling,⁹ but rather a consequence of the flattening of the fermionic self-energy at high frequencies. Based on our analysis, we find evidence for an upper cutoff scale of the boson spectrum of about 300 meV in the cuprates. This is consistent with the assumed value in the marginal Fermi-liquid phenomenology,⁴ and also with the measured width of the spin-fluctuation spectrum.¹⁰

The Kubo expression for the optical conductivity can be written as¹¹

$$\sigma(\omega) = \frac{\omega_{pl}^2}{4\pi} \int d\epsilon \frac{f(\epsilon) - f(\omega + \epsilon)}{i\omega} \frac{1}{-\omega - \Sigma^*(\epsilon) + \Sigma(\omega + \epsilon)}, \quad (1)$$

where ω_{pl} is the bare plasma frequency and Σ is the retarded fermion self-energy (in this paper we ignore any momentum-dependent effects). Within the same approximation, the fermion self-energy can be expressed as

$$\Sigma(\omega) = \int \frac{d\Omega}{\pi} \int d\epsilon \alpha^2 F(\Omega) \frac{n_B(\Omega) + f(\epsilon)}{\omega - \epsilon + \Omega + i\delta}, \quad (2)$$

with n_B the Bose function and f the Fermi function. $\alpha^2 F$ is the boson spectral function multiplied by the square of the coupling strength to the fermions and the (bare) fermion density of states (and, thus, is a dimensionless quantity). For $T=0$, the imaginary part of the self-energy becomes

$$-\text{Im} \Sigma(\omega) = \int_0^\omega d\Omega \alpha^2 F(\Omega). \quad (3)$$

The real part can be obtained by Kramers-Kronig transformation. From these expressions, one can easily calculate the real and imaginary parts of the conductivity and the phase angle.

Alternately, one can examine the generalized Drude expression for the conductivity,²

$$\sigma(\omega) = \frac{\omega_{pl}^2}{4\pi} \frac{1}{1/\tau(\omega) - i\omega m^*(\omega)}. \quad (4)$$

An approximation for $1/\tau$ (i.e., $\text{Im} \Sigma_{\text{opt}}$) can be obtained¹¹ by expanding the denominator of Eq. (1) to lowest order, integrating over frequency, and then inverting the result, again using the lowest order expansion, to get $\sigma^{-1}(\omega)$. We call this the Allen approximation. Within this approximation,

$$\frac{1}{\tau(\omega)} = \frac{2}{\omega} \int_0^\omega \text{Im} \Sigma(\Omega) d\Omega = \frac{2}{\omega} \int_0^\omega d\Omega (\omega - \Omega) \alpha^2 F(\Omega). \quad (5)$$

The optical mass, $m^*(\omega) = 1 + \text{Re} \Sigma_{\text{opt}}/\omega$ can then be obtained by Kramers-Kronig.

Surprisingly, we have found that for a broad spectrum of bosons, $1/\tau$ determined exactly from Eq. (1) matches the Allen approximation to a high precision over the entire fre-

quency range,¹² and, therefore, for the purposes of this paper, either expression can be used interchangeably. Because of this, we can easily perform a finite T calculation by using the finite T version of the Allen approximation derived in Ref. 13,

$$1/\tau(\omega) = \frac{1}{\omega} \int_0^\infty d\Omega \alpha^2 F(\Omega) \left[2\omega \coth\left(\frac{\Omega}{2T}\right) - (\omega + \Omega) \coth\left(\frac{\omega + \Omega}{2T}\right) + (\omega - \Omega) \coth\left(\frac{\omega - \Omega}{2T}\right) \right]. \quad (6)$$

In addition, there is the impurity contribution. We assume an energy-independent fermion density of states, so that the impurity contribution to $\text{Im } \Sigma$ is a constant, which we denote as Γ_i , thus, the contribution to $1/\tau$ is $2\Gamma_i$ (with no change to the optical mass).

