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Classification

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Short Communication

Spin fluctuation effects on a quasi-2D itinerant electron system : a microscopic model for the marginal Fermi liquid

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Abstract. — We study a model of itinerant two-dimensional electron system exhibiting Van Hove and nesting singularities of the Fermi surface at half-filling of the band. We consider the spin fluctuation electron-electron scattering as the dominant scattering mechanism. This yields a marginal Fermi liquid behaviour at half-filling and a crossover from a normal Fermi liquid to a marginal one away from half-filling. Density of states, magnetic susceptibility, spin excitation spectrum, resistivity, thermopower and the phase diagram using BCS theory obtained by this simple model are in a qualitative agreement with high T_c superconductors.

1. Introduction.

The high values of T_c found in the cuprate oxide superconductors [1], as well as many quite singular properties of their normal phases have lead many theorists to propose original models which discard the normal Fermi liquid picture [2]. Some of them, indeed, proposed a phenomenological model describing the electrons as a marginal Fermi liquid [3]. Such a phenomenological theory seems to provide a satisfactory account of many « abnormal » properties. The purpose of this paper is to show that a model of two-dimensional Fermi liquid near an antiferromagnetic instability, exhibiting nesting property of the Fermi surface [4, 5] as well as Van Hove singularity [6-8] at the Fermi energy is able to reproduce a marginal Fermi liquid behaviour, and therefore to interpret a lot of experimental data such as magnetic susceptibility, neutron scattering, resistivity and thermopower. Moreover, a phase diagram for superconductivity is obtained within a BCS model taking into account spin fluctuations.

Several weak coupling models have been proposed in literature, which differ by the type of approximations and by the choice of spin susceptibility used in the theoretical treatment,

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because of the difficulty of performing an exact analytical calculation. Kampf and Schrieffer [4] have carried out a study of the self-energy and of the density of states assuming a model susceptibility (not obtained from their model Hamiltonian). They have also calculated the density of states numerically using the RPA susceptibility at zero temperature. They have obtained a pseudogap in the density of states, earlier predicted by Friedel [6]. Likewise Viroszek and Ruvalds [5] have proposed a « nested Fermi liquid » theory. The self-energy and the magnetic susceptibility were calculated considering the density as a constant and therefore did not take into account, of course, the Van Hove singularity in the density of states. Some normal state properties studies have been performed using the RPA approximation [9, 10].

Our work first investigates in detail the behaviour of the density of states and the formation of the pseudogap due to spin fluctuations as a function of temperature, electron interaction strength and band filling from *ab initio* calculations consistent with the theoretical model used to describe the nested Fermi surface. Then, we calculate the consequences of the quasiparticle spectrum on the thermodynamic and transport properties. The marginal Fermi liquid behaviour as well as the crossover to a normal Fermi liquid behaviour, which we have discussed in detail, are implied from both the nesting property of the Fermi surface and the Van Hove singularity.

2. The model and the approximations.

The purpose of this paper is not to give accurate quantitative calculations of the real systems, but to propose a very simple model containing the main qualitative ideas. Because of the strongly two-dimensional character of the electron states near the Fermi level, we describe the electrons by a two-dimensional Hubbard model for a square lattice. The tight binding dispersion relation may be written as $E_k = -2t(\cos k_x a + \cos k_y a) - \mu$ where μ is the chemical potential. The case $\mu = 0$ corresponds to the half-filled band, i.e. for example, to pure La_2CuO_4 . Such a simple model exhibits two peculiar properties which will be essential for describing the electrons: (i) a perfect nesting property at $\mu = 0$ and (ii) a Van Hove singularity in the density of states. The Coulomb electron interactions are included in the intra-atomic approximation and will be always considered as smaller than the bandwidth W ($W = 8t$):

$$H = \sum_{ks} E_k c_{ks}^+ c_{ks} + U/N \sum_{kk'qs} c_{k+qs}^+ c_{ks} c_{k'-q-s}^+ c_{k'-s} \quad (1)$$

