Normal state pseudogap and $(\pi, 0)$ feature in the underdoped high-$T_c$ cuprates. A microscopical theory.

F Onufrieva and P Pfeuty

Laboratoire Leon Brillouin CE-Saclay 91191 Gif-sur-Yvette France

We show that a simple 2D electron system on a square lattice with hoping between more than nearest neighbors exhibits in the presence of electron spin exchange interaction properties strikingly similar to those observed in the underdoped cuprates. It is a normal state pseudogap, its behaviour with doping and $T_c$, a form of the spectrum around $(0, \pi)$ etc. The reason is that the anomalous electron spectrum can be obtained from both AF and SC ordered phases. This way is of the same which leads to SC instability and SDW instability around the point $T = 0$ of (0, $\pi$) - features). The problem of the electronic anomalies above $T_c$ is quite untrivial in the case of hoping between more than one fermions interacting with bosonic field, the equations corresponding quantum critical point (QCP) $\delta = \delta_c$, $T = 0$ ($\delta = 1 - n$) combines two independent aspects of criticality, the ordinary one related to logarithmic singularities in thermodynamical properties and the untrivial one: this point is the end point of the critical line related to Kohn singularities in 2D electron polarizability.

Quite trivial consequence of this ETT is a developing of density wave (DW) and SC instabilities around the point $\delta = \delta_c$, $T = 0$ in the presence of interaction and therefore an existence of critical bosonic fluctuations in the disordered metallic state above $T_c$. The untrivial aspects concerning to DW degrees of freedom are: (i) strong asymmetry between regimes $\delta < \delta_c$ and $\delta > \delta_c$ and (ii) very long (in doping and temperature) memory about DW instability in the disordered state on one side of ETT, $\delta < \delta_c$. This encourages us to continue our analysis and to consider now the interaction of bare electrons with DW bosonic field that is the aim of the present paper.

The basic equations are following. The spectral function corresponding to the renormalized Green function, $A(k, \Omega) = \lim_{\gamma \to 0} |ImG((k, \Omega + i\gamma))|$, is given by

$$A(k, \Omega) = \frac{|Im\Sigma(k, \Omega)|}{\Omega - \epsilon_k - Re\Sigma(k, \Omega)^2 + |Im\Sigma(k, \Omega)|^2}$$

(1)

with the irredudcible part $\Sigma(k, i\Omega_n)$ determined as

$$\Sigma(k, i\Omega_n) = \sum_p \int \frac{d\omega}{\pi} (J^2_F) Im\chi(p, \omega)\left[\frac{n^B(\omega) + n^F(\tilde{\epsilon}_{p + k, \sigma})}{i\Omega_n + \omega - \tilde{\epsilon}_{p + k, \sigma}} + \frac{1 + n^B(\omega) - n^F(\tilde{\epsilon}_{p + k, \sigma})}{i\Omega_n - \omega - \tilde{\epsilon}_{p + k, \sigma}}\right].$$

(2)

We work with electron spin exchange interaction, the same which leads to SC instability and SDW instability. Being practically standard for the case of fermions interacting with bosonic field, the equations lead to results which explicit form crucially depends on explicit forms of the bare electron spectrum $\epsilon_{k, \sigma}$ and of the bosonic Green function (or corresponding susceptibility $\chi$). In our approach we use the susceptibility calculated for the considered 2D electron system in the disordered state above both SDW and SC instabilities. And we use the spectrum which possesses SP : in the form...
\[ \epsilon_k = -2t(cosk_x + cosk_y) - 4t'cosk_xcosk_y \]  
for numerical calculations and in the form

\[ \tilde{\epsilon}_k = \epsilon_k - \mu = -Z + ak_x^2 - bk_y^2, \]

for analytical estimations. In \( \tilde{k}_x, \tilde{k}_y \) are distances from SP wavevector \( (0, \pi) \), \( a = t - 2t', b = t + 2t' \). The important parameter is \( Z \), defined as \( Z = \mu - \epsilon_s (\epsilon_s = -4t'/t \) is SP energy) and measured the energy distance from ETT: \( Z \propto \delta_\Delta - \delta_\Sigma \). This parameter determines a new energy scale in the system. As we will see, results for \( \Sigma \) and therefore for the renormalized electron Green function are very different from those obtained in \[ 3 \] where the SP in the bare spectrum was ignored.