Since we are addressing data in the normal state, we consider electrons interacting with a broad spectrum of bosons. We have considered two models. First, a Lorentzian spectrum,

$$\alpha^2 F(\Omega) = \text{Im} \frac{\Gamma}{\gamma - i\Omega}, \quad (7)$$

which has been introduced in the context of spin-fluctuation exchange,^{14,15} and used for the charge propagator as well.¹⁶ In our case, we will also incorporate a high-frequency cutoff into Eq. (7). Second, a gapped marginal Fermi liquid¹⁷ (MFL) with

$$\alpha^2 F(\Omega) = \text{Im} \frac{1}{\pi} \frac{\Gamma}{\omega_2 - \omega_1} \ln \frac{\omega_2^2 - (\Omega + i\delta)^2}{\omega_1^2 - (\Omega + i\delta)^2}. \quad (8)$$

This model yields a flat $\alpha^2 F(\Omega)$ between the lower (ω_1) and upper (ω_2) cutoffs. Both spectra give similar results.

We start with the MFL model. At $T=0$, the imaginary part of the fermion self-energy is

$$\begin{aligned} -\text{Im } \Sigma &= \Gamma_i \quad \omega < \omega_1, \\ \Gamma_i + \Gamma \frac{\omega - \omega_1}{\omega_2 - \omega_1} &\quad \omega_1 < \omega < \omega_2, \\ \Gamma_i + \Gamma &\quad \omega_2 < \omega, \end{aligned} \quad (9)$$

where Γ is the frequency-integrated spectral weight for $\alpha^2 F$. The real part of the self-energy is easily determined by Kramers-Kronig,

$$\begin{aligned} \text{Re } \Sigma &= \frac{-\Gamma}{\pi} \left(\frac{\omega - \omega_1}{\omega_2 - \omega_1} \ln \frac{|\omega - \omega_2|}{|\omega - \omega_1|} + \frac{\omega + \omega_1}{\omega_2 - \omega_1} \ln \frac{|\omega + \omega_2|}{|\omega + \omega_1|} \right. \\ &\quad \left. + \ln \frac{|\omega + \omega_2|}{|\omega - \omega_2|} \right). \end{aligned} \quad (10)$$

The expressions for the real and imaginary parts of the optical self-energy in the Allen approximation are

$$1/\tau = 2\Gamma_i, \quad \omega < \omega_1,$$

$$\begin{aligned} 2\Gamma_i + \frac{\Gamma}{\omega} \frac{(\omega - \omega_1)^2}{\omega_2 - \omega_1}, \quad \omega_1 < \omega < \omega_2, \\ 2\Gamma_i + 2\Gamma - \frac{\Gamma}{\omega} (\omega_2 + \omega_1), \quad \omega_2 < \omega, \end{aligned} \quad (11)$$

$$\begin{aligned} \text{Re } \Sigma_{\text{opt}} &= \frac{\Gamma}{\pi \omega (\omega_2 - \omega_1)} [(\omega - \omega_2)^2 \ln |\omega - \omega_2| \\ &\quad + (\omega + \omega_2)^2 \ln |\omega + \omega_2| - (\omega - \omega_1)^2 \ln |\omega - \omega_1| \\ &\quad - (\omega + \omega_1)^2 \ln |\omega + \omega_1| - 2\omega_2^2 \ln \omega_2 + 2\omega_1^2 \ln \omega_1]. \end{aligned} \quad (12)$$

For finite T , a simple analytic expression for $1/\tau(\omega)$ can be obtained only at frequencies $\omega > \omega_2$,

$$1/\tau_{\text{high}} = 2\Gamma_i + \frac{\Gamma}{\omega_2 - \omega_1} \left[4T \ln \frac{\sinh(\omega_2/2T)}{\sinh(\omega_1/2T)} - \frac{\omega_2^2 - \omega_1^2}{\omega} \right]. \quad (13)$$

We determine $1/\tau$ by numerical integration of Eq. (6) at frequencies below 0.5 eV, and use Eq. (13) above this frequency. The optical mass is then determined by numerical Kramers-Kronig.

