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Dan Wulin, Benjamin M. Fregoso, Hao Guo, Chih-Chun Chien, and K. Levin

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Conductivity in Pseudogapped Superconductors: A Sum-Rule Consistent Preformed Pair Scenario

Dan Wulin [1], Benjamin M. Fregoso [1], Hao Guo [3], Chih-Chun Chien[2] and K. Levin[1]
[1] *James Franck Institute and Department of Physics, University of Chicago, Chicago, Illinois 60637, USA*
[3] *Department of Physics, University of Hong Kong and*
[2] *Theoretical Division, Los Alamos National Laboratory, MS B213, Los Alamos, NM 87545, USA*
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We calculate the dc conductivity σ in a pseudogapped high T_c s perconductor within a precursor superconductivity theory which is consistent with gauge invariance. Our results contain physical effects beyond those identified previously. Rather than presuming that lifetime effects dominate the T dependence of transport, here we show (consistent with growing experimental support) that the temperature dependence of the effective carrier number is a natural consequence of the pseudogap, and demonstrate reasonable agreement with dc transport in the underdoped cuprates.

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Understanding the T dependence of the dc resistivity, particularly near optimal doping, was one of the first puzzles posed by the high temperature superconductors. A number of different models based on spin-charge separation to marginal Fermi liquid phenomenology were invoked to explain the unusual power laws observed. With our increased understanding of the pseudogap phase (which extends over most of the phase diagram, including optimal doping), it has become clear that earlier theories must be modified to accomodate the pseudogap[1] and related Fermi arc effects. Moreover, the nature of this pseudogap is currently under heated debate as to whether it derives from precursor and/or fluctuation superconductivity[2] or an alternative order parameter[3]. It is therefore essential to build a systematic and properly conserving transport theory within each of these schools and their variants.

In this paper we use a pre-formed pair, sum rule- compatible approach to address the dc conductivity $\sigma(T)$ in the cuprates. Our goals are to determine (i) the effects of a pseudogap on $\sigma(T)$, (ii) the experimentally deduced temperature dependence of the lifetime, (iii) how to understand superconducting coherence effects in $\sigma(\omega \approx 0, T)$[4] from above to below T_c, (iv) the role of the Fermi arcs as well as (v) what is the source of the "bad metallicity"[5] in the cuprates. Our approach is based on the notion that the attraction is stronger than in BCS theory; this leads to finite center of mass pair excitations of the normal and the condensed state. The formal machinery used here for addressing transport is well established[6–8]. These pair fluctuations are a natural consequence of the short coherence length, as well as generally high T_c. They are to be distinguished from phase fluctuations; as a mean field approach we do not include superconducting fluctuations which dominate in the critical region.

For illustrative purposes, it is helpful, first, to present our expression for the dc conductivity for s-wave jellium, and thereby illustrate what is the role of pre-formed or non-condensed pairs. We find

$$\sigma(T) = \frac{1}{3\pi^2}\int_0^\infty dk \frac{k^4}{m^2}\frac{E_{\mathbf{k}}^2-\Delta_{\rm pg}^2}{E_{\mathbf{k}}^2}\left(-\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\right)\tau_\sigma(T) \quad (1)$$

Here $E_{\mathbf{k}}$ is the usual BCS dispersion, $E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$ where the excitation gap consists of two contributions from non-condensed (pg) and condensed (sc) pairs: via $\Delta_{\mathbf{k}}^2 \equiv \Delta_{pg,\mathbf{k}}^2+\Delta_{sc,\mathbf{k}}^2$, $f(E_{\mathbf{p}})$ is the Fermi function and τ_σ is the effective lifetime. The gap $\Delta_{\mathbf{k}}$ remains relatively T-independent, even below T_c, as observed, because of the conversion of non-condensed ($\Delta_{pg,\mathbf{k}}$) to condensed ($\Delta_{sc,\mathbf{k}}$) pairs as the temperature is lowered. This transport equation is for the weak scattering limit and when $\Delta_{pg} = 0$ it reduces to strict BCS theory, where below T_c, we consider $\omega \to 0^+$.

