Effect of a Normal-State Pseudogap on Optical Conductivity in Underdoped Cuprate Superconductors

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We calculate the c-axis infrared conductivity $\sigma_c(\omega)$ in underdoped cuprate superconductors for spinfluctuation exchange scattering within the CuO$_2$-planes including a phenomenological d-wave pseudogap of amplitude $E_g$. For temperatures decreasing below a temperature $T^\ast \sim E_g/2$, a gap for $\omega < 2E_g$ develops in $\sigma_c(\omega)$ in the incoherent (diffuse) transmission limit. The resistivity shows 'semiconducting' behavior, i.e. it increases for low temperatures above the constant behavior for $E_g = 0$. We find that the pseudogap structure in the in-plane optical conductivity is about twice as big as in the interplane conductivity $\sigma_c(\omega)$. in qualitative agreement with experiment. This is a consequence of the fact that the spinfluctuation exchange interaction is suppressed at low frequencies as a result of the opening of the pseudogap. While the c-axis conductivity in the underdoped regime is described best by incoherent transmission, in the overdoped regime coherent conductance gives a better description.

Numerous experiments have established the fact that the underdoped cuprate superconductors exhibit a 'pseudogap' behavior in both spin and charge degrees of freedom below a characteristic temperature $T^\ast$ which can be well above the superconducting transition temperature $T_c$. Many interpretations of the pseudogap have been advanced (see, e.g. the discussion in Ref. 1), however, no consensus has been reached so far, which of the various microscopic theories is the correct one. It has been shown by Williams et al. that specific heat, susceptibility and NMR data of many underdoped cuprates can successfully be modeled using a phenomenological normal-state pseudogap having d-wave symmetry and an amplitude which is temperature independent but increases upon lowering the doping level into the underdoped regime. This strong anisotropy of the pseudogap is also in accordance with angle-resolved photoemission spectroscopy (ARPES) experiments on underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8-\delta}$ (Bi2212). This model yields a smooth evolution of the normal state pseudogap into the superconducting gap as has been found in scanning-tunneling (STM) experiments. Also, measurements of resistivity, Hall coefficient and thermoelectric power can be reconciled with this model. However, measurements of the dynamical conductivity within or perpendicular to the CuO$_2$-planes consistently show pseudogap structures having a size which only weakly depends on doping in the underdoped regime, in marked contrast to the model above. In addition, while the c-axis conductivity in YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) shows a pseudogap having a size of approximately 300-400 cm$^{-1}$, the size of the pseudogap extracted from ab-plane conductivity is of the order of 600-700 cm$^{-1}$. This difference cannot be attributed to the charge reservoir layers between the CuO$_2$-planes, as it has been convincingly shown recently that the pseudogap seen in c-axis conductivity has its origin in the CuO$_2$-planes.

Here, we try to address these apparent inconsistencies in an effort to come to a consistent phenomenological description of the pseudogap. We calculate the c-axis and ab-plane conductivity in the presence of a temperature independent, but doping dependent pseudogap as is suggested by the work of Williams et al. To do so it is necessary to take into account some scattering mechanism within the CuO$_2$-plane. We choose to study spinfluctuation exchange scattering within the so-called selfconsistent fluctuation-exchange (FLEX) approximation for the two-dimensional Hubbard model, which has proven to give a good qualitative description of the high-$T_c$ cuprates in the optimally doped regime. Especially, the selfconsistently calculated interaction due to exchange of spin and charge fluctuations yields a quasiparticle scattering rate which varies linearly with frequency in the normal state, and exhibits a gap-like suppression at lower frequencies in the superconducting state. At the same time the effective mass ratio is increased at lower frequencies in the superconducting state. Thus, FLEX approximation accounts for the damping and mass enhancement needed to extend the theory for thermodynamical quantities by Williams et al. to dynamical quantities.

We have shown previously that such a theory is capable of describing qualitatively a number of different experiments in underdoped cuprates like Knight-shift, nuclear-spin relaxation rate, neutron scattering, ARPES, STM,
and ab-plane conductivity experiments. In particular, the pseudogap leads to a gap-like suppression of the scattering rate at lower frequencies below the linear frequency extrapolation in accordance with the observed in-plane conductivity. The $T_c$, which is calculated selfconsistently from the strong-coupling gap equation is suppressed in proportion to the magnitude of the pseudogap. The behavior of the Knight-shift, nuclear-spin relaxation rate, and density of states is described correctly as the temperature is decreased through $T_c$, showing a smooth evolution of the pseudogap into the superconducting gap.