We have also examined Lorentzian models with either a hard or a soft cutoff. To impose a hard cutoff, we cut $\alpha^2 F(\Omega)$ in Eq. (7) at some $\omega_c \gg \gamma$, to impose a soft cutoff, we add a quadratic frequency term to the denominator of Eq. (7). We obtained similar results in both cases. For brevity, we only present the results for the hard cutoff case. The self-energy at $T=0$ is given by

$$\begin{aligned} -\text{Im } \Sigma &= \Gamma_i + \frac{\Gamma}{2} \ln \frac{\omega^2 + \gamma^2}{\gamma^2}, \quad \omega < \omega_c, \\ \Gamma_i + \frac{\Gamma}{2} \ln \frac{\omega_c^2 + \gamma^2}{\gamma^2}, \quad \omega > \omega_c. \end{aligned}$$

The expressions for the imaginary part of the optical conductivity in the Allen approximation is

$$\begin{aligned} 1/\tau &= 2\Gamma_i + \Gamma \left(\ln \frac{\omega^2 + \gamma^2}{\gamma^2} - 2 + \frac{2\gamma}{\omega} \tan^{-1} \frac{\omega}{\gamma} \right), \quad \omega < \omega_c, \\ 2\Gamma_i + \Gamma \left(\ln \frac{\omega_c^2 + \gamma^2}{\gamma^2} - 2 \frac{\omega_c}{\omega} + \frac{2\gamma}{\omega} \tan^{-1} \frac{\omega_c}{\gamma} \right), \quad \omega > \omega_c. \end{aligned}$$

We start with some general observations. The behavior of the optical self-energy is similar in the two models. $\text{Re } \Sigma_{\text{opt}}$ is initially linear for small frequencies, then bends over, passing through a maximum near the cutoff, with a decay at higher frequencies. $1/\tau$ is linear (except at the lowest frequencies) up to the cutoff. Beyond this, it continues to rise, but much more slowly. It should be noted that in the linear regime, the slopes of $\text{Im } \Sigma$ and $1/\tau$ are almost identical, unlike the impurity contribution which differs by a factor of 2. This can be understood quite simply from Eq. (3). Therefore, we expect that the energy derivative of the scattering rates

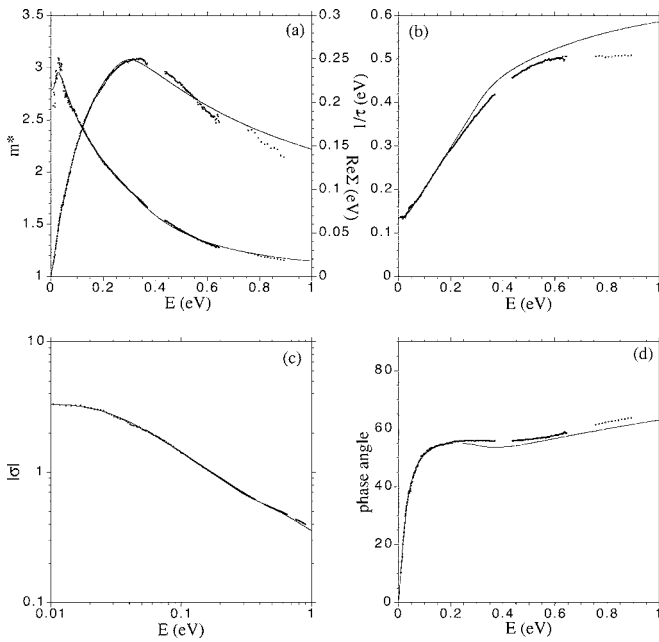


FIG. 1. Fit of the MFL model to $T=260$ K data of van der Marel *et al.* on optimal doped $\text{Bi}_2\text{Sr}_2\text{Ca}_{0.92}\text{Y}_{0.08}\text{Cu}_2\text{O}_{8+\delta}$ (Ref. 6). Parameters are (meV) $\Gamma_i=67.5$, $\Gamma=270.5$, $\omega_1=15.5$, and $\omega_2=301$. Plotted are (a) the optical mass and $\text{Re}\Sigma_{\text{opt}}$, (b) $1/\tau$, (c) the modulus of σ , and (d) the phase angle, $\tan^{-1}(\sigma_2/\sigma_1)$.

