The Two Component Optical Conductivity in the Cuprates: A Necessary Consequence of Preformed Pairs

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We address how the finite frequency real conductivity $\sigma(\omega)$ in the underdoped cuprates is affected by the pseudogap, contrasting the behavior above and below $T_c$. The f-sum rule is analytically shown to hold. Here we presume the pseudogap is associated with non-condensed pairs arising from stronger-than-BCS attraction. This leads to both a Drude and a mid infrared (MIR) peak, the latter associated with the energy needed to break pairs. These general characteristics appear consistent with experiment. Importantly, there is no more theoretical flexibility (phenomenology) here than in BCS theory; the origin of the two component conductivity we find is robust.

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The behavior of the in-plane ac conductivity $\sigma(\omega)$ in the underdoped high temperature superconductors has raised a number of puzzles [1] for theoretical scenarios surrounding the origin of the mysterious pseudogap. At the same time, there has been substantial recent progress in establishing experimental constraints on the interplay of the pseudogap and $\sigma(\omega)$[2]. A key feature of $\sigma(\omega)$ is its two component nature consisting of a “coherent” Drude like low $\omega$ feature followed by an approximately $T$-independent mid-infrared (MIR) peak [1,3]. The latter “extends to the pseudogap boundary in the phase diagram at $T^*$.” [2] Crucial to this picture is that “high $T_c$ materials are in the clean limit and that ... the MIR feature is seen above and below $T_c$” [4]. Thus, it appears that this feature is not associated with disordered superconductivity and related momentum non-conserving processes, but rather it is “due to the unconventional nature of the [optical] response” [1].

It is the purpose of this paper to address these related observations in the context of a preformed pair Gor’kov based theory that extends BCS theory to the strong attraction limit [5]. Our expressions for $\sigma(\omega)$ are equivalent to their BCS analogue when the pseudogap vanishes. This approach is microscopically based and the level of phenomenological flexibility [6,7] is no more than that associated with transport in strict BCS superconductors. Alternative mechanisms for the two component optical response include Mott related physics [8] and d-density wave [9] approaches, which have acknowledged inconsistencies [10], as well as approaches that build on inhomogeneity effects [11]. Distinguishing our approach is its very direct association with the pseudogap. In an evidently less transparent way, a two component response arises numerically [8] in the presence of Mott-Hubbard correlations above $T_c$. However, experiments show how the MIR feature must persist in the presence of superconductivity, suggesting that pseudogap physics affects superconductivity below $T_c$, as found here.

Unique is our capability to address both the normal (pseudogap) and superconducting phases. Moreover, we are also able to establish [6,7] compatibility with the transverse f-sum rule without problematic negative conductivity [8] contributions. Finally, our approach is to be distinguished from the phase fluctuation scenario that appears problematic in light of recent optical data related to imaginary THz conductivity [12]. In experimental support of our scenario is the claim based on $\sigma(\omega)$ data [12] that the “doping dependence suggests a smooth transition from a BCS mode of condensation in the overdoped regime to a different mode in underdoped samples, [as] in the case of a BCS to Bose-Einstein crossover.”

Our analysis leads to the following physical picture: the presence of non-condensed pairs both above and below $T_c$ yields an MIR peak. This peak occurs around the energy needed to break pairs and thereby create conducting fermions. Its position is doping dependent, and only weakly temperature dependent, following the weak $T$ dependence of the excitation gap $\Delta(T)$. The relatively high frequency spectral weight from these pseudogap effects, present in the normal phase, is transferred to the condensate as $T$ decreases below $T_c$, leading to a narrowing of the low $\omega$ Drude feature, as appears to be experimentally observed. Even relatively poor samples are in the clean limit [1,4], so that an alternative pair creation/annihilation contribution associated with broken translational invariance cannot be invoked to explain the observed MIR absorption.

