Theory of the leading edge gap in underdoped cuprates

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We present the theory of the leading edge gap in the normal state of underdoped high-$T_c$ materials. The consideration is based on a magnetic scenario for cuprates. We show that as doping decreases, the increasing interaction with paramagnons gives rise to a near destruction of the Fermi liquid and this in turn yields precursors to $d$–wave pairing. We argue that the leading edge gap at $\sim 30\meV$ and a broad maximum in the spectral function at $\sim 150\meV$ are byproducts of the same physical phenomenon.

One of the most intriguing experimental facts about underdoped cuprates is that they display superconducting properties already at temperatures which can be few times larger than $T_c$. This phenomenon, which has been observed in the NMR, transport and optical measurements, is most directly seen in photoemission experiments on 2212$Bi$ compounds: the leading edge of the photoemission curve remains at a finite distance from zero energy well above the actual $T_c$ and displays an angular dependence, similar to that of a true $d$–wave superconducting gap. This pseudogap behavior is however rather peculiar as the leading edge gap (LEG) is not accompanied by the quasiparticle peak. Instead, the spectral function is rather flat above the LEG and only displays a broad maximum at a frequency $\sim 150\meV$ which is 5 times larger than the gap. This last frequency is comparable to the spin exchange integral $J$, and this caused the speculations that the high-frequency maximum can be due to the precursors to antiferromagnetism. A challenging observation for this conjecture is that the LEG and the broad maximum at high frequencies seem to emerge at the same doping concentration and therefore are likely to be byproducts of the same physical phenomenon.

In this paper, we show that both, the LEG and the broad maximum at higher frequencies can simultaneously be explained in the magnetic scenario for cuprates. This scenario implies that the low-energy physics of cuprates is described by the spin-fermion model in which itinerant fermions interact with their collective spin degrees of freedom by

$$\mathcal{H}_{s-f} = g \sum c_{k,\alpha} \bar{c}_{\alpha,k} (\bar{\sigma} \cdot q) \xi S_{-q}^\dagger.$$ (1)

Here $g$ is the coupling constant which is assumed to increase as the system approaches half-filling, and $\sigma_i$ are the Pauli matrices. This model can be obtained from the underlying Hubbard-type model by integrating out high-energy fermions and performing the RPA summation in the particle-hole channel.

The propagator for low-energy fermions is assumed to have a Fermi-liquid form $G_0(k, \omega_n) = Z_0/(i\omega_n - \epsilon_k)$ where for $\epsilon_k$ we use a tight binding form $\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$. For the photomission experiments on the overdoped cuprates, the collective variables $S_q$ are characterized by their bare spin susceptibility $\chi_0(q, \omega) = \chi/(1 + (\tilde{q} \xi)^2 - \omega^2/\Delta^2)$, where $\xi$ is the spin correlation length, $\Delta = v_s \xi^{-1}$ where $v_s$ is the spin-wave velocity, and $\tilde{q} = Q - q$ where $Q$ is either equal or very close to the antiferromagnetic momentum $(\pi, \pi)$. Observe that we did not introduce the damping term $\propto \omega$ into $\chi_0$. We argue that for $T \ll J$, the key source of spin damping is the decay of a spin fluctuation into a particle-hole pair. In this situation, spin damping is not an input parameter in the theory, but rather should be obtained self-consistently within the spin-fermion model.

The quasiparticle residue $Z_0$ is generally a function of $T$, and it becomes a constant only below some $T^*$, when quantum fluctuations start to dominate over classical fluctuations. In this paper, we assume for simplicity that classical fluctuations can be completely neglected below $T^*$ and set $Z_0(T) = Z_0(T^*)$. In practical terms, this implies that we in fact will be computing the LEG right above $T_c$ where it is maximal and will not discuss how this gap is destroyed by thermal fluctuations. For the rest of the paper we absorb both $Z_0(T^*)$ and $\chi$ into the coupling constant: $g Z_0(T^*) \sqrt{\chi} \to g$.

