Normal state understanding within a Fermi liquid approach

I. Sfar\textsuperscript{1,2}, S. Charfi-Kaddour\textsuperscript{1,*}, M. Héritier\textsuperscript{2}, and R. Bennaceur\textsuperscript{1}

\textsuperscript{1} LPMC, Département de Physique, Faculté des Sciences de Tunis, Campus Universitaire 1060 Tunis, Tunisia
\textsuperscript{2} Laboratoire de Physique des Solides, UMR CNRS-Paris XI, Bat. 510, 91405 Orsay, France

Received 1 September 2003, revised 7 March 2004, accepted 8 March 2004
Published online 23 April 2004

PACS 74.20.Mn, 74.72.–h

Using the Hubbard model in the weak coupling limit within a Fermi liquid approach, we have studied spin fluctuation effects in quasi-2D superconductors such as high critical temperature superconductors. We show that, due to nesting properties of the Fermi surface, the magnetic and the transport properties are different from the behaviours we should observe in usual metal, because of strong magnetic fluctuation effect. We distinguish different regions in the normal state with different dependences as a function of temperature for several properties, such as the resistivity, NMR relaxation rate and spin susceptibility. We show that the pseudo-gap region is strongly related to the existence of a pseudo-gap in the density of states at the Fermi level.

© 2004 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

1 Introduction

The high value of $T_c$ found in the cuprate oxide superconductors, as well as many quite singular properties of their normal state phases have led many theorists to propose various original models [1–3], which have been strongly debated for the past fifteen years. Some important fundamental questions are addressed to the physicist trying to understand the nature of High Critical Temperature Superconductivity:

(i) Is this phenomenon simply resulting from a “conventional” mechanism, taking advantage of exceptionally favourable conditions (such as a singular density of state, a quasi-two-dimensional structure, a quite strong electron-phonon coupling etc...) or are we confronted to an essentially novel phenomenon, in which, in particular, magnetic interactions or magnetic fluctuations might play a crucial and quite original role ?

(ii) A subsequent question immediately arises: what is the relevant theoretical description of the “normal state” in these superconductors, stable above the critical temperature? The standard basis of the quantum theory of solids, used in particular in the BCS theory of conventional superconductivity, is the Landau theory of normal Fermi liquids, which describes the correlated electrons, in the limit of low energy and low temperature excitations, as a gas of weakly coupled well defined and long lived “quasi-particles”, near enough the Fermi level.

Experimental data impose severe constraints on the various possible responses to this question. In particular, the generic phase diagram of the High Critical Temperature Superconductors (HCTS) exhibits a quite unusual behaviour above the critical temperature. Three different regimes separated by crossover lines are observed. With increasing the hole content, first a “pseudo-gap” regime, then a “strange metal” behaviour and finally a usual Fermi liquid are found in strong contrast with the usual behaviour of a normal Fermi liquid phase. These observed data in (HCTS) have cast some doubt about the validity of the Landau theory of Fermi liquid and lead many theorists to discard it and to propose the electron corre-
strange metal correlations are too strong to allow the existence of well defined quasi-particles: Coulomb correlations are believed to be so strong that the so-called “normal” phase in no longer Fermi liquid [1]. In this non-Fermi liquid picture, the under-doped materials, such as La$_2$CuO$_4$ or YBa$_2$Cu$_3$O$_{6.5}$ is a Mott-Hubbard or a Charge Transfer insulator, where the electrons are localised by Coulomb correlations.

Some authors [2], indeed, have proposed a phenomenological model describing the electron system as a Marginal Fermi liquid. Although these phenomenological models cannot provide a microscopic description of the phenomenon, such marginal Fermi liquid theories seem to give a satisfactory account of many abnormal properties. Undoubtedly, it would be quite interesting if we were able to find a microscopic theoretical description able to account for such a marginal Fermi liquid behaviour. It is important, also, to emphasise an essential property: the normal state phase clearly exhibits a crossover behaviours, with characteristic energy scales which depend on the doping for all the HCTS.

In this work, we would like to discuss a weak correlation limit, which, surprisingly, seems to account for most of the normal phase anomalies. While the experimental data are definitely incompatible with the usual properties of standard Fermi liquids, it can be shown that this is no longer the case if we consider, instead of a standard Fermi liquid, a model of two-dimensional Fermi liquid in close vicinity of an antiferromagnetic instability. It is well known, from many experiments, that HCTS exhibits nesting properties of the Fermi surface [3–7], as well as Van Hove singularity [8] in the neighbourhood of the Fermi level. Such anomalous features strongly modify the usual standard Fermi liquid behaviour and can reproduce a marginal Fermi liquid behaviour. Therefore, such a simple theoretical model might provide a possible interpretation of a lot of experimental data such as magnetic susceptibility, neutron scattering, resistivity...