Here, we will show that the selfconsistency of the spin-fluctuation interaction with the single particle properties, especially with the pseudogap itself, provided by the FLEX approximation will lead to a natural understanding of the differences in size of the pseudogap seen in ab-plane and c-axis conductivity. Also, the semiconducting behavior of the c-axis resistivity can be understood qualitatively. However, we will also see that such a simple ansatz for the pseudogap is not sufficient to understand the doping independence of the size of the gap observed in ab-plane and c-axis conductivity.

Measurements of the c-axis conductivity suggest that conductivity in c-direction is coherent in the overdoped regime, successively becoming incoherent in the underdoped regime. We will therefore study the two limits of coherent and incoherent c-axis conductivity. We will see that indeed within our model incoherent conductance gives a good description of the underdoped regime, while coherent conductance is more appropriate for the overdoped regime, confirming previous interpretations of the c-axis conductivity.

The coherent conductivity along the interplane c-direction is given to lowest order in the inter-layer hopping $t_\perp$ by

$$
\sigma_c(\omega) = \frac{e^2t_\perp^2c_0\pi}{\hbar a_0^2} \int_{-\infty}^{\infty} d\omega' [f(\omega') - f(\omega' + \omega)]
\times \frac{1}{N} \sum_k \left| N(k,\omega + \omega)N(k,\omega) + A_1(k,\omega + \omega)A_1(k,\omega) + A_g(k,\omega + \omega)A_g(k,\omega) \right|, \tag{1}
$$

where $c_0$ and $a_0$ are the c-axis and ab-plane lattice constants. Here, $N$ is the normal spectral function and $A_1$ and $A_g$ are the anomalous spectral functions with respect to the superconducting gap and the pseudogap, respectively. These spectral functions are taken from a selfconsistent solution of the FLEX equations in the presence of the pseudogap and are given by:

$$
N(k,\omega) = -\frac{1}{\pi} \text{Im} \frac{\omega Z + \epsilon_k + \xi}{(\omega Z)^2 - (\epsilon_k + \xi)^2 - E_g^2 - \phi^2}, \tag{2}
$$

$$
A_1(k,\omega) = -\frac{1}{\pi} \text{Im} \frac{\phi}{(\omega Z)^2 - (\epsilon_k + \xi)^2 - E_g^2 - \phi^2}, \tag{3}
$$

$$
A_g(k,\omega) = -\frac{1}{\pi} \text{Im} \frac{E_g}{(\omega Z)^2 - (\epsilon_k + \xi)^2 - E_g^2 - \phi^2}. \tag{4}
$$

![FIG. 1. The coherent dynamical c-axis conductivity (Eq. \ref{1}) for three temperatures $T=0.1t$ (solid line), $0.05t$ (dashed), and $0.03t$ (dotted) (a) for a pseudogap amplitude $E_g = 0$ (b) for $E_g = 0.15t$. The dashed-dotted line in (a) holds for the superconducting state for $E_g = 0$ ($T_c = 0.023t$) at $T = 0.017t$.](image)

We want to emphasize that it is necessary to include the bubble contribution due to $A_g$ into the conductivities and susceptibilities. Neglection of this term leads to severe disagreement with the data. Following Ref. \ref{1}, for the pseudogap we assume the form

$$
E_g(k) = E_g [\cos k_x - \cos k_y] \tag{5}
$$

where $E_g$ is temperature independent and increases with decreasing doping level below the optimal doping level. The FLEX equations are solved selfconsistently in the presence of this pseudogap and yield the quasiparticle selfenergy components $Z(k,\omega)$ and $\xi(k,\omega)$ as well as the superconducting gap $\phi(k,\omega)$. Within FLEX the effective spin and charge fluctuation interactions are given by the RPA expressions

$$
\frac{3}{2} U^2 \frac{\chi_{s0}}{1 - U\chi_{s0}} \quad \text{and} \quad \frac{1}{2} U^2 \frac{\chi_{c0}}{1 + U\chi_{c0}}, \tag{6}
$$

where the bubble spin susceptibility $\chi_{s0}$ is calculated selfconsistently from the expression...
\[ \text{Im} \chi_{s0}(q, \omega) = \pi \int_{-\infty}^{\infty} d\omega' \left[ f(\omega') - f(\omega + \omega) \right] \]
\[ \times \frac{1}{N} \sum_{k} \left[ N(k + q, \omega' + \omega) N(k, \omega') + A_1(k + q, \omega' + \omega) \times A_1(k, \omega', \omega) \right] \]
\[ \times A_2(k, \omega') + A_3(k + q, \omega' + \omega) A_3(k, \omega') \]
and thus depends on the pseudogap via the spectral functions. The charge susceptibility \( \chi_{s0} \) has the opposite sign in front of the anomalous terms in Eq. (8). For the on-site Coulomb repulsion we take an effective \( U(q) \) with maximum value \( U = 3.6 \) at \( q = Q = (\pi, \pi) \), as has been discussed in Ref. [17]. For the bandstructure \( c_k \) we take the tight-binding band

\[ \epsilon_k = t \left( -2 \cos k_x - 2 \cos k_y + 4B \cos k_x \cos k_y - \mu \right) \]

where \( t \) is the in-plane hopping matrix element and we take \( B = 0.45 \) and \( \mu = -1.1 \) which describes approximately the Fermi surfaces of the YBCO and Bi2212 compounds.