We now proceed with the calculations. Our strategy is the following: we first demonstrate that when the coupling exceeds some typical value $g_0$, the self-energy corrections to the fermionic propagator nearly completely destroy the Fermi liquid in the vicinity of $(0, \pi)$ and related points. Then we use the renormalized form of $G$ to compute the pairing susceptibility in the $d_{x^2-y^2}$ channel. We show that this susceptibility is attractive, and for $g > g_0$ yields a $d$–wave LEG above $T_c$. Finally, we show how the leading edge gap transforms into a true superconducting gap below $T_c$.

We begin by reviewing the earlier results for the fermionic and bosonic self-energies in the spin-fermion model. The bosonic self-energy gives rise to a damping term in the full spin susceptibility: $\chi^{-1}(q, \omega) = \chi_0^{-1}(q, \omega) + i\chi^{-1} \omega/\omega_{sf}$ where $\omega_{sf} \approx (3/16) v^2 \xi^{-1}(g_0/g)^2$, $g_0^2 = 4\nu v \xi/3$ and $\nu$ is the Fermi velocity at the points where $\epsilon_k = \epsilon_{k+Q} = \mu$. For the $\epsilon_k$ which we are using, these points (hot spots) are located near $(0, \pi)$ and symmetry related points.

The fermionic self-energy in the spin-fermion model is highly nontrivial even for finite $\xi$ due to a hidden singu-
larity at $\omega \to 0$ which needs to be regularized, and has the form

$$
\Sigma(k, \omega) = -\left( \frac{g}{g_0} \right)^2 \frac{2\omega}{1 + \sqrt{1 - i\omega/\omega_s f}} \times \frac{\epsilon_{k+Q}^2}{\omega^2} - \epsilon_{k+Q} \Phi_2 \left( \frac{\epsilon_{k+Q}}{\omega_s f} \right)
$$

(2)

where the two scaling functions have the following limiting behavior: $\Phi_1(0) = 1$, $\Phi(x \gg 1) \sim x^{-1/2}$, $\Phi_2(0) = 1$, $\Phi_2(y \geq 1) = 4\ln y/(\pi y)$. Apparently, $\Sigma(k, \omega)$ is large for $g > g_0$. However, substituting $\omega_s f$ into the scaling functions, we find that for $g \gg g_0$, $y \gg 1$ and hence $\Phi_2(y) \ll 1$. In this situation, $\Sigma(k, 0)$ depends on $g$ only logarithmically and in fact saturates if we impose an upper cutoff in the spin susceptibility at $\omega_{\text{max}} \sim 2J$.

We computed $\Phi_2(y)$ beyond logarithmical accuracy and found that $(g/g_0)^2 \Phi_2(y)$ is always smaller than 1 (it saturates at about 0.4 for $g/g_0 \to \infty$). In this situation, the Fermi surface evolution wouldn’t start, and one preserves a large, Luttinger-type Fermi surface [3].

On the other hand, the frequency dependent term in $\Sigma$ still scales as $(g/g_0)^2$ in a region where $x \lesssim 1$, i.e., where $\epsilon_{k+Q}^2 \lesssim 2\nu^2(\omega/\omega_1)$ where $\omega_1 = 2\omega_s f^2$. In this range, the bare $\omega$ term becomes overshadowed by the self-energy for $g > g_0$. Moreover, for $\epsilon_k^2 < (9/8)\nu^2(\omega/\omega_1)$, the self-energy overshadows both $\omega$ and $\epsilon_k$, and to a good accuracy, the renormalized $G$ acquires a universal, momentum independent form

$$
G^{-1}(\omega) = -\Sigma(\omega) = \frac{1}{Z} \frac{2\omega}{1 + \sqrt{1 - i\omega/\omega_s f}}
$$

(3)

where $Z = (g_0/g)^2$. The two conditions on $\epsilon_k$ and $\epsilon_{k+Q}$ select a region around a hot spot with the width $\sim \omega_1/\omega_2$. We will see below that the dominant contribution to the LEG comes from the frequencies $\omega \sim \omega_1$. For these frequencies, Eq. (3) is valid over a substantial fraction of the Brillouin zone which e.g. includes the $(0, \pi)$ point.