from photoemission and optics should coincide, which is indeed the case.¹⁸

Angle-resolved photoemission spectroscopy (ARPES) has yet to address the question of saturation at high frequencies, but optics has. Earlier studies indicated that the linear frequency dependence of $1/\tau$ persists to energies of order 1 eV, but recently van der Marel *et al.*⁶ have seen evidence for saturation. The difference from earlier work has to do with the choice of ϵ_∞ and $\omega_{pl} - 1/\tau$ and m^* are related to the dielectric function ϵ as $\omega^2 m^* + i\omega/\tau = \omega_{pl}^2 / (\epsilon_\infty - \epsilon)$.¹⁹ From an analysis of their data, these authors gave evidence for quantum-critical scaling.⁶ In fact, the tendency for saturation in $1/\tau$, as noted above, is actually indicative of being above the quantum-critical regime.

To see this point more clearly, we show a fit to their data using the MFL model in Fig. 1. We chose to fit the highest temperature data (260 K) as the data at lower temperatures give evidence for a pseudogap effect, which is known from ARPES to be present up to around 200 K for optimal doped samples.²⁰ The fit was performed to the optical mass using Eq. (12). The $T=0$ expression was used as it is analytic and, thus, can be employed in any nonlinear fitting routine.

Some remarks are in order. First, the low-frequency cutoff is evident as a peak in the optical mass at about 15 meV. The high-frequency cutoff is evident as a peak in $\text{Re}\Sigma_{\text{opt}}$ at about 300 meV. Therefore, even without the fit, these values can be read off directly from the data. We should remark that the low-frequency cutoff is not that important (it simply assures that the optical mass does not diverge at low frequencies), and, thus, the fit to $\text{Re}\Sigma_{\text{opt}}$ is essentially a two parameter one (Γ and ω_2). Second, the upper cutoff is also visible where $1/\tau$ deviates from linear behavior. We note that the mismatch

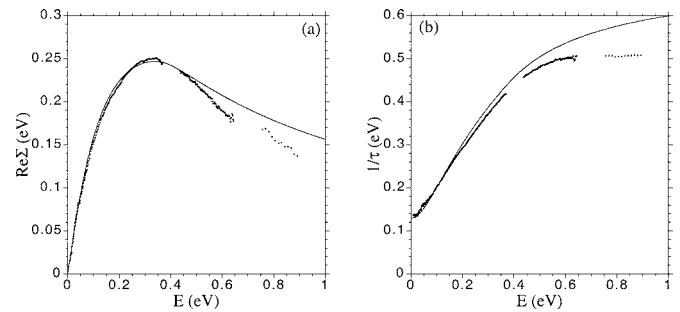


FIG. 2. Fit of the Lorentzian model to $T=260$ K data of van der Marel *et al.* (Ref. 6). Parameters are (meV) $\Gamma_i=65$, $\Gamma=172$, $\gamma=75$, and $\omega_c=380$.

between the fit and data for $1/\tau$ at high frequencies can be compensated by a small shift in the assumed value of ϵ_∞ and so is not a serious issue. Third, the fit gives an excellent reproduction of the modulus of σ , and, in particular, the exponent value of -0.65 . Therefore, the fact that this value is fractional does not necessarily imply quantum-critical physics with a sublinear exponent. Moreover, we note that the phase angle is well reproduced by the fit.