We first calculate the electron self-energy, in which we consider only the electron-electron scattering terms corresponding to antiferromagnetic spin fluctuations near a Spin Density Wave instability. These terms are expected to be particularly dominant because of nesting and Van Hove singularities (which lead to a logarithm squared divergence for $\mu = 0$):

$$\Sigma(\mathbf{k}, \omega_n) = -\frac{3U^2}{2\beta} \int \frac{d^2q}{4\pi^2} \sum_{\nu_m} G(\mathbf{k}-\mathbf{q}, \omega_n - \nu_m) \chi(q, \nu_m) \quad (2)$$

where χ is the magnetic susceptibility, which we will approximate by the R.P.A. expression

$$\chi^{\text{RPA}} = \frac{\chi^0}{1 - U\chi^0} \quad \text{where} \quad \chi^0(q, \omega) = -\sum_k \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\omega + \varepsilon_k - \varepsilon_{k+q}} \quad (3)$$

To maintain an analytic approach of the problem, we only keep in the spin fluctuation spectrum the $\mathbf{q} = \mathbf{Q}$ component, in which $\mathbf{Q} = (\pm \pi/a, \pm \pi/a)$ is the nesting wave vector of the half-filled band case. In our simple model, the real nesting vector would depend on band

filling [11]. However, commensurability effects may pin it at \mathbf{Q} , as in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, which justifies our approach. In contrast with previous calculations, we obtain an analytical fit of the imaginary part of the RPA susceptibility, which allows us to perform the calculation of the self-energy and of the electron Green's function $G^{\text{ret}}(k, \omega)$, which we will use to calculate many properties of the electron system varying the chemical potential, the temperature for different values of U/W . We shall see that this model provides a microscopic justification for the marginal Fermi liquid approach.

3. Origin of the marginal Fermi liquid behaviour.

It is well known that the electron inverse life time near the Fermi surface in a normal Fermi liquid obeys a law $\hbar/\tau_k \sim (k_B T/\varepsilon_F)^2$. In our model, both Van Hove and nesting singularities, in the half-filled band case, make the $\mathbf{q} = \mathbf{Q}$ scattering processes so large that other Fourier components may be neglected, which, in practice put an additional constraint on the final scattered states. This amounts in reducing by one the dimensionality of the phase space available for the scattering processes, which gives an inverse electron life-time $\hbar/\tau_k \sim k_B T/\varepsilon_F$, as in a marginal Fermi liquid and, therefore is much larger than in a usual Fermi liquid. This temperature dependence has been already suggested by different authors as a consequence of nesting property or Van Hove singularity [5, 8, 12]. More generally, this marginal behaviour, but also a crossover to a normal behaviour away from half-filling, which is a more general statement than the temperature dependence of a given physical quantity, are implied by our microscopic derivation of the self energy. Indeed, away from half-filling Van Hove and nesting singularities disappear. For electron energies smaller than the characteristic energy 2μ violating the nesting condition, we thus recover a normal Fermi liquid behaviour, while at electron energy much larger than 2μ , we still have a marginal behaviour and a crossover between these two regimes at intermediate energies. This will be observed in all the physical properties derived in our model. However, our approximation which consists in keeping only the term $\mathbf{q} = \mathbf{Q}$ makes the cross over between the two regimes too abrupt. It would be smoothed by taking into account other Fourier components.

4. Consequences on the physical properties.

4.1 DENSITY OF STATES. — We calculate the single particle density of states from the imaginary part of the Green function. The contribution of spin fluctuations to the self energy will introduce a pseudogap in the density of states [4], related to antiferromagnetic short range order, which takes the place of the real gap in the Spin Density Wave ordered phase. This pseudogap will strongly influence many properties of the normal phase. We have studied in detail its dependence as a function of the band filling, of the temperature and of the U/t ratio. The smaller W/U or T or μ , the stronger the pseudogap (see Fig. 1).