Importantly, this scheme is associated with the standard[9–11] pseudogap self energy, which we derived even earlier within our microscopic formalism[12]

$$\Sigma_{pg}(K) = -i\gamma + \frac{\Delta_{pg,\mathbf{k}}^2}{i\omega_n+\xi_{\mathbf{k}}+i\gamma} \quad (2)$$

Here γ represents a damping related to the interconversion of pairs and fermions. (Rather than introducing two different γ's in the first and second term, we minimize the number of parameters and take them equal.)

Physically, Eq. (1) implies that *the dc conductivity is affected by the pseudogap or pre-formed pairs, via a reduction as well as a temperature dependence of effective carrier number* $(n/m(T))_{\rm eff}$. The first of these arises from the Fermi function derivative, which reduces the number of carriers through a gap effect. The second of these appears via the pre-factor $-\Delta_{pg}^2$ which reflects the fact that when fermions are tied up into pairs the carrier number is decreased. Indeed, there is an increasing experimental awareness[13,14], that "the dc resistivity of cuprates $\rho_{dc}(T)$ is governed not only by the relaxation processes but also by temperature-dependent numbers of carriers".

Formalism A central question here is how to incorporate the widely used Eq.(2) into a consistent treatment of transport. Based on Eq.(2), one can write for the full Green's function including condensed pair (sc) effects

$$G_K = \Big(i\omega_n - \xi_{\mathbf{k}} + i\gamma - \frac{\Delta^2_{pg,\mathbf{k}}}{i\omega_n + \xi_{\mathbf{k}} + i\gamma} - \frac{\Delta^2_{sc,\mathbf{k}}}{i\omega_n + \xi_{\mathbf{k}}}\Big)^{-1} \quad (3)$$

Note that there can be no finite lifetime effects associated with the condensed pairs.

Within a BCS-like formulation, transport properties will involve terms of the form $F_{sc,K}$ which represent the usual Gor'kov functions as a product of one dressed (G) and one bare (G_0) Green's function (GG_0),

$$F_{sc,K} \equiv -\frac{\Delta_{sc,\mathbf{k}}}{i\omega_n + \xi_{\mathbf{k}}}(i\omega_n - \xi_{\mathbf{k}} - \frac{\Delta^2_{\mathbf{k}}}{i\omega_n + \xi_{\mathbf{k}}})^{-1} \quad (4)$$

To address transport we consider the EM kernel $\mathbf{J} = -\overleftrightarrow{K}\mathbf{A}$, with $\overleftrightarrow{K}(Q) = e^2\big(\overleftrightarrow{n}/m\big)_{dia} + \overleftrightarrow{P}(Q)$, where the paramagnetic contribution, given by $\overleftrightarrow{P}(Q)$, is associated with the normal current from fermionic and bosonic excitations.

The diamagnetic current (with electronic dispersion $\xi_{\mathbf{k}}$), is $(\overleftrightarrow{n}/m)_{dia} = 2\sum_K(\partial^2\xi_{\mathbf{k}}/\partial\mathbf{k}\partial\mathbf{k})G_K$. We integrate this expression by parts and use the generalized Ward identity to obtain[7] an alternate form (above T_c)

$$\Big(\frac{\overleftrightarrow{n}}{m}\Big)_{dia} = -2\sum_K \frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}\Big[G_K^2 + \sum_P t_{pg}(P)G^2_{0,P-K}G^2_K\Big] \quad (5)$$

In applying the Ward identity to arrive at Eq. (5), we are considering a t-matrix approach in which the self energy can be written as $\Sigma_{pg}(K) = \sum_Q t_{pg}(Q)G_0(Q-K)$, with $t_{pg}(Q) = (U^{-1} + \chi_{pg}(Q))^{-1}$ where $\chi_{pg}(Q) = \sum_K G_K G_{0,Q-K}$. Here U is the strength of an attractive interaction which is unspecified. The presence of GG_0 in the non-condensed pair t-matrix, t_{pg} follows from the GG_0 form of the Gor'kov function (Eq. (4)). We define $K = (\mathbf{k}, i\omega_n)$ ($Q = (\mathbf{q}, i\Omega_m)$) where $i\omega_n$ ($i\Omega_m$) is a fermionic (bosonic) Matsubara frequency.