Eq. (4) is obtained to second order in $g$ but using the renormalized form of the spin susceptibility. It turns out [4] that higher-order self-energy and vertex corrections to both, fermionic self-energy and spin damping scale in the same way as the momentum dependent term in (2), i.e., they depend on $g$ only logarithmically and in practice reduce to just constants. We have checked that numerically, all third-order corrections are rather small and can be safely neglected. For example, for $(g/g_0)^2 = 3$, the inclusion of the vertex correction into the self-energy yields only 4% correction to Eq. (3).

We now discuss which ratio $g/g_0$ we expect for cuprates. For optimally doped 2212Bi materials, photoemission data imply that $v \approx 1.2t \sim 0.4eV$ [4]. Using $\xi \sim 2.5$ inferred from NMR in 214 and 123 materials near $T^*$ at optimal doping [5], we obtain $\omega_s f \sim 30(g_0/g)^2meV$. Experimentally, $\omega_s f \sim 10meV$ [4] which implies that $(g/g_0)^2 \sim 3$. Underdoped materials should have even larger ratio of $g/g_0$. For $(g/g_0)^2 \geq 3$, we found that the full $G(k, \omega)$ and its strong-coupling version, Eq. (4), yield virtually equivalent results for the spectral function (see Fig. 1), i.e., for this $g/g_0$ the spectral weight is almost completely transformed into the incoherent part of $G$, and the quasiparticle peak is hardly visible.

Notice that though the Green’s function in Eq. (3) does not give rise to a quasiparticle peak, it has a non-Fermi-liquid form $G \propto e^{-\pi/4(\omega|\omega_s f|)^{-1/2}s\text{gn}\omega}$ only for $|\omega| > \omega_s f$. For smaller $\omega$, we have $G^{-1} \propto (\omega + i\omega|\omega|/(4\omega_s f))$. This is a conventional Fermi-liquid form of the fermionic Green’s function right at the Fermi surface. The peculiarity of the present case is that the strong self-energy corrections effectively freeze the system at the Fermi surface even if actual $k$ deviates from $k_F$ and moves over the region where Eq. (3) is valid. Away from this region, the self-energy corrections get smaller and one should recover some renormalized dispersion on a scale of $t$. Notice that this behavior is fully consistent with the “flat dispersion” observed near optimal doping [4].

Having obtained the form of the quasiparticle Green’s function, we now consider what happens in the pairing channel. The pairing interaction is obtained from $V_{\text{pair}}(\mathbf{k}, \mathbf{p}, \omega) = dk d\mathbf{p} \Gamma(|\omega|)$ where $dk = (\cos k_x - \cos k_p)$ and $\Gamma(|\omega|)$ is a decaying function of the transferred frequency with the limiting behavior
where $\Gamma(\omega) \propto \ln \omega$ and $\Gamma(|\omega|) \propto \omega^{-2}$ for $|\omega| \gg \omega$. Numerically, $\Gamma(|\omega|)$ is rather flat for $|\omega| < \omega_1$ and decreases at higher frequencies. To simplify the analysis, we set $\Gamma(|\omega|) = \Gamma = \text{const}$ for $|\omega| < \omega_1$ and zero for $|\omega| > \omega_1$. The constant is chosen such that the area under $\Gamma(\omega)$ is the same as in the exact expression. This procedure yields $\Gamma = -0.16(\omega_f/\xi)^2 = -3.57 \omega_f^2/Z^2$. Using this approximation, we explicitly can sum up RPA series in the particle-particle channel and obtain a $d_{x^2-y^2}$ pairing susceptibility in the form $\chi^{\text{sc}}(k+q,k,\Omega) = d_k^2 \chi^{\text{sc}}(q,\Omega)$ where

$$\chi^{\text{sc}}(q,\Omega) = \frac{3}{2} \frac{\Gamma_3\Pi_3(q,\Omega)}{(1 + 3\Gamma_3\Pi_3(q,\Omega))}$$

and $\Pi_3(q,\Omega) = \int d^2p G(p)G(\Omega - p)d^2q$ is a $d$-wave polarization operator. The prime to the integration sign indicates that the momentum integration goes over the region where Eq. (3) is valid. In this region, the polarization operator is independent on $q$.

