On the Normal State of the High Temperature Superconductors

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(September 25, 1996)

Based on a Fermi liquid model, we present several results on the normal state of the optimally doped and overdoped cuprate superconductors. Our main result is an analytic demonstration, backed by self-consistent numerical calculations, of the linear in temperature resistivity and linear in $1/\text{energy}$ optical conductivity, provided the interacting Fermi liquid has strong peaks in its density of states (van-Hove singularities in 2 dimensions) near the chemical potential. Moreover, we find that the interactions tend to pin these strong peaks close to the chemical potential. This fact compares favorably with experiment on a variety of cuprates. Finally, we show that the above scenario yields naturally the low energy dependence of the experimentally determined susceptibility, without reference to spin waves.

On the scattering rate of the cuprates

We consider a 2-dimensional fermionic model with a tight-binding dispersion $\epsilon_k$ (with nearest neighbor hopping $t$, and next nearest neighbors of the desired order), chemical potential $\mu$, and some bare coupling constants $\{U_i\}$ (where the indices may stand for the usual Hubbard $U$, a constant Coulomb coupling etc.) \[1\]. This is a reasonable starting point for the description of the quasi-particles in the planes of the optimally doped and overdoped cuprates.

We write a diagrammatic Baym-Kadanoff self-consistent approximation for this system, which can be solved numerically \[1\]. The main characteristic of this approach of interest here, is that the self-energy $\Sigma$ is given as the convolution of the dressed Green’s function $G$ times an effective potential $V$. The latter arises as a combination of the couplings $\{U_i\}$ and the susceptibility $\chi(q,\omega_m)= -T \sum_{k,\epsilon_n} G(k+q,\epsilon_n+\omega_m)G(k,\epsilon_n)\ (\epsilon_n,\omega_m$ being Matsubara energies).

The numerical solution of the many-body system yields always an interesting result for the self energy at finite temperature. $\text{Im}\Sigma(k,\epsilon)$ turns out to be essentially linear in energy in an interval $\epsilon_1<\epsilon<\epsilon_2$. However it does have the correct parabolic Fermi liquid behavior for $\epsilon \to 0$. The parabolic region shrinks with decreasing filling $n$. Furthermore, the energy interval of linear behavior expands as the van-Hove singularities ($\nabla \epsilon_k=0$) at the points $q_0= (\pm \pi, 0), (0, \pm \pi)$ become stronger (there are no other van-Hove singularities for the dispersion we used).

We give an analytic derivation of this result. It can easily be shown \[2\] that $\text{Im}\Sigma(k,\epsilon)$ is given by the following formula at finite temperature:

$$\text{Im}\Sigma^R(k,\epsilon) = \sum_{q,\omega} \text{Im}G^R(q,\epsilon-\omega)\text{Im}V^R(k-q,\omega)\left\{\coth(\omega/2T) + \tanh((\epsilon-\omega)/2T)\right\}. \quad (1)$$

Taking

$$\text{Im}G^R(k,\epsilon) = -\pi\delta(s_{k,\epsilon}), \quad s_{k,\epsilon} = \epsilon + \mu - \epsilon_k, \quad (2)$$

we obtain

$$\text{Im}\Sigma^R(k,\epsilon) = -\pi \sum_q \text{Im}V^R(k-q,s_q,\epsilon)\left\{\coth(s_q,\epsilon/2T) + \tanh((\epsilon-\mu)/2T)\right\}. \quad (3)$$

Setting $\text{Im}G(k,\epsilon)$ equal to a delta function appears to be a reasonable approximation for this purpose, since numerically it is small compared to the band energy - typically $\text{Im}G(k,\epsilon)<t/20$ for $\{U_i\} \leq t$, with a magnitude roughly proportional to $\{U_i\}$. In fact, the difference of $\text{Im}\Sigma(k,\epsilon)$, as seen in our numerical calculation, for small and large coupling constants is mostly quantitative rather than qualitative!