Eq.(5) is important because it has cast the diamagnetic response in the form of a two particle correlation function. That there is no Meissner effect in the normal state is related to a precise cancellation between the diamagnetic and paramagnetic terms. Noting $\overleftrightarrow{P}(0) = -e^2(\overleftrightarrow{n}/m)_{dia}$, we may extend $\overleftrightarrow{P}(0)$ to finite Q and infer that in the normal state

$$\overleftrightarrow{P}(Q) = 2e^2\sum_K \frac{\partial\xi_{\mathbf{k}+\mathbf{q}/2}}{\partial\mathbf{k}}\frac{\partial\xi_{\mathbf{k}+\mathbf{q}/2}}{\partial\mathbf{k}}\Big[G_K G_{K+Q} + \sum_P t_{pg}(P)G_{0,P-K-Q}G_{0,P-K}G_{K+Q}G_K\Big]. \quad (6)$$

One can alternatively[7,8] introduce the Aslamazov-Larkin and Maki-Thompson diagrams to arrive at the above equation[9]. The condensate contribution is similarly associated with a t-matrix. $\Sigma(K) \equiv \Sigma_{sc}(K) + \Sigma_{pg}(K)$ and $\Sigma(K) = \sum_Q t(Q)G_0(Q-K)$. where $t(Q) \equiv t_{sc}(Q) + t_{pg}(Q)$. Since $t_{sc}(Q) = -\delta(Q)\Delta^2_{sc,\mathbf{k}}/T$, this yields the superconducting contribution in Eq. (3)

$$\Sigma_{sc}(K) = \frac{\Delta^2_{sc,\mathbf{k}}}{i\omega_n + \xi_{\mathbf{k}}} \quad (7)$$

Then, in the same spirit as our previous[12] derivation of Eq.(2) we take note of the fact that up to $T \approx T^*/2$, where T^* is the pairing onset temperature (ie, where the pair chemical potential is small), $t_{pg}(Q)$ is strongly peaked at small P. This leads us to identify $\Delta^2_{pg} = -\sum t_{pg}(Q)$ and clarifies the parameters of Eq. (2). We rewrite Eq. (6), now including the usual condensate contribution as

$$\overleftrightarrow{P}(Q) \approx 2e^2\sum_K \frac{\partial\xi_{\mathbf{k}+\mathbf{q}/2}}{\partial\mathbf{k}}\frac{\partial\xi_{\mathbf{k}+\mathbf{q}/2}}{\partial\mathbf{k}}\Big[G_K G_{K+Q} + F_{sc,K}F_{sc,K+Q} - F_{pg,K}F_{pg,K+Q}\Big] \quad (8)$$

$$\text{with} \quad \mathrm{F_{pg,K}} \equiv -\frac{\Delta_{\mathrm{pg},\mathbf{k}}}{\mathrm{i\omega_n + \xi_k + i\gamma}}\mathrm{G_K} \quad (9)$$

From Eq.(8) and $\mathrm{Re}\,\sigma^{para}(\Omega) \equiv \big(\frac{-\mathrm{Im}\,P_{xx}(\Omega)}{\Omega}\big)$, the paramagnetic contribution to the dc conductivity is

$$Re\sigma^{para}(0) \approx -\lim_{\mathbf{q}\to 0}\mathrm{Im}\sum_K\Big[\frac{2e^2}{i\Omega_m}\Big(\frac{\partial\xi_{\mathbf{k}}}{\partial k_x}\Big)^2\Big(G_K G_{K+Q} - F_{pg,K}F_{pg,K+Q} + F_{sc,K}F_{sc,K+Q}\Big)\Big]_{i\Omega_m\to 0^+} \quad (10)$$