In Fig. 2(a) we show the coherent conductivity \( \sigma_c(\omega) \) calculated in this way from Eq. (9) for different temperatures. Here we took \( E_g = 0 \). For decreasing temperatures \( T \) a coherent Drude peak develops at low frequencies. Such a development of a coherent Drude peak has been observed in overdoped cuprates, where the pseudogap is absent or small. Thus, our coherent conductance results account well for this observation in the overdoped compounds. In the superconducting state a suppression of \( \sigma_c(\omega) \) at intermediate frequencies sets in as shown by the dashed-dotted line in Fig. 2(a) for \( T = 0.017t \). Here, \( T_c = 0.023t \). At the same time the Drude peak continues to sharpen. Fig. 2(b) shows the normal-state coherent conductivity \( \sigma_c(\omega) \) at intermediate frequencies, the coherent Drude peak at low frequencies still remains and even sharpens, similar to the superconducting state in Fig. 2(a). These results are completely different from the experimental results in the normal state of underdoped cuprates, showing instead of a coherent Drude peak a gap-like suppression at low frequencies. Thus, it is not sufficient to simply turn on a pseudogap in order to account for the c-axis conductivity in underdoped compounds. As has been noted earlier, the c-axis conductance at the same time becomes incoherent in the underdoped regime and therefore it is necessary to calculate the incoherent conductivity in the presence of a pseudogap. Incoherent conductivity corresponds to diffuse c-axis transmission and amounts in taking the averages of the spectral functions \( N(k, \omega) \), \( A_1(k, \omega) \), and \( A_2(k, \omega) \) over all momenta (see the discussion in Ref. [14]). This means that \( N(k, \omega) \) is replaced by the density of states

\[ N(\omega) = \frac{1}{N} \sum_k N(k, \omega) \]

while the averages of \( A_1 \) and \( A_2 \) vanish due to the \( d \)-wave symmetry of the superconducting and the pseudogap.

Then we find:

\[ \sigma_{c, \text{incoh}}(\omega) = \frac{e^2 t_c^2 c_0 \pi}{h a_0} \int_{-\infty}^{\infty} d\omega' \left[ f(\omega') - f(\omega' + \omega) \right] \]
\[ \times N(\omega' + \omega) N(\omega'). \]

**FIG. 2.** The incoherent dynamical c-axis conductivity (Eq. (10)) for three temperatures \( T = 0.1t \) (solid line), 0.05t (dashed), and 0.03t (dotted) and two values of \( E_g = 0 \) (upper three curves) and 0.15t (lower three curves).

Fig. 2 shows the incoherent conductivity \( \sigma_{c, \text{incoh}}(\omega) \) for \( E_g = 0 \) and \( E_g = 0.15t \) for three different temperatures \( T = 0.1, 0.05, \) and 0.03t. For \( E_g = 0.15t \) a gap develops below a threshold frequency of about \( \omega \sim 2\tilde{E}_g \) upon lowering the temperature while the conductivity stays almost constant for frequencies above this threshold energy. Here, \( \tilde{E}_g = 2E_g / \text{Re}Z(E_g) \) is the renormalized amplitude of the \( d \)-wave pseudogap, and \( \text{Re}Z(\omega) \) is the average mass renormalization at the Fermi surface which is of the order of 2 for the parameters considered here. For \( E_g = 0 \), \( \sigma_{c, \text{incoh}} \) is very much frequency and temperature independent. These results are in qualitative agreement with the measured interplane conductivity in underdoped YBCO compounds. The gap in the c-axis conductivity \( \sigma_{c, \text{incoh}}(\omega) \) for frequencies \( \omega \) below \( 2\tilde{E}_g \) develops below a characteristic temperature \( T^* \sim \tilde{E}_g / 2 \).