2 Normal state properties

Because of the observed anomalies and their implication on the validity of the Fermi liquid picture, a great interest has been devoted to the discussion of the normal state properties. In this section, we remind briefly the most important experimental data reported on the HCTS properties. There are three distinct regions where the normal state properties are very different. The first region is the pseudo-gap regime which corresponds to the under-doped region, below a cross-over temperature defined as $T^*$. The second region roughly corresponds, near $T_c$, to optimal doping (i.e. where $T_c$ is maximum), this region becomes broader as $T$ increases. Finally, the third region corresponds to the strongly over-doped region below a second cross-over temperature, defined as $T'^*$. In the pseudo-gap region of the phase diagram, a large variety of experiments definitely show evidence of a strong suppression of spectral weight in the low energy part of the excitation spectrum. This phenomenon has been named in the literature as the pseudo-gap [9]. The behaviours, as a function of
temperature, of the magnetic susceptibility, of the nuclear relaxation rate and of the transport measurements clearly show deviations from the usual properties of conventional Fermi liquids.

In a conventional metal, the Pauli susceptibility is, in principle, temperature independent. Such a behaviour has been observed, indeed, in YBa$_2$Cu$_3$O$_7$. However, for lower oxygen content, a different behaviour has been found [10]. A general feature appears, which is the first observed signature of the pseudo-gap. The magnetic susceptibility displays a reduction at low temperature. The closer the antiferromagnetic phase, the more pronounced the susceptibility reduction. This pseudo-gap effect in the magnetic susceptibility is also observed in other cuprates [11]. It is generally believed that this effect is restricted to the under-doped region.

Usually, in a metallic state, the NMR spin-lattice relaxation rate divided by the temperature $1/(T_1T)$ is temperature independent, as predicted by the Korringa law. In the cuprates, the NMR data for the copper nucleus show an important temperature dependence of $1/(T_1T)$ with a maximum value at a temperature close to the pseudo-gap temperature $T^*$. This enhancement of $1/(T_1T)$ depends on the hole doping. This effect could reflect the existence of the antiferromagnetic (AF) fluctuations. Moreover, the pseudo-gap effect observed by NMR experiments in the under-doped samples disappeared completely in the over-doped samples [11].

A considerable amount of inelastic neutron scattering (INS) experiments have been performed [12]. The experimental data provide a clear evidence of the persistence of antiferromagnetic fluctuations. Magnetic fluctuations are observed, depending on the compounds, to be either commensurate peaked at AF wave vector $Q_{AF} = (\pi, \pi)$ or incommensurate away from $Q_{AF}$.

One major feature of the non Fermi liquid behaviour of HCTS is the electrical resistivity temperature dependence. Many experiments have shown a linear $T$ dependence of the resistivity in the ($a$, $b$) plane, obeyed over a quite large temperature range, with a very small $T = 0$ intercept. As well as the linearity, one should note that the resistivity is high: these are poor metals. A linear $\rho(T)$ of course expected from electron-phonon interaction in a normal metal at temperature larger than the characteristic Debye temperature $\theta_D$. However, one knows, from studies of low $T_c$ samples that the range of validity of the linear law extends at much lower temperatures. Careful analysis of the resistivity have been made in the whole phase diagram. In single and double layered Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_y$, in the under-doped region, Konstantinovic et al. [13] observe a downward deviation of the resistivity from the high temperature law: $\rho(T) = \rho_0 + \alpha T$ starting at a characteristic temperature $T^*$, which corresponds fairly well to the opening of the pseudo-gap. This temperature $T^*$ shifts systematically to higher temperatures as doping decreases. This phenomenon is also observed in La$_{2-x}$Sr$_x$CuO$_4$ and YBa$_2$Cu$_3$O$_7$ compounds.

### 3 Theoretical approach: magnetic fluctuation effects on the normal state

The electronic systems under discussion are described by a simple two-dimensional one-band Hubbard model, where $U$ is the intra-atomic Coulomb interaction.

$$H = \sum_{k,s} \epsilon_k c_{k,s}^\dagger c_{k,s} + \frac{U}{N} \sum_{k,q,s} c_{k+q,s}^\dagger c_{k,s} c_{p-q,s}^\dagger c_{p,s},$$

where $c_{k,s}$ indicates electron annihilation operator corresponding to a Bloch state with wave vector $k$ and a spin $s$, $\epsilon_k$ is the energy band dispersion law and $N$ is the number of sites. In the Hubbard approximation, $U$ is usually the “bare” local on-site Coulomb integral. However, the sensible value of $U$ to be put in the Hubbard hamiltonian treated in the RPA is obviously not the “bare” one, but an effective one which is reduced by screening or other many body effects [14].