In previous work in the literature[11,15] only the first term involving GG was included, which was recognized as inadequate[11]. Note also that Eq (1) follows directly from Eq. (10) in the limit of small $\gamma \approx \tau_\sigma^{-1}$. For consistency we rewrite Eq. (5), also adding in the usual BCS condensate terms

$$\Big(\frac{n_{xx}}{m}\Big)_{dia} \approx -2\sum_K\Big(\frac{\partial\xi_{\mathbf{k}}}{\partial k_x}\Big)^2\Big[G_K G_{K+Q} - F_{sc,K}F_{sc,K+Q} - F_{pg,K}F_{pg,K+Q}\Big] \quad (11)$$

We are now in a position to demonstrate compatibility with the important conductivity sum rule $\int_0^\infty d\Omega Re\sigma(\Omega) = (1/2)e^2(n_{xx}/m)_{dia}$. Note that $Re\sigma(\Omega) = -ImP_{xx}(\Omega)/\Omega + \pi\delta(\Omega)[ReP_{xx}(\Omega) + e^2\big(n_{xx}/m\big)_{dia}]$. Integrating the first term over frequency we find $= -\pi P_{xx}(0)$, while the second (delta function) term yields a term $+\pi P_{xx}(0)$, which leaves only the diamagnetic contribution and yields the desired sum rule. *Note that this sum rule is intimately connected to the absence (above T_c) and the presence (below T_c) of a Meissner effect.* Importantly, since $\big(\frac{n_{xx}}{m}\big)_{dia}$ can be viewed as essentially independent of temperature, when there are approximations in evaluating the transport

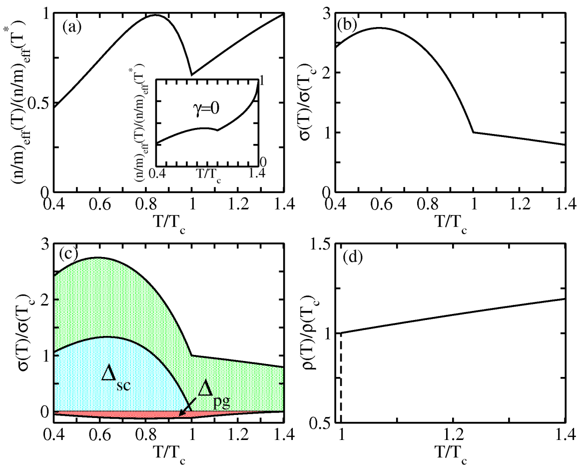

Figure 1: (Color online)Conductivity in an overdoped sample (a) The effective carrier number. The inset shows the effective carrier number for $\gamma/\Delta(T_c) = 0$. (b) $\sigma(T/T_c)$. (c) Different contributions to Re$\sigma(T/T_c)$: the contributions due to Δ_{sc} and Δ_{pg} are labeled and the total value of $\sigma(T/T_c)$ is the unlabeled region. Panels (b) and (d) compare favorably with experiment[4,16].