As shown in \[ 1 \], the susceptibility in the regime \( \delta < \delta_{DW} \) of the disordered metallic state can be roughly presented in the form

\[ \chi(q, \omega) = \frac{1}{4J} \left( \frac{1 - \kappa^2}{\kappa^2 + A(q - Q_{SP})^2} \right) \]

valid for low energies \( \omega \ll \omega_c \), \( \kappa \propto 1/Z \), with \( C(0) \propto 1/Z \), the parameter \( \kappa^2 \) describes a proximity to the DW instability line. The important parameter is the energy \( \omega_0 = \frac{C(0)}{\kappa^2} \) for which \( Im\chi(q, \omega) \) is maximum, the parameter which determines the second energy scale in the system. The behaviour of \( \kappa^2, C(0), \) and \( \omega_0 \), as functions of \( \delta \) and \( T \) is quite untrivial, we discuss this point later on.

Analytical calculations for \( T = 0 \) performed with the spectrum \[ 1 \] and susceptibility \[ 1 \] for \( k = k_{SP} = (0, \pi) \) give for \( \Omega \) corresponding to the bare spectrum \( \epsilon_{k_{SP}} = -Z \).

\[ Im\Sigma(k_{SP}, \Omega = \epsilon_{k_{SP}}) \propto -\frac{1}{C(0)} \ln(\frac{ZC(0)}{\kappa^2}) \ln\left(\frac{2C(0)}{m}\right) \]

\( (m = (1/a + 1/b)/2) \) while for low energies \( \Omega \ll \omega_c \) they give: \( |Im\Sigma(k, \Omega)| \propto \Omega^2 \). Numerical calculations performed with the full spectrum \[ 8 \] and with the calculated RPA susceptibility give the results shown in Fig.\[ 2 \]. Both numerical and analytical calculations show that \( Im\Sigma \) taken for fixed \( Z \) becomes singular at \( \Omega = \epsilon_{k_{SP}} = -Z \) when \( \kappa^2 \to 0 \) and that for very low energies the Fermi liquid behaviour survives. The corresponding behaviour of \( Re\Sigma \) is presented in Fig.\[ 2 \] together with the line \( \Omega - \epsilon_k \) since the equation \( \Omega - \epsilon_k = Re\Sigma(k, \Omega) = 0 \) determines new poles. One can see that there are three poles for small \( \kappa^2 \). The position of the pole at the intermediate energy is close to the position of the pole in the bare spectrum while the two external poles are precursors of the new bands in the ordered DW phase, see \[ 8 \]. The important point is that the spectral function exhibits maxima approximately at the energies corresponding to the new poles while it is minimum at the position of the bare pole, see Fig.\[ 2 \]. This occurs due to the singularity (or maximum in the case of finite \( \kappa^2 \) in \( |Im\Sigma| \) just at \( \Omega \) corresponding to the position of the bare spectrum. Such a behaviour means an appearence of two new modes of the spectrum instead of one in the bare spectrum. For intermediate \( \kappa^2 \) the poles at negative \( \Omega \) disappear, however the peak in the spectral function at negative \( \Omega \) survives being now a resonance peak.

FIG. 1. \( Im\Sigma, Re\Sigma \) and spectral functions as functions of \( \Omega \) for \( k = k_{SP} \) and different values of \( \kappa^2 = 0.05, 0.01, 0.001 \) depending on \( t/J \) (\( T = 0, Z/t = 0.2, t'/t = -0.3 \)).

Calculations of \( Im\Sigma \) for \( k \) along different directions \( \phi \) traversing SP show that the effect of the maximum in \( |Im\Sigma| \) is preserved for wavevectors located in some distance \( \Delta k(\phi) \) from \( (\pi, 0) \), see for example Fig.\[ 2 \] corresponding to the direction \( \pi(1 - k, k) \) which traverses the ”hot spot”. The \( \Omega^2 \) behaviour at low \( \Omega \) is also preserved. [One should note that there is no square-root behaviour \[ 8 \] for \( \Omega > \omega_0 \) in the presence of SP.] This picture is valid for all directions including \((0, \pi) - (\pi, \pi)\) and \((0, \pi) - (0, 0)\). The maximum of \( |Im\Sigma| \) (when exists) occurs at \( \Omega^* = -[Z + a\omega_0 + b(\Delta k(\phi))^2] \). Above some threshold value of \( \Delta k^*(\phi) \), \( Im\Sigma \) becomes almost unstructured.