We now compute $\Pi_0(0,0)$ and show that for the fully incoherent $G$ from (3), the $d$-wave pairing interaction is strongly enhanced, but there is no real instability up to $T = 0$. Indeed, the momentum integration in the polarization operator goes over the area $\sim \omega/\omega_1$. Integrating then over frequency we obtain $\Pi \sim Z^2/\omega_{sf} \int_{\omega_{sf}} d\omega/(\omega/\omega_1)$. This integral is clearly dominated by $\omega \sim \omega_1$, and yields $\Pi \sim Z^2/\omega_{sf} \sim \Gamma^{-1}$, i.e., $\Pi_0(0,0) = O(1)$ independent on $g$. Collecting all numbers, we obtain $3\Pi_3(0,0) \approx -0.7$. We see that $1 + 3\Pi_3(0,0)$ is reduced but still remains positive, i.e., fully incoherent $G$ does not give rise to actual superconductivity. It does however give rise to $d$-wave precursors as we now show. For this, we construct the pairing self-energy using $\chi^{\text{sc}}$ and obtain

$$\tilde{G}^{-1}(k,\omega) = G^{-1}(\omega) + d_k^2 \int \chi^{\text{sc}}(q,\Omega)G(-\omega + \Omega)$$

(5)

Here $\tilde{G}$ is the full quasiparticle Green’s function, and $G$ plays the role of the bare Green’s function for the Cooper channel. For the $\delta$-functional form of $\chi^{\text{sc}}(q,\Omega)$, Eq. (5) reduces to a conventional Gorkov’s equation for the simple $\tilde{G}$. In our case, $\chi^{\text{sc}}$ is enhanced, but it never acquires a $\delta$-functional peak. Nevertheless, we can do the same trick as with the SDW precursors (4), expand $G(-\omega + \Omega) = G(-\omega) + G'$ and check whether $G'$ is relevant. Without $G'$, (3) has the same form as in the true superconducting state. The relative corrections due to $G'$ depend the ratio of the typical width of $\chi^{\text{sc}}(q,\Omega)$ and the typical frequency shift obtained by solving the Gorkov’s equation without $G'$. If this ratio is small, then the corrections are also small. Physically, this means that when the amount of a shift is larger than the width of a pairing susceptibility, the latter can be approximately considered as a $\delta$-function at the energy scales comparable to the shift.

We now present the results of computations. Let us first neglect $G'$. Solving (5) we then obtain

$$\tilde{G}(\omega) \propto \frac{\omega (1 + \sqrt{1 - i}\omega)}{\omega^2 - b_k^2(1 + \sqrt{1 - i}\omega)^2}$$

(6)

where $\omega = \omega/\omega_{sf}$ and $b_k = Z\Delta_{d}(k)/2\omega_{sf}$ where $\Delta_{d}^2(k) = 2\int d^2q \Omega \chi^{\text{sc}}(q,\Omega)$. The $q$-integration in the last formula again runs over the area where Eq. (5) is valid and for $\Omega \sim \omega_1$ which, as we will see, dominates the frequency integral, yields $O(1)$. The integration over $\Omega$ is not formally restricted, but the polarization operator decreases with increasing $\Omega$ such that one progressively loses the enhancement in the $d$-wave channel. We found that the polarization operator changes sign at $|\Omega| = \omega_1$. To a reasonable accuracy, we can then approximate $\Pi(\Omega)$ as $\Pi(\Omega) = \Pi(0)(1 - (\Omega/\omega_1)^2)$. Substituting this result into $\chi^{\text{sc}}$, performing the integration and collecting all numbers, we obtain $b_k = 0.82\xi d_k$ which is a large number near $(0, \pi)$ (notice that $b_k$ does not depend on $q$). A simple analysis then shows that the pole in $\tilde{G}$ is located almost along imaginary frequency axis, at $\omega = -i\omega^*(k)$, where $\omega^*(k) = \omega_{sf} b_k^2 = 0.34 d_k^2 \omega_1$. As a result, the spectral function which emerges from (5) does not acquire a quasiparticle pole but rather a shift by $\omega \sim \omega^*$. For $k$ near $(0, \pi)$ we then have

$$A(\omega) \propto \frac{\sqrt{\omega}}{\omega + \omega^*(k) + (\omega^*(k))^2}$$

(7)