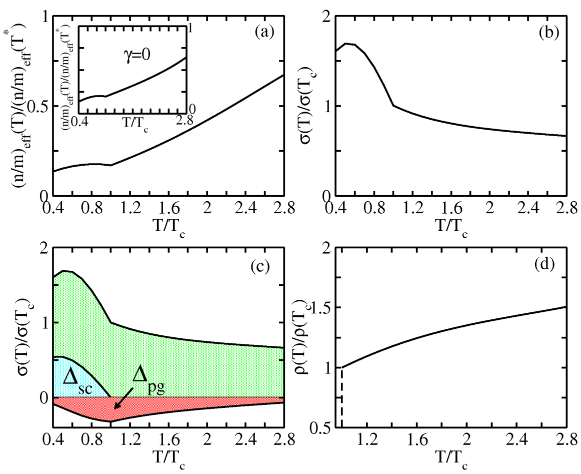

Figure 2: (Color online)Transport in an underdoped sample. (a) The effective carrier number. The inset shows the effective carrier number for $\gamma/\Delta(T_c) = 0$.(b) $\sigma(T/T_c)$. (c) Various contributions to Re$\sigma(T/T_c)$. Corresponding (d) resistivity. Panels (b) and (d) compare favorably with experiment[4,16].

diagrams, it is appropriate to evaluate the chemical potential μ based on the T-independence in Eq(11).

Numerical Results For our numerical calculations we have essentially two fitted parameters T^* and T_c, representing hole doping, and these in turn constrain the attraction U. We obtain μ and $\Delta_{\mathbf{k}}(T)$ from the mean field equations where the mean field transition temperature is T^*. Rather than using a more numerically intensive approach[9] we simplify the decomposition of pg and sc contributions so that $\Delta_{pg,\mathbf{k}}(T) = (T/T_c)^{3/4}\Delta_{\mathbf{k}}(T)$ for $T < T_c$ and for $T > T_c$, $\Delta_{pg,\mathbf{k}}(T) = \Delta_{\mathbf{k}}$. This parametrization of the gaps is very close to the full numerical solution[9]. The values for γ were chosen to give rough agreement with the observed Fermi arc lengths. Although it is not particularly critical, we take the form $\gamma \propto (T/T_c)^3$ for $T < T_c$. This is based on fitting the temperature dependence of the spectral function peak width to the measured quasi-particle scattering rate[17]. We define the effective carrier number $(n/m(T))_{\text{eff}} \equiv \gamma(T)\sigma(T)$. It should not be surprising that the effective carrier number increases with temperature because of the presence of an excitation gap and related non-condensed pairs. This T-dependent carrier number is precisely what is found in a strict BCS superconductor below T_c. This contribution leads to a nonmetallic tendency with σ *increasing* with T above T_c.

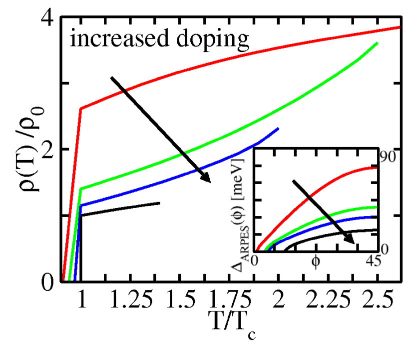

Figure 3: (Color online) Doping dependence of resistivity (below T^*) and (inset) ARPES gaps showing Fermi arcs. The normalization ρ_0 is defined as $\rho(T_c)$ for the highest doping case ($\gamma/\Delta(T_c) = 0.67$). The change in doping is associated with different ratios of $\gamma/\Delta(T_c) = 0.07, 0.20, 0.35, 0.67$ for increased doping.

Experimentally[1], one finds an increasing resistivity with T and a quasi-linear T dependence. Conventionally this is explained by assuming that $(n/m(T))_{\text{eff}}$ is T-independent, but that the inverse lifetime is linear in temperature. We have just shown that due to the pseudogap, the carrier number necessarily increases with T. This suggests that $\gamma(T)$ must be a higher power than linear. It is not implausible to assume that the gapless Fermi arcs lead to a more conventional, Fermi liquid behavior; thus we choose $\gamma \propto (T/T_c)^2$.