A careful study has been done to determine the shape of the Fermi surface. It seems clear that in all the cuprates, the Fermi surface exhibits a nesting property which is more or less perfect, depending on the compound. The best nesting is probably observed in the Bi-2212 compound [15].

Let us consider a metal with a nearly perfect nesting with a $Q$ wave vector, i.e. in which the following relationship is almost exactly verified:

$$\epsilon_{k+Q} = -\epsilon_k - Q \theta.$$
Here, $\omega_0$ is considered as the deviation from perfect nesting. The spin susceptibility for non-interacting electrons is given by the following relation:

$$\chi^0(q, \omega) = \sum_k \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\omega + \epsilon_k - \epsilon_{k+q}},$$

where $f$ is the Fermi–Dirac distribution. The imaginary part of this susceptibility at the $Q$ wave vector is then

$$\text{Im } \chi^0(Q, \omega) = \frac{1}{2} N^0 \left( \frac{\omega}{2} - \frac{\omega_0}{2} \right) \frac{\sinh \frac{\omega}{2kT}}{\cosh \frac{\omega}{2kT} + \cosh \frac{\omega_0}{2kT}},$$

where $N^0$ is the density of states of the non-interacting electrons.

### 3.1 Over-doped region

We have considered the RPA approximation to calculate the magnetic and transport properties in this region where

$$\chi^{\text{RPA}} = \chi^0 1-U.$$ 

Actually, the NMR relaxation rate is given by the relation

$$\frac{1}{T_1 T} = \lim_{\omega \to 0} \sum_q \frac{\text{Im } \chi^{\text{RPA}}(q, \omega)}{\omega} \approx \lim_{\omega \to 0} \frac{\text{Im } \chi^{\text{RPA}}(Q, \omega)}{\omega},$$

where $Q$ is the best nesting vector corresponding to the less imperfect nesting.

We will try first to understand the $T^{*}$ line by taking into account the effect of moderate spin fluctuations on the normal state properties. Our calculations of the spin relaxation rate reveal that $1/(T_1 T)$ have a peak as a function of the temperature. The temperature corresponding to this maximum is in fact very sensitive to nesting which is related to the strength of the spin fluctuations. Indeed, this peak vanishes rapidly when $\omega_0$ increases. It is commonly known that, by moving from an antiferromagnetically correlated system to a more usual metallic system, we gradually recover the Korringa law. As a consequence, we should have a maximum of $1/(T_1 T)$ shifted to higher temperatures and the temperature $T^{*}$ is then an increasing function of hole doping.

Since the spin fluctuations play an essential role in the normal state, these fluctuations should also contribute significantly to the resistivity. A simple way to determine this contribution is to calculate the following resistivity due to AF fluctuations using the approach considered for nearly magnetic systems [16]:

$$\rho(T) = \frac{1}{T} \int_0^{2k_f} \int_q \text{Im } \chi^{\text{RPA}}(q, \omega) \omega e^{\omega/T} (e^{\omega/T} - 1)^{-2} \, d\omega.$$ 

Starting from optimal doping, as the doping increases, the antiferromagnetic fluctuations effects are progressively reduced. These fluctuations less and less affect the quasi-particles and the usual $T^2$ electron-electron Fermi liquid damping will be progressively dominating. This is in agreement with the observed gradual crossover of $\rho(T)$ at low temperatures from $\rho(T) \sim T$ near optimal hole concentration towards $\rho(T) \sim T^2$ in the over-doped region.

© 2004 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
3.2 Under-doped region

The nesting property induces the existence of strong antiferromagnetic fluctuations, which are not strong enough to induce a SDW state, but are able to yield important consequences on many physical properties by inducing a pseudo-gap in the density of states. This pseudo-gap, obtained by different authors [3, 5, 6], is the key point to elucidate the unusual properties in the under-doped region and the $T^*$ line. This pseudo-gap have quite important consequences in the under-doped region for the following reason. When the hole doping concentration is small, the spin fluctuations are rather strong because of the good Fermi surface nesting. In that case, the pseudo-gap of the density of states is deep. In this situation, the Fermi level sits inside the pseudo-gap and the density of states at the Fermi energy, $N(q_0)$, is very low. Moreover, it is well known that the properties of a metal are directly related to the density of states at the Fermi energy. Therefore, all these electronic properties will be considerably affected because of the strong reduction of $N(q_0)$, compared to a normal metal value.