Eqs. (5) and (7) are the key results of the paper. We see that already in the normal state the spectral function rapidly (as $\sqrt{\omega}$) increases at low frequencies, reaches half a maximum at $\omega \approx 0.2 \omega^*$, then passes through a maximum at $\omega = \omega^*$, and very slowly decreases reaching half a
maximum only at $\omega \sim 5\omega_c$. This behavior has a striking resemblance with the LEG behavior observed in photoemission (see Fig. 2). The position of LEG coincides with the half-maximum at low frequencies; the broad maximum is located at frequencies which are few times larger. This is quite consistent with the data. The magnitude of $\mu$ is located at frequencies which are few times larger.

We now estimate the corrections due to $G'$. Formally, the frequency shift and the width of $\chi''$ are both of the order of $\omega_1$. However, if the pairing susceptibility is strongly enhanced such that $1 + 3\Gamma\Pi(\omega) = \delta \ll 1$, then the width of the pairing susceptibility scales as $\omega_1\sqrt{\delta}$. In this situation, the relative corrections due to $G'$ scale as $\delta^{1/2}$ and are small. In our case, $\delta \approx 0.3$. We computed the leading correction to the pairing self-energy due to $G'$ and found that near $(0, \pi)$ it accounts for $\sim 50\%$ correction for $\omega = \omega_c$, and for only $10\%$ correction for $\omega = \omega'$. Though corrections are not that small, we expect that they somewhat reduce the amplitude of the LEG, but do not change substantially the overall shape of $A(\omega)$.

So far we completely neglected the coherent part of $G$, $G_{coh} = Z/(i\omega - Z\epsilon_k)$. This piece contributes a conventional, logarithmical in $T$ term to the polarization operator and therefore gives rise to a finite $T_c$. We computed $T_c$ in a standard manner and found $T_c \sim vZe^{-c}$ where $c \approx 1$. We see that as the doping decreases, $T_c$ actually goes down because the correlation length increases. Suppose now we are below $T_c$. Then the opening of the superconducting gap yields a strong negative feedback effect on the spin damping. This gives rise to a rapid increase of $\omega_{sf}$ compared to the perturbative result, and, hence, to a decrease in $b_k$. The latter yields a gradual shift of the pole in $G$ in $\omega$ from an imaginary to a real axis, which gives rise to a gradual transformation of the LEG into the quasiparticle peak (see Fig. 3). This is precisely what has been observed in the experiments [3, 5]. At $T \ll T_c$, $b_k \ll 1$, and the typical frequencies for the pairing problem are much smaller than $\omega_{sf}$. At these frequencies, we have a conventional attractive Fermi liquid, which is just frozen at the Fermi surface in some $k$–range. The pairing then gives rise to a conventional quasiparticle pole at $\omega = \omega^{qp} = 2b_k\omega_{sf} = Z\Delta(k)$ (we assume that the total spectral weight in $\chi''$ does not change as $T$ goes below $T_c$). Notice that the position of the pole does not depend on $\omega_{sf}$ and hence does not change with temperature. Therefore we can directly compare the locations of $\omega^{qp}$ and $\omega_c$. Substituting the numbers, we find $\omega^{qp} = (6/\xi(T_c))\omega_c$. For underdoped cuprates, $\xi(T_c) \sim 4 - 5$. Then $\omega^{qp}$ is slightly larger than $\omega_c$, which fully agrees with the data.

To summarize, in this paper we have shown that the exchange of magnetic fluctuations can account for the observed LEG in underdoped cuprates. The LEG and the broad maximum of the spectral function at $\sim 5$ times larger frequencies turn out to be byproducts of the same physical effect.

A final point. In the above discussion we assumed that the Fermi surface is not modified by interactions. In fact, when LEG is formed, the spin damping goes down because of a feedback effect from the LEG, and the momentum-dependent piece of the self-energy increases. Eventually, this increase should trigger the evolution of the Fermi surface towards small hole pockets. This evolution is accompanied by the suppression of the $d$–wave attraction by vertex corrections [1, 3]. This last effect is probably relevant only at very low densities, but it nevertheless suppresses not only $T_c$ but also the LEG before the system reaches half-filling. How precisely this happens, however, requires further study.

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