In Fig. 1 we plot results for a prototypical overdoped system with $T^*/T_c = 1.4$ and $\gamma/\Delta(T_c) = 0.67$. In the upper left inset we also plot $(n/m(T))_{\text{eff}}$ in the limit that $\gamma \to 0$, so that there is no distinction between condensed and non-condensed pairs and Fermi arcs are not present. The lowest T considered is $T/T_c = 0.4$ where the numerics are well controlled and impurity effects are less important. The highest temperatures considered correspond to T^*, above which the simple form for the fermionic self energy of Eq. (2) is no longer valid. It should be noted that both σ and $(n/m(T))_{\text{eff}}$ vanish at strictly zero temperature, as we do not include a self consistent treatment of d-wave localization[18]. Plotted in Fig.1(a) is the corresponding effective carrier number $(n/m(T))_{\text{eff}}$. From this figure one can see that the carrier number begins to rise once T exceeds T_c. Because the difference between the inset and main figure are not dramatic, we see that the arcs are not crucial for this aspect of transport. In Fig.1(b) we plot Re$\sigma(T/T_c)$, which exhibits a maximum below T_c, as has been been observed experimentally[4]. This is associated with the onset of order via Δ_{sc}, which increases σ (Eq. (10)). Above T_c, we see that the conductivity of the normal state is appropriately metallic, but suppressed by the excitation gap. In Fig.1(c) we plot and label the Δ_{sc} and Δ_{pg} components of Reσ arising from the three different contributions on the right in Eq. (10) as well as the total dc conductivity. The (pg) contribution from the non-condensed pairs lowers the conductivity because the presence of non-condensed pairs means fewer fermions are available for *dc* transport. The resistivity ρ, shown in Fig.1(d) has a nearly linear temperature dependence, but rises faster than T near T^* because the effective carrier number is nearing its normal state value.

The counterpart results for an underdoped sample with a much larger gap and $\gamma/\Delta(T_c) = 0.07$ and $T^*/T_c = 4$, are shown in Fig.2. The effective carrier number is plotted in Fig.2(a), and the inset shows the results for $\gamma = 0$. Above T_c, the curvature of $(n/m(T))_{\rm eff}$ changes to convex bowing, whereas it is concave in the overdoped case. This is to be expected as this larger value for $\Delta(T_c)$ suppresses the carrier number. The conductivity plotted in Fig.2(b) is similar to its experimental counterpart and the difference between this and the overdoped case is made apparent in Fig.2(c). One sees that the contribution from non-condensed pairs is much larger at lower doping due to the larger pseudogap. The larger depression in $(n/m(T))_{\rm eff}$ in turn leads to a concave bowing in the resistivity, seen in Fig.2(d).

Figure 3 presents a plot of normal state resistivities and (inset) spectral gaps associated with the fermionic spectral function for dopings that interpolate between the underdoped and overdoped cases. The resistivities are normalized by the value $\rho_o = \rho(T_c)$ for the case of highest doping. We may characterize each curve, in order of increasing doping, by the ratio $\gamma/\Delta(T_c) = 0.07, 0.20, 0.35, 0.67$, which lead to progressively larger arcs. The size of the resistivities decreases as one increases the hole concentration and this reflects the change in gap size and effective carrier number. One can see from the figure that there is a change in the nearly linear slope with increased doping from concave to convex bowing, which may have been seen experimentally[16]. The spectral gaps at T_c, displayed in the inset of Fig.3 show the general experimental trend[1,11] where the arc length increases with doping.

Conclusions Our main observation of T-dependence in the carrier number (and its implications for dc transport) seems quite natural and general, although the community focus has been on the T dependence of the scattering time. The present pre-formed pair approach is importantly demonstrably consistent with conservation laws and extendable below T_c (merging into a BCS ground state). By contrast, other papers in the literature[2,11,15] are restricted to $T > T_c$ and, unlike Ref. 3 do not establish sum rule consistency. The collapse of the Fermi arcs and the so-called two-gap physics (through Eq. (3)) are also evident[19] here, as is the anomalously low conductivity, or "bad-metal" behavior[5]. The (gapless) Fermi arcs appear to be more important for the relaxation time than for the carrier number.

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