We assume that

$$\text{Im}V^R(q,\omega) = \sum_{n=0}^{\infty} \frac{V_q^{(2n+1)}(0)}{(2n+1)!} x^{2n+1}, \quad (4)$$

where $V_q^{(n)}(0)$ is the $n$-th derivative of $\text{Im}V(q,\omega=0)$ with respect to $\omega$. This is true for an electronically mediated interaction, with a polarization which is a regular function of $\omega$ (see also below).
First we consider the low $T$ limit. The sum over $q$ is dominated by the van-Hove singularities at the points $q_o$. Assuming that $\epsilon_{eH} = \epsilon_{q_o}$ is close to $\mu$, the tanh has a vanishing contribution at the vicinity of $\epsilon_q \sim \mu$ (note that for $\epsilon_q < \mu$ and $\epsilon_q > \mu + \epsilon$ the contributions of tanh and and coth annihilate each other in the low $T$ limit). Hence

$$Im\Sigma^R(k,\epsilon) \simeq -\pi \sum_{q>q_o} \sum_{n=0}^{\infty} \frac{V^{(2n+1)}_{k-q}(0) (s_{k,\epsilon})^{2n+1}}{(2n+1)!} ,$$

(5)

where we assumed that $\mu > \epsilon_{eH} = \epsilon_{q_o}$. For sufficiently small $V^{(n)}_{q}(0), \forall n > 1$, we obtain

$$a_k = \sum_{q>q_o} V^{(1)}_{k-q}(0) \gg \sum_{q>q_o} \sum_{n=1}^{\infty} \frac{V^{(2n+1)}_{k-q}(0) (\epsilon + c)^{2n}}{(2n+1)!} ,$$

(6)

where $c = \mu - \epsilon_{eH}$. This relation is valid for $\epsilon + c < \epsilon_c$, where the latter is the characteristic energy beyond which the infinite sum on the right becomes comparable to the $V^{(1)}_{q}(0)$ term. Also, for energies beyond the bandwidth $8t$, $Im\chi_o$, and hence $ImV$ (see below), decay to zero. These considerations permit the identification

$$\epsilon_1 = \mu - \epsilon_{eH} , \quad \epsilon_2 = \min\{\epsilon_c + \epsilon_{eH} - \mu, 8t + \epsilon_{eH} - \mu\} .$$

(7)

The assumption above for $a_k$ yields

$$Im\Sigma^R(k,\epsilon) \simeq -\pi a_k (\epsilon + c) , \quad \epsilon_1 < \epsilon < \epsilon_2 .$$

(8)

Finally, we note that, if the Fermi surface approaches a van-Hove singularity at $q_o$, $V^{(1)}_{k-q}(0)$ should become bigger, being proportional to $1/(\nabla\epsilon_{k,p}, \vec{k}p)$ (as implied by the standard Fermi liquid result for the imaginary part of the susceptibility).

We consider now the high temperature limit $T \gg \epsilon$. We see immediately that

$$Im\Sigma^R(k,\epsilon) = -\pi \sum_{q} ImV^R(k-q, s_{q,\epsilon}) \{2T/s_{q,\epsilon} + O(s_{q,\epsilon}/2T)\} .$$

(9)

(Note that the term of order $T$ of this sum is reminiscent of the left-hand side of the sum rule - c.f. Pines and Nozières \cite{8} - $\lim_{q \to 0} \int_0^{\infty} d\omega Im\chi_o(q,\omega)|\epsilon(q,\omega)|^2/\omega = -N\pi/mc^2_s$, with $N$ being the total particle number, $c_s$ the speed of sound, $m$ the effective mass, and $\epsilon(q,\omega)$ the dielectric function.) The sum is dominated by the van-Hove singularities at the points $q_o$, thus yielding

$$Im\Sigma^R(k,\epsilon) \simeq -2T\pi \sum_{q>q_o} V^{(1)}_{k-q}(0) = -2\pi a_k T .$$

(10)

Here we made use of the condition above for $a_k$.