We have obtained similar results by fitting to a Lorentzian with a high-frequency cutoff (Fig. 2).²¹ Therefore, the high-frequency data should not be taken as being dependent on having a marginal Fermi-liquid bosonic spectrum, but rather is a generic feature of electrons interacting with a broad spectrum of bosons. This is evident as well from the work of Hwang *et al.*²²

In Figs. 1 and 2, a rather large value is needed for Γ_i to fit the zero-frequency limit of $1/\tau$. As is obvious from the linear T dependence of the resistivity, most of this term is actually inelastic. To examine this in more detail, we show the variation of the modulus of the conductivity and the phase angle as a function of Γ_i (Fig. 3) and T (Fig. 4). Both variations are similar, and reproduce well the experimental variation with temperature.⁶ Note that the phase angle is always zero at zero energy unless $T=0$, $\Gamma_i=0$, where it becomes 90° .

What are the implications of this work? First, we see that the apparent scaling behavior over a wide frequency range is actually unrelated to quantum criticality and is just the consequence of the flattening of $1/\tau$, accompanied by a decrease in $\text{Re}\Sigma_{\text{opt}}$. Second, we see that the behavior of the single particle and optical self-energies is very similar for the marginal Fermi-liquid phenomenology, and the Lorentzian

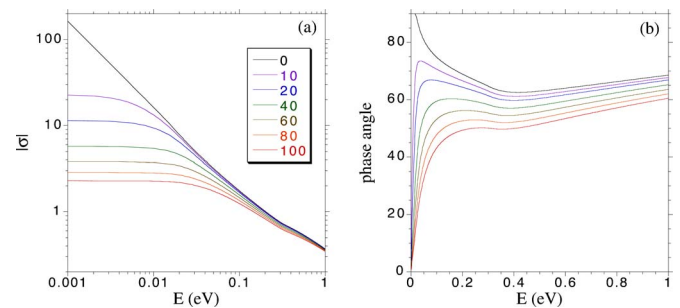


FIG. 3. (Color online) Variation of the MFL model results with impurity scattering strength Γ_i (meV). Same parameters as Fig. 1.

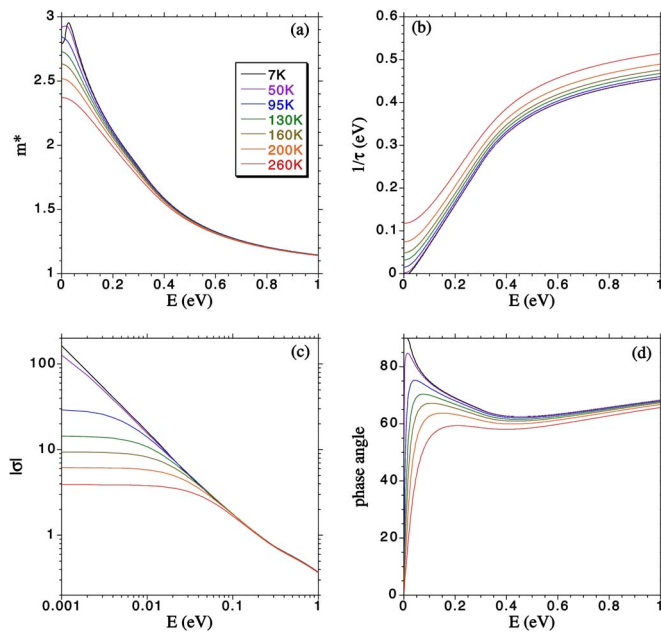


FIG. 4. (Color online) Variation of the MFL model results with temperature. Same parameters as Fig. 1, except $\Gamma_i=0$.

model used in microscopic fermion-boson theories. Third, the data give strong evidence for an upper cutoff of the boson spectrum of around 300 meV. A cutoff of this scale was suggested in the original marginal Fermi-liquid phenomenology.⁴ Such a large energy scale would imply that the source of the boson spectrum is collective electronic excitations rather than phonons. Inelastic neutron scattering data show magnetic spectral weight up to this energy scale,¹⁰ and, thus, spin fluctuations or possibly other electronic excitations are a natural explanation for the boson spectrum. This would be in support of an electronic origin for cuprate superconductivity.

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