We want to stress that the temperature evolution of all physical quantities arises exclusively from the Fermi and Bose functions occurring in the FLEX equations in our real-frequency formulation [15] and in the expressions for the susceptibilities (see Eq. (7)), since we assumed that the pseudogap \( E_g(k) \) defined in Eq. (3) is temperature independent, following Ref. [1]. Physically, this means that above \( T^* \) the effect of the pseudogap is smeared out such that the normal state behavior (corresponding to the FLEX equations for \( E_g = 0 \)) is recovered while the effect of the pseudogap on the quasiparticle and spin excitation spectra increases as \( T \) decreases below \( T^* \) towards \( T_c \).

From our incoherent conductivity we can extract the c-axis resistivity \( \rho_c = [\sigma_{c, \text{incoh}}(\omega = 0)]^{-1} \) in the presence
of the pseudogap. The temperature dependence of \( \rho_c \) is shown in Fig. 3 for different values of the pseudogap amplitude \( E_g \), 0.1t, 0.15t, and 0.2t, corresponding to different doping levels. For \( E_g = 0, \) \( \rho_c \) is almost constant. For finite \( E_g \) it starts to increase above the curve for \( E_g = 0 \) at lower temperatures. This 'semiconducting' behavior of \( \rho_c \) is directly related to the depth of the pseudogap at zero frequency in \( \sigma_c^{\text{incoh}}(\omega = 0) \) which increases for increasing \( E_g \) and decreasing temperature (see Fig. 3). The results in Fig. 3 are consistent with the estimate of the characteristic temperature given above, i.e. \( T^* \sim E_g/2 = E_g/ReZ \), because the steep rise of \( \rho_c \) for a given \( E_g \) appears approximately below \( T^* \). Our results are in qualitative agreement with c-axis resistivity data on underdoped YBCO[16]. We remark that the definition of the characteristic temperature \( T^* \sim E_g/2 \) corresponds to the scaling procedure in Ref. 1 where it has been shown that the NMR Knight shift \( N^g(K_0(T)) \) for a wide range of doping values follows closely a universal scaling curve if the data are plotted against a scaling parameter \( z = 2T/E_g \). The downturn of \( N^g(K_0(T)) \) for decreasing \( T \) occurs at about \( z = 1 \) which corresponds to a \( T^* \sim E_g/2 \).

In Fig. 4 we show \( \sigma_c(\omega) \) at a fixed temperature \( T = 0.03t \) and different values of \( E_g \). From Fig. 4 we see that the renormalized size \( 2E_g \) of the gap in \( \sigma_c^{\text{incoh}} \) follows \( E_g \). If one assumes that \( E_g \) strongly changes with doping level, as has been proposed in Ref. 1, the results shown in Fig. 4 cannot provide an explanation for the doping independence of the pseudogap seen in c-axis conductivity on underdoped cuprates. This is an apparent inconsistency of the model by Williams et al, which can describe well thermodynamic quantities, but does not give a satisfactory account of the doping dependence of ab-plane and c-axis conductivity, which are dynamical quantities. Our results rather indicate that there are two independent energy scales involved in the pseudogap problem: first, the width of the pseudogap (here \( 2E_g \)) as it is seen in the \( \omega \)-dependence of the c-axis and ab-plane conductivity, being largely doping independent, and second, the depth of the pseudogap as it is seen in the \( \omega = 0 \) value of the incoherent c-axis conductivity corresponding to the characteristic temperature \( T^* \) for the c-axis resistivity and the thermodynamic quantities, which increases upon lowering the doping level. Such two energy scales could be introduced into the problem by considering more complicated forms for the pseudogap than Eq. (3). For example, the pseudogap could have a frequency dependence or a momentum dependence which changes with temperature as suggested by a recent analysis of ARPES data[14].

The lower solid line in Fig. 4 shows the result for the incoherent c-axis conductivity in the superconducting state for \( T = 0.017t \) and \( E_g = 0 \) (\( T_c = 0.023t \)). This compares well with the experimental results on optimally doped YBCO[3] showing a suppression at low frequencies, similar to the suppression due to the normal-state pseudogap. In addition, a weak enhancement at the gap edge develops. Again, this behavior is completely different from the corresponding behavior of the coherent c-axis conductivity (see the dashed-dotted line in Fig. 4 a).