In all, we showed that the scattering rate $\tau^{-1}(k,\epsilon)$ of the quasiparticles obeys

$$\tau^{-1}(\epsilon) \simeq a\epsilon , \quad T \ll \epsilon , \quad \tau^{-1}(T) \simeq bT , \quad T \gg \epsilon ,$$

(11)

with a ratio $b/a = 2$. We note that the $T$ and $\epsilon$ dependence of $\tau^{-1}_k$ is independent of $k$ - thus leading necessarily to a linear in $T$ resistivity and a linear in $1/\epsilon$ optical conductivity, even with inclusion of vertex corrections in the calculation.

Numerically $ImV(q,\omega)$ is seen to be linear in $\omega$ for small $\omega$, and then it has 2 or 3 distinct peaks, before decaying to zero for $\omega$ greater than the bandwidth $8t$. This behavior closely follows $Im\chi_o(q,\omega)$, as in fact

$$ImV = Im\chi_o |\epsilon| |\epsilon| (U_1, Re\chi_o, Im\chi_o)|^2 ,$$

(12)

with $\epsilon$ being a rational function of its arguments. The overall behavior of $ImV(q,\omega)$ follows from any screened interaction between the carriers. Hence the argument for the linear in energy and temperature behavior of $\tau^{-1}(T,\epsilon)$ is equally generic. It relies on a large coefficient for the linear in energy term of $ImV$, and the presence of strong peaks in the density of states - van-Hove singularities in 2-dimensions - near the chemical potential. What is more, in our numerical solution we observe that the energy $\epsilon_{eH}$ of the singularities is pushed by the interactions close to the chemical potential. The shape of the imaginary part of the self-energy $Im\Sigma(k,\epsilon)$ of the interacting system...
being responsible for the modification of the density of states \(N(\epsilon)\), through the relation \(N(\epsilon) = -Tr\ ImG(k, \epsilon)/\pi\) \((Im\Sigma(k, \epsilon)\) has a peak below \(\mu\) and a dip above it, which account for the transfer of the spectral weight). This feedback effect reinforces the role of the singularities, which are more effective in producing a linear scattering rate the closer they are to the Fermi surface. In fact this seems to be a plausible explanation for the common characteristic of a good many cuprates whose van-Hove singularities are located between 10-30 meV below the Fermi surface \([4]\).

It is interesting that the electron doped \(Nd_{2−x}Ce_xCuO_{4+δ}\) which has a van-Hove singularity much below the Fermi surface, i.e. at approximately \(μ-350\) meV, as shown by ARPES \([2]\), has a usual Fermi liquid \(τ^{-1}(T) = const. T^2\) \([3]\). This lends support to the picture described above.

Let us note here that in all likelihood the present mechanism cannot explain the experimentally observed \(T^2\) dependence of the Hall resistivity of the cuprates. A successful way to explain it has been found by Stojkovic and Pines \([7]\), using an electron interaction peaked at \(Q= (±\pi, ±\pi)\). Their argument can be slightly modified, so that it works for our form of the electron potential \(V\), but with a modified susceptibility peaked at \(Q\), as we propose elsewhere \([8]\).

### On the susceptibility of the cuprates

The Millis-Monien-Pines susceptibility \([8]\)

\[
\chi_{MMP}(q, \omega) = \frac{\xi^2 X_1}{1 + \xi^2(q - Q)^2 - i\omega/\omega_{SF}},
\]

has been used to fit the susceptibility of the cuprates for low \(\omega\) from both NMR and inelastic neutron scattering (INS) experiments. The short range antiferromagnetic order, a remnant of the parent antiferromagnetic materials, with correlation length \(ξ\), is responsible for the peak of the susceptibility for \(q\) near \(Q\). Typically \(ξ\) is of the order of the lattice constant, while \(ω_{SF} ≈ 10 - 40\) meV.

The origin of the small magnitude of \(ω_{SF}\) has remained elusive thus far. Chubukov, Sachdev and Sokol have interpreted it as a damped spin wave mode \([9]\). Spin waves are clearly observable in underdoped cuprates. However to date, experimental evidence has it that spin waves are overdamped in the normal phase of the optimally doped and overdoped regimes.