FIG. 2. \( Im\Sigma(k, \Omega) \) as functions of \( \Omega \) for wavevectors in the direction \( \pi(1 - k, k) \). \( T = 0, Z/t = 0.3, t/J = 1.8, (\kappa^2 = 0.066, \omega_0/t = 0.08 \).

There are number of important consequences of such a behaviour. The first is the form of the spectrum in the vicinity of \((\pi, 0)\): the bare spectrum splits into two branches, and a gap opens, see Fig.\[ 2 \] for the spectrum obtained from maxima of spectral functions. Secondly, the splitting into two branches and the gap disap-
pear above some threshold wavevector when one goes far away from SP, the bare spectrum is restored. The corresponding density of states (DOS) calculated for the same conditions as the spectrum in Fig.3a is shown in Fig.3b. It exhibits a pseudogap and two new peaks instead of the SP peak in the bare spectrum.

Thirdly, being directly related to the energy scale $Z \propto \delta_c - \delta$, the gap increases with $Z$ or by other words with decreasing doping, see Fig.4. The coefficient of proportionality depends on interaction increasing with $J/t$. Fourthly, due to high value of $|Im\Sigma|$ for $\Omega$ corresponding to the lower branch this branch is strongly damped in the vicinity of $(0, \pi)$. The damping decreases when one goes away from SP and the well-defined bare spectrum is restored. All these features are in a very good agreement with ARPES. There is, however one important difference: the upper well-defined branch characterized by new SP located almost on FL is not observed experimentally. This could come from finite $T$ effect.

FIG. 3. Electron spectrum along directions $(0, \pi)-(\pi, \pi)$ and $(\pi, \pi)-(0, 0)$ in two temperature regimes, I ($T \ll \omega_0$, $\omega_0 \ll 1$) and II ($T > \omega_0$) for fixed $Z$. Calculations are done for (a) $T=0$ and (c) $T/t=0.16$, in both cases for $Z/t=0.3$ ($\delta = 0.1$). For the regime I the corresponding DOS is shown for comparison (b). Results for the regime II are compared with ARPES data [3] for the underdoped BSCO (d). The dashed lines in (a), (b), (c) correspond to the bare spectrum.

To check let’s study a behaviour at finite $T$. After the analysis similar to that performed for $T=0$, one can realize that there are four different regimes in $T$. For the first three, the lower branch in the spectrum keeps its main features while the upper branch changes its behaviour. Namely, in the low temperature regime I, $T \ll \omega_0$, $\kappa^2 \ll 1$, the energy $\epsilon_B$ is negative and the upper branch traverses FL at some point in the direction $(0, \pi)-(\pi, \pi)$ as in Fig.3a. FS exists being open but quite close to the critical form. In the crossover regime, $T \sim \omega_0$, one has $\epsilon_B \approx 0$, the new SP in the upper branch traverses FL while this branch becomes much more damped than in the regime I. In the regime II, $T > \omega_0$, the SP energy moves to positive $\Omega$, $\epsilon_B > 0$, and what is most important the upper branch does not traverses FL anymore (see spectral functions in Fig.3b and the spectrum obtained from their maxima in Fig.3d): Fermi surface disappears. And finally in the regime III, $T < \omega_0$ while both parameters are not very small, the spectral functions have a form shown in Fig.3d. The gap is filled up, the bare spectrum is restored although it remains quite damped at $(\pi, 0)$.

Areas in $\omega_0 - \delta$ plane where each regime takes place depend on behaviour of $\omega_0$ as a function of $\delta$ and $T$. This behaviour is analyzed in Fig.4. We remind that $\omega_0$ (taken at fixed doping $\delta < \delta_{DW}$), slightly decreases with increasing $T$ below $T^*_{DW}(\delta) = \alpha(\delta_c - \delta)$, remains constant until another temperature, $T^*_{FL}(\delta) = \beta(\delta_c - \delta)$ and then increases with $T$. This leads to the phase diagram in Fig.4.
where we show one more regime, the regime IV, \(T > \omega_0\). For it a gap opens for all \(k\) in the direction \((1 - k, k)\), the spectrum has the form as in the ordered phase, see Fig.6 in [13]. The origin is a peak in \(|Im\Sigma(k, \Omega)|\) at \(\Omega = -\delta_{DW}\) existing for all \(k\). This regime corresponds to the quasistatic regime analysed in [7] (although the authors did not note that the gap opens for all wavevectors along \((k, 1 - k)\)). It is important to emphasize that it takes place only in the intime vicinity of AF instability whatever its origin (SDW or the spin-localized as in [7]).