Before doing detailed calculations, it is possible to an-
can be understood as deriving from the fact that when dc conductivity \( \sigma_{DC} \) distribution becomes; that is, pseudogap effects lower the pseudogap. It reflects processes that require a minimal presence of stronger than BCS attraction, we observe this second contribution, a novel pair breaking effect of the pseudogap. It reflects processes that require a minimal presence of stronger than BCS attraction, we observe this second contribution, a novel pair breaking effect of the pseudogap.

We have derived the optical conductivity \( \sigma(\omega) \) in previous work \([\text{54} \text{, 52} \text{, 14}]\). The current-current correlation function is \( \chi_{jj} = \hat{P} + \frac{\mu}{\gamma} - C_\chi \), where \( C_\chi \) is associated with collective modes, which do not enter above \( T_c \) nor in the transverse gauge below \( T_c \).

For notational convenience we define \( E \equiv E_k = \sqrt{\xi_k^2 + \Delta^2} \) as the fermionic excitation spectrum, \( \xi_k \) is the normal state dispersion, \( f \equiv f(E) \) is the Fermi distribution function, and the pairing gap \( \Delta = \Delta_{sc} + \Delta_{pg} \) is found \([\text{54} \text{, 52} \text{, 14}]\) to contain both condensed (\( sc \)) and non-condensed (\( pg \)) terms. In the d-wave case, we write \( \Delta = \Delta_{k} + \Delta_{q} \), \( \xi_k = -2t(\cos k_x + \cos k_y) - \mu \), and \( E_k = \sqrt{\xi_k^2 + \Delta_k^2} \), where \( \varphi_k = (\cos k_x - \cos k_y)/2 \) is the d-wave form factor.

The full expression for the current-current response kernel was discussed elsewhere \([\text{54} \text{, 7}]\)

\[
\hat{P}(Q) \approx 2 \sum \frac{\delta \xi_{k+\alpha/2} \delta \xi_{k+\beta/2}}{\delta k} \left[ G(K) G(K+Q) + F_{sc,K} F_{sc,K+Q} + F_{pg,K} F_{pg,K+Q} \right] \tag{1}
\]

where \( Q = (q, i\Omega_m) \), \( i\Omega_m \) is a bosonic Matsubara frequency, and the three forms of propagators, introduced in earlier work \([7]\) are

\[
G(K) = \left( i\omega_n - \xi_k + i\gamma - \frac{\Delta_{pg,k}^2}{i\omega_n + \xi_k + i\gamma} - \frac{\Delta_{sc,k}^2}{i\omega_n + \xi_k} \right)^{-1}
\]

\[
F_{sc,K} = -\frac{\Delta_{sc,k}}{i\omega_n + \xi_k} \frac{1}{i\omega_n - \xi_k - \Delta_{sc,k}^2 / i\omega_n + \xi_k}
\]

\[
F_{pg,K} = -\frac{\Delta_{pg,k}}{i\omega_n + \xi_k + i\gamma} G(K) \tag{2}
\]

where \( K = (k, i\omega_n) \) and \( i\omega_n \) is the fermionic Matsubara frequency. The real part of the conductivity can be extracted from \( \hat{P}(Q) \) using the definition \( \text{Re} \sigma(\omega \neq 0) \equiv -\lim_{q \to 0} \text{Im} P^{xx}((i\Omega_m \to \omega + i0^+,q)/\omega \). Here \( \gamma \) represents the damping associated principally with the interconversion of fermions and bosons. The first equation representing the full Green’s function is associated with a BCS self energy \( \propto \Delta_{sc,k}^2 \) and a similar contribution from the non-condensed pairs \( \propto \Delta_{pg,k}^2 \). The latter is fairly standard in the literature \([13]\) and importantly was derived microscopically in our earlier work \([10]\).

Above, \( F_{sc} \) represents the usual Gorkov-like function associated with condensed pairs and we can interpret \( F_{pg} \) as their non-condensed counterpart. The full excitation gap \( \Delta(T) \) does not have a strong temperature dependence in the underdoped regime; below \( T_c \) this is because of a conversion of non-condensed to condensed pairs as \( T \) is reduced.