In order to take into account the electron interactions in the calculation of the spin susceptibility and this important modification of the density of states, we consider $N^{corr}$, the density of states of the antiferromagnetically correlated system, instead of $N^0$ which are defined by

$$N^0(\omega) = -\sum_k \frac{1}{\pi} \text{Im} G^0(k, \omega) \quad \text{and} \quad N^{corr}(\omega) = \sum_k \frac{1}{\pi} \text{Im} G(k, \omega)$$

where $G^0$ is the non interacting Green function and $N^{corr}$ is the density of states calculated by the Green function $G$ of the correlated system taking into account self-energy corrections. Then the imaginary part of the susceptibility $\text{Im} \chi(Q, \omega)$ becomes:

$$\text{Im} \chi(Q, \omega) = \frac{1}{2} N^{corr} \left( -\frac{\omega}{2} - \frac{\omega_0}{2} \right) \frac{\sinh \frac{\omega}{2kT}}{\cosh \frac{\omega}{2kT} + \cosh \frac{\omega_0}{2kT}}.$$

Therefore, we should expect an important effect on the Pauli susceptibility $\chi(Q = 0)$ which depends directly on the density of states at the Fermi level. The energy scale of the observed pseudo-gap in the Pauli susceptibility is then the width of the pseudo-gap. Since the spin fluctuations are reduced as the hole doping grows, the pseudo-gap width of the density of states is reduced and consequently $T^*$ decreases as a function of doping. In the other hand, the nuclear relaxation rate and the electrical resistivity which are related to $\text{Im} \chi$ will be also reduced at low temperature ($T < T^*$) due to the pseudo-gap.

3.3 Strange metal region

In the strange metal region, in the under-doped region, if we consider the temperature at which the pseudo-gap is going to be filled, the density of states will become almost constant for higher temperatures and the pseudo-gap effect will vanish. In that case, we should have an almost constant magnetic susceptibility. The imaginary part of the susceptibility corresponding to the best nesting will behave roughly as follows:

$$\text{Im} \chi(Q, \omega) \approx \frac{\omega}{T} \quad \text{for} \quad \omega < T.$$

In the overdoped region, we show that the resistivity is linear for temperatures higher than a certain temperature depending on $\omega_0$. Indeed, in this region, the thermal excitations are enough to allow the spin fluctuations, those corresponding to imperfect nesting with the Q wave vector. Hence, the $q = Q$ scattering is so large in these conditions that other fourier components may be neglected, which put an additional constraint in the final scattered state and lead to a marginal Fermi liquid behaviour at high temperature.
Our microscopic approach leads to theoretical predictions which verify the basic hypotheses of the phenomenological marginal Fermi liquid. They are, indeed, in good agreement with the experimental observations. We can conclude that the $T^*$ observed in the under-doped region is a characteristic energy related to the width of the density of state pseudo-gap and that the $T^{**}$ line is related to energy corresponding to the deviation from perfect nesting.

We should note that important studies have been carried in this field to explain the pseudo-gap effect and photoemission experiments [17].

4 Conclusion

We have proposed microscopic interpretations of the normal state properties on the basis of weak electron coupling theories. We have tried to give a coherent interpretation of the normal state experimental observations. We have shown that the pseudo-gap regime is governed by the pseudo-gap formed in the single particle density of states by the magnetic short range order. This pseudo-gap in the density of states gets deeper and wider as the antiferromagnetic phase is approached, i.e. at low doping. In this regime, the width of the density of states pseudo-gap is the pertinent energy scale which is directly connected to $T^*$ and the normal state properties are directly affected by this pseudogap. In the strange metal region, due to thermal activation, the normal state behaves now like a marginal Fermi liquid where the spin fluctuations are responsible for the temperature dependence of the normal state properties. For higher doping, the usual Fermi liquid behaviour is gradually recovered due to a weakening of the spin fluctuations.

The weak coupling limit used in this simple theoretical calculation is certainly too schematic. It is known that the electron correlations are probably not very weak. In a more realistic description, one should certainly improve this point, for example by using a Dynamical Mean Field Theory to take into account more precisely the correlation effects. However, we believe that the properties of a Fermi liquid in close vicinity of a magnetic instability and properly modified by the existence of a two-dimensional Van Hove singularity provide a qualitatively correct description of the normal state.

Acknowledgement We acknowledge the financial support from CMCU to project 01/F1303.

References