An alternative explanation is a fermionic origin for \(ω_{SF}\). Suppose we write the total susceptibility as

\[
\chi(q, \omega) = \chi_{AF}(q, \omega) + \chi_0(q, \omega), \ \ q → Q,
\]

\[
\xi^2 \chi_1
\]

\[
1 + \xi^2(q - Q)^2 - f(\omega)
\]

\[
\chi_0(q, \omega) = \frac{\chi_0}{1 - i\omega/\omega_0}.
\]

\(\chi_0\) is the fermionic susceptibility, while \(\chi_{AF}\) has an antiferromagnetic origin - being due, e.g., to the localized Cu spins. Note that a similar proposal for the susceptibility has been put forward by Onufrieva and Rossat-Mignod \([10]\). If \(|f(\omega)| ≪ ω/ω_0\) we recover essentially \(\chi_{MMP}(q, \omega)\) - which is itself an approximate form of the true susceptibility - with \(ω_{SF} = ω_0\).

Hence the origin of small \(ω_0(q) = \nabla\epsilon_k \nabla\) is the proximity of the Fermi surface to a van-Hove singularity - c.f. the discussion in the context of the scattering rate above. From the numerical solution of our system, we easily obtain values of \(ω_0\) comparable to the experimentally relevant ones, when the chemical potential is near \(ε_{H}\). Actually this is the case with a good number of cuprates. In ref. \([1]\) there is a compilation of several cuprates, the van-Hove singularities of which are located between 10 - 30 meV below the Fermi level. Also, Blumberg, Stojkovic and Klein (BSK) \([1]\) suggest that this characteristic may be true irrespective of the doping, as long as the latter is appropriate for superconductivity. This is based on ARPES experiments on the bilayer \(YBa_2Cu_2O_{7−δ}\). Unfortunately, it has not proved possible yet to perform measurements on many compounds, especially the monolayers \(La_{1−x}Sr_xCuO_4\) and \(Tl_2Ba_2CuO_{6+δ}\). The point here is the following. By fitting the ARPES data, BSK show that one of the two effective bands - the anti-bonding one - formed by hybridization of the two layers by interlayer coupling has a chemical potential only some 20 - 50 meV above the van-Hove singularity at \((0, π)\), irrespective of the doping regime. It is then clear that these carriers, with a large density of states, give rise to a small \(ω_0\) as discussed above. Hence it is very interesting to know how universal this characteristic of the cuprates is, as it may explain naturally the
magnitude of $\omega_0$. Furthermore, it would be interesting to determine experimentally, e.g. by NMR, the value of $\omega_0$ for $Nd_{2-x}Ce_xCuO_4+\delta$. In that case, $\omega_0$ should be enhanced as a result of the van-Hove singularities being far away from the Fermi surface.

Finally, we have checked that within a weakly-disordered model for the planes, we do not obtain a small $\omega_0$, as might have been expected. The rationale behind this model is the disorder inherent in the cuprates. The dopants are randomly positioned in the crystal structure, thereby creating an effective disorder potential for the carriers in the planes.

Summary

In summary, we have shown that a fermionic model, with strong van-Hove singularities located close to the chemical potential $\mu$, is able to account in a natural and consistent manner for a number of characteristics of the optimally doped and overdoped cuprates. The list includes the linear in $T$ resistivity, the linear in $1/\epsilon$ optical conductivity, the pinning of the van Hove-singularities close to $\mu$, and the low energy dependence of the susceptibility. Existing experimental evidence is quite favorable for the model, while some new experiments are proposed in light of the model. We will report elsewhere on the implications of our approach for the superconducting transition.

The author has enjoyed useful discussions with Yia-Chung Chang, Gordon Baym, Girsh Blumberg, Antonio Castro Neto, Tony Leggett, Qimiao Si and Branko Stojkovic. This work was supported by the Research Board of the University of Illinois, the Office of Naval Research and NSF.

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