We may rewrite \( \hat{P}(Q) \) in the regime of very weak dissipation \( \gamma \to 0 \) where the behavior is more physically transparent. For simplicity we will illustrate this result for s-wave pairing

\[
\hat{P}(\omega, q) = \sum \frac{kk}{m^2} \left[ \frac{E_+ + E_-}{E_+ E_-} \left( 1 - f_+ - f_- \right) \right.
\]

\[
\times \frac{E_+ E_- - \xi_+ \xi_- - \delta \Delta^2}{\omega^2 - (E_+ + E_-)^2} - \frac{E_+ - E_-}{E_+ E_-} \left( f_+ - f_- \right) \left. \right]
\]

\[
\times \frac{E_+ E_- - \xi_+ \xi_- + \Delta \Delta^2}{\omega^2 - (E_+ - E_-)^2} \left( f_+ - f_- \right), \tag{3}
\]

where \( f_\pm = f(E_\pm) \) and \( \delta \Delta^2 = \Delta_{sc,k}^2 - \Delta_{pg,k}^2 \), \( \xi_\pm = \xi_{k \pm 1/2} \), and \( E_{\pm} = E_{k \pm 1/2} \).

In addition, the total number of particles can be written as \( n = \sum k (1 - \xi_+ - \xi_-) / E_k \). In this way, it is seen \([7]\) that \( \text{Re} \sigma(\omega \to 0) = (\pi\tau_\sigma/m) \delta(\omega) \). Since \( \Delta_{sc,k}^2 = \Delta_{pg,k}^2 \), one can see that pseudogap effects, through \( \Delta_{pg,k}^2 \), act to lower the superfluid density; the excitation of these non-condensed pairs provides an additional mechanism, beyond the fermions, for depleting the condensate with increasing temperature.

We introduce a transport lifetime \( \tau \equiv \gamma^{-1} \) into Eq\( \text{4} \) via the replacement \( \delta(\omega - (E_k^+ \pm E_k^-)) \approx \lim_{\tau \to \infty} \frac{-\text{Im} P^{xx}((i\Omega_m \to \omega + i0^+,q)/\omega \}}{\pi} \), to yield (for the more general d-wave case)

\[
\text{Re} \sigma(\omega \neq 0) \approx \sum \frac{4\sin^2 k_x t^2 \Delta_{pg,k}^4(2\Delta_{pg,k}^2 E_k^2 - 1 - 2f(E_k) - 2E_k)}{E_k^2}
\]

\[
\times \left[ \frac{1}{1 + (\omega - 2E_k)^2 + 1 + (\omega + 2E_k)^2} \right]
\]

\[
-2\frac{E_k - \Delta_{pg,k}^2 \varphi_k}{E_k^2} \frac{\delta f(E_k)}{\delta E_k} \frac{\tau}{1 + \omega^2 \tau^2} \tag{4}
\]

where we have dropped a small term associated with the derivative of the d-wave form factor \( \varphi_k^2 \). Here \( \Delta_{sc,k} = \Delta_{sc}(T) \varphi_{k \pm 1/2} \) and \( \Delta_{pg,k} = \Delta_{pg}(T) \varphi_{k \pm 1/2} \). Because of
Conversely, the proportion of the spectral weight residing at high energies on the order of $10^6 \text{cm}^{-1}$ increases with temperature.