The in-plane conductivity \( \sigma_{ab}(\omega) \), neglecting vertex corrections, is given by

\[
\sigma_{ab}(\omega) = \frac{2e^2 \pi}{h\epsilon_0}\int_{-\infty}^{\infty} d\omega' [f(\omega') - f(\omega + \omega)]
\]

\[
\times \frac{1}{N} \sum_k \left[ v_{k,x}^2 + v_{k,y}^2 \right] N(k,\omega' + \omega)N(k,\omega') + A_1(k,\omega' + \omega)A_1(k,\omega') + A_2(k,\omega' + \omega)A_2(k,\omega') \]

\[
+ A_1(k,\omega' + \omega)A_2(k,\omega') + A_2(k,\omega' + \omega)A_1(k,\omega') \right]
\]

where \( v_{k,i} = \partial \epsilon_k / \partial k_i \) are the band velocities within the ab-plane. Our results for \( \sigma_{ab}(\omega) \) (see Fig. 6 in Ref. [17]) are very similar to those for the coherent c-axis conductivity shown in Fig. 4. The in-plane conductivity is coherent in character and shows a Drude peak at low fre-
However, the size of the pseudogap structure seen in ab-plane conductivity on underdoped YBCO has been measured to be 600-700 cm$^{-1}$, while the gap extracted from c-axis conductivity in the same compounds is of the order of 300-400 cm$^{-1}$. In Fig. 5 we show our results for $\sigma_{ab}(\omega)$ and $\sigma_{c}^{\text{incoh}}(\omega)$ for $E_g = 0.15t$ and $T = 0.03t$ along with the density of states $N(\omega)$ Eq. (9) and the quasiparticle damping rate $\text{Im}Z(k_n, \omega)$ at the antinodal momentum $k_n$ at the Fermi surface (arbitrary units). Here we see that the size of the pseudogap appearing in these four quantities is quite different. In fact, the gaps have an approximate relation of 1:2:3:4 in the density of states, incoherent c-axis conductivity, quasiparticle damping rate, and ab-plane conductivity, respectively. Especially, we find that the gap structure in $\sigma_{ab}(\omega)$ is about twice as big as in $\sigma_{c}^{\text{incoh}}(\omega)$, being about $4\tilde{E}_g$ in $\sigma_{ab}(\omega)$ while only $2\tilde{E}_g$ in $\sigma_{c}^{\text{incoh}}(\omega)$ with $\tilde{E}_g \approx 0.12t$, in rough agreement with experiment. This relation of the gaps is a direct consequence of the electronic origin of the spinfluctuation scattering process and the selfconsistency of the FLEX equations: the opening of the pseudogap leads to a suppression of the spinfluctuation interaction via Eqs. (8) and (9) at frequencies below $\sim 2\tilde{E}_g$. This in turn results in a reduction of the self-energy below $\sim 3\tilde{E}_g$ and a corresponding structure at $\sim 4\tilde{E}_g$ in $\sigma_{ab}(\omega)$. However, in the incoherent c-axis conductivity only a gap of size $\sim 2\tilde{E}_g$ appears because of the momentum average of the spectral functions, resulting in a frequency convolution of the density of states with itself. The appearance of a $4\Delta_0$-gap in the ab-plane conductivity in the superconducting state for an electronic pairing mechanism has been noted earlier in connection with marginal Fermi liquid theory. Here we suggest that a corresponding effect is taking place in the pseudogap state of underdoped high-$T_c$ compounds.

The pseudogap structures in the curves in Fig. 5 appear to be washed out somewhat and show more complex behavior than a simple suppression at the effective pseudogap. This is due to the fact that the pseudogap Eq. (8) is renormalized due to self-energy effects. The structures seen in the conductivity, density of states, and quasiparticle damping rate do not display a pure $d$-wave gap, but a renormalized one, similar as in the superconducting state (see Ref. [13]). More detailed discussions of the density of states and the quasiparticle damping rate can be found in Refs. [13–17].

To summarize, we have investigated the influence of a normal-state pseudogap of the form suggested by Williams et al. on the c-axis and ab-plane conductivity for spinfluctuation exchange scattering within the self-consistent FLEX approximation. We find that coherent conductance can describe the c-axis conductivity in the overdoped compounds, while it is necessary to consider incoherent c-axis conductance in the underdoped regime. Incoherent conductance can account well for the dynamical c-axis conductivity and the c-axis resistivity in the underdoped compounds, showing 'semiconducting' behavior. However, it is difficult to reconcile the doping dependence of the amplitude of the pseudogap, as suggested by the work of Williams et al., with the doping independent size of the pseudogap seen in dynamical c-axis and ab-plane conductivity. This suggests that the pseudogap has a nontrivial momentum or frequency dependence, which changes with temperature. We find that the difference in size of the pseudogap in ab-plane conductivity as opposed to c-axis conductivity finds a natural explanation in the electronic origin of spinfluctuation scattering and its selfconsistency with the single-particle properties. This leads to a gap structure of size $\sim 4\tilde{E}_g$ in the ab-plane conductivity, while the gap seen in the incoherent c-axis conductivity only has a size of $\sim 2\tilde{E}_g$.

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