![Fig. 6. Calculated phase diagram for \(t - t'\) electron system in the presence of \(J\)-interaction. \(T_{DW}\) is the line of DW instability [11], \(T_{sc}\) of SC instability [12], different crossover regimes are discussed in the text. \(t'/t = -0.3\), \(t/J = 1.8\).](image)

All regimes discussed have been obtained in ignoring a superconductivity. In the presence of the latter (SC instability also develops around the QCP as discussed in [12,11]) the regimes I, IV are unaccessible being covered by SC phase. It is the regime II which occupies the space in the presence of the latter (SC instability 

![Fig. 7. The function \(A(k, \omega)n^F(\omega)\) for \(Z/t=0.3\), \(T/t=0.16\) and four characteristic wavevectors. \(t'/t = -0.3\), \(t/J = 1.8\).](image)

With the same aim to compare with experiment we show in Fig.7 the response function \(A(k, \omega)n^F(\omega)\) corresponding to that measured by ARPES for four most characteristic wavevectors: for \((\pi, 0)\) to emphasize the untrivial \(\Omega\) dependence, for two wavevectors located not far from \((\pi, 0)\) in two directions \((\pi, 0) - (\pi, \pi)\) and \((\pi, 0) - (0, 0)\) to emphasize the absence of crossing of FL, and for the wavevector close to \(k_F\) in \((1, 1)\) direction to emphasize the ordinary FL form of the response function. The behaviour is very close to that observed experimentally [4]. All these regimes are related to the DW fluctuations. The question arises about a precursor of the superconductivity. Do corresponding fluctuations succeed in opening a pseudogap. The answer is that it is indeed so but only in the intime vicinity of \(T_{sc}(\delta)\) in the same way as for the regime IV with respect to the line \(T_{DW}(\delta)\): the details will be discussed elsewhere.

Summarizing, we have found that a simple 2D electron system on a square lattice exhibits in the presence of electron spin exchange interaction properties strikingly similar to those observed in the underdoped cuprates, the normal state pseudogap, its behaviour with doping, its existence below \(T_{gap}^*\) increasing with decreasing \(\delta\), the shape of the spectrum around \((0, \pi)\) etc.: the fact which is quite impressive in a view that we did not use any external hypothesis or adjustable parameters. The motor is EIT which due to two-dimensionality gets new features \([1],[2]\) with respect to well-studied 3D case, see \([4],[11]\). The effects disappear in the nesting case, \(t' = t'' = ... = 0\): the regimes \(\delta < \delta_c\) and \(\delta > \delta_c\) become symmetrical, for both regimes the bosonic field is incommensurate and rapidly weakening with increasing \(\delta_c - \delta\) and \(T\) \([1]\). The results are in a good agreement with exact diagonalization study for \(t - t' - J\) model \([3]\). The general picture is not sensitive to values of microscopical parameters, \(t'/t\) and \(t/J\) (only positions of the characteristic points, \(\delta_c\), \(\delta_{DW}\), \(\delta_{DW}\) depend on them). The theory predicts a quite interesting behaviour for the spectrum and spectral functions for positive \(\omega\) that would be interesting to check by photoemission experiment.

[1] H.Alloul et al, Phys.Rev.Lett. 63, 1700 (1989).
[2] S.L. Cooper et al, Phys.Rev.B 40, 11358 (1989)
[3] D.S. Marshall et al, Phys.Rev.Lett. 76, 4841 (1996)
[4] H.Ding et al, Nature (London), 382, 51 (1996)
[5] C.Kim et al, Phys.Rev.Lett. 80, 4245 (1998)
[6] A.P.Kampf, J.R.Schrieffer, Phys.Rev.B 42, 7967 (1990)
[7] J.Schmalian, D.Pines et al, PRL 80, 3839 (1998)
[8] A. Chubukov et al, Phys.Rev.B 57, R11085 (1998)
[9] B.Janko et al, Phys.Rev.B 36, R11407 (1997)
[10] J.Raninger et al, PRL 74, 4027 (1995)
[11] F.Onufrieva et P.Pfuty, cond-mat/9804263
[12] F. Onufrieva et al, Phys.Rev.B 54, 12464 (1996)
[13] M.Kisselev et al., cond-mat/9804191
[14] I.M. Lifshitz, Zh. Eskp. Teor. Fiz. 33, 1569 (1960)
[15] A.Varlamov et al, Adv.Phys. 38, 469 (1989)