To more deeply analyze this redistribution of spectral weight, the difference of the frequency integrated conductivity between $1.4T_c$ and $0.6T_c$ of the present theory is plotted as a function of $\omega/t$ in the inset of the bottom panel in Figure 1. Here we define $W(\omega, T) = (2/\pi) \int_0^\infty d\omega' \sigma(\omega', T)$ and $\Delta W(\omega) = W(\omega, 1.4T_c) - W(\omega, 0.6T_c)$. For comparison, we plot a counterpart “BCS-like” spectral weight change which is derived by effectively neglecting the terms involving $\Delta_{pg}^2$ in Eq. 4. Both conductivities are normalized by their independently calculated change in superfluid densities, $\Delta n_s/m$. The present theory leads to the full integrated (normalized) spectral weight by $\omega \approx 1 \text{eV}$, while the BCS-like curve counterpart corresponds to $\omega \approx 60 \text{meV}$. One can see that the presence of non-condensed pairs redistributes an appreciable amount of spectral weight to higher energies. Experimentally, there have been claims that very high energy scales ranging from $1.5-2 \text{eV}$ may be needed to satisfy the sum rule. This figure shows how pseudogap contributions can be, at least partly, responsible for these high energy scales.

We present a more detailed set of comparisons between theory and experiment in Fig. 2 where, for the latter, we reproduce the $y = 6.75$ plots in Fig. 4 from Ref. 2 in panels (a)-(c) and the bottom panel of Fig. 5 from the same work in panel (d). Panels (e)-(g) in Fig. 2 are associated with $T/T_c = 1.4, 0.4$, and 0.2 and should be compared with the plots in (a)-(c). Here one sees rather similar trends. Importantly the Drude peak narrows and increases in height as $T$ decreases. The MIR peak position is relatively constant, (as seen experimentally) and in the theory roughly associated with $2\Delta$, the value of which is identified in each figure (e)-(g). That $\Delta(T)$ is roughly constant through the displayed temperature range, reflects the inter-conversion of non-condensed to condensed pairs.

It should be noted, however, that the height of the MIR peak in the data is more temperature independent than found in theory. This would seem to suggest that there are non-condensed pair states at $T = 0$ perhaps associated with inhomogeneity or localization effects. This interpretation of the optical data appears consistent with our previous studies of angle resolved photoemission (ARPES) data from which we have inferred that the ground state in strongly underdoped samples may not
be the fully condensed d-wave BCS phase. Rather there may be some non-condensed pair or pseudogap effects which persist to T=0. In ARPES experiments one could attribute this persistence to the fact that the T=0 gap shape is distorted relative to the more ideal d-wave form found in moderately underdoped systems [19]. Similar observations are made from STM experiments [20].

We show in Fig. 2(h) a plot of the MIR peak location $\omega_{\text{mid}}$ as a function of $T^*$ as calculated in our theory; this plot suggests that the MIR peak position scales (nearly linearly) with the pairing gap or equivalently with $T^*$. This observation is qualitatively similar (within factors of 2 or 3) to Fig.2(d), reproduced from Ref.2. Finally, we stress that we have investigated the effects of varying $\gamma$ as well as its $T$ dependence and find that our results in Fig.2 remain very robust.

At the core of interest in the optical conductivity is what one can learn about the origin of the pseudogap. We earlier discussed problematic aspects of alternative scenarios for the two component optical response. We reiterate that the observed tight correlation with the two component optical response and the presence of a pseudogap [2] is natural in the present theory, where the MIR peak is to be associated directly with the breaking of meta-stable pairs. Such a contribution does not disappear below $T_c$, until all pairs are condensed. In summary, our paper appears compatible with the very important experimental conclusion in Ref. 2 that “Our findings suggest that any explanation of the MIR peak should take into account the correlation between the formation of the mid IR absorption and the development of the pseudogap.”

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Appendix A: Further numerical studies

In this Appendix we present a comparison figure, Fig.3, for the optical conductivity in the case where we take the parameter $\gamma$ to be constant in temperature for three different values of $\gamma$. The first column in Fig.3 reproduces the experimental data from Ref. 2. The remaining columns show the theoretical results for decreasing values of $\gamma$. Each row corresponds to decreasing temperature from top to bottom. This shows that are results are robust over a large range of $\gamma$ and very much independent of what values or temperature dependences are assumed for the lifetime broadening.

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Figure 3: Illustrative figure for the case of constant gamma. The numerical values indicated are quoted relative to those we showed in the paper.

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