It is important to notice that in the intermediate region between the antiferromagnetic and the superconducting phases, the spin fluctuations are quite strong and the pseudogap is deep. Because of the disorder, an Anderson localisation could occur for the states in the bottom of the pseudogap, therefore near the Fermi level.

4.2 SUPERCONDUCTIVITY. — The main observed superconducting properties may be coherently interpreted within the B.C.S. theory [6, 7]. However, deviations from the B.C.S. standard value (0.5) have been observed for the isotopic effect coefficient, but calculations using the logarithmic 2D density give quantitative results close to experiments [8]. In fact, the isotopic effect is very sensitive to density of states variations [13]. A phase diagram of the superconductivity has been derived *versus* the band filling ratio assuming a quasi-2D itinerant

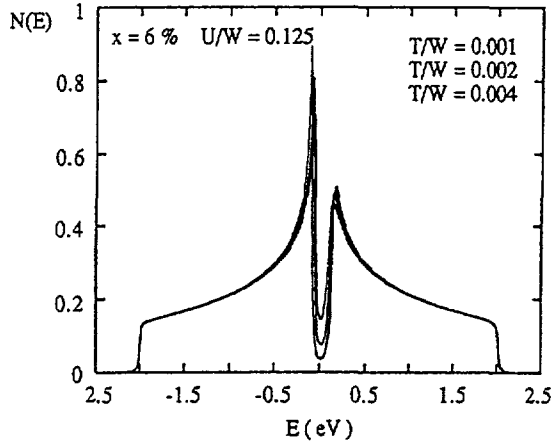


Fig. 1. — Density of states for 6% hole doping with $U/W = 0.125$ at different temperatures $T/W = 0.001, 0.002$ and 0.004 .

system submitted to a Fröhlich attractive interaction in the presence of short range antiferromagnetic correlations. The B.C.S. gap equation calculated using the Green functions dressed by the spin fluctuations is :

$$1 = g \int \frac{d^2k}{4\pi^2} k_B T_c \sum_n e^{-i\omega_n \eta} \frac{1}{(-i\omega_n - \varepsilon_k - \Sigma(-k, -\omega_n))(i\omega_n - \varepsilon_k - \Sigma(k, \omega_n))} \quad (4)$$

This treatment only assumes the existence of a Fröhlich effective attractive interaction between electrons with a coupling constant g , without specifying its microscopic origin. In the simplest model the attraction would be due to an exchange of phonons, but a more exotic mechanism, such as an exchange of spin fluctuations could also have been considered. However, in that case, RPA would be inadequate to discuss mixing of Copper and Zero sound channels. To reproduce an order of magnitude of the critical temperature analogous to La_2CuO_4 , we have assumed g to be equal to $W/6$ with a Debye energy equal to $W/40$. A smaller value of the Debye energy would require a larger value of g .

The calculated phase diagram (Fig. 2) is similar to the experimental one obtained for the one CuO_2 plane compounds [2]. Qualitatively, for a small hole (or electron) doping, the Fermi level is located at the bottom of the pseudogap and the critical temperature is very small. If the doping increases, the Fermi level moves towards the peak of the pseudogap and T_c increases. For large doping, T_c decreases owing to the decrease of the density.

4.3 NORMAL STATE PROPERTIES.

4.3.1 Magnetic susceptibility. — In the normal state, a large temperature dependence of the magnetic susceptibility χ in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [2] and in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ [14] has been observed. For small Sr concentration x , χ is an increasing function of the temperature but for high concentrations, the susceptibility behaves reversely. We propose that this temperature dependence is linked to the Pauli susceptibility given by $\chi^{\text{Pauli}} = 2 \mu_B^2 N(\varepsilon_F)$ where $N(\varepsilon_F)$ is the density of states at the Fermi level and μ_B is the Bohr magneton. In fact, because of the temperature dependence of the pseudogap, the density of states at the Fermi level varies differently whether the Fermi level is inside or outside the pseudogap : for small μ , the density increases with temperature and for higher μ , it is the reverse (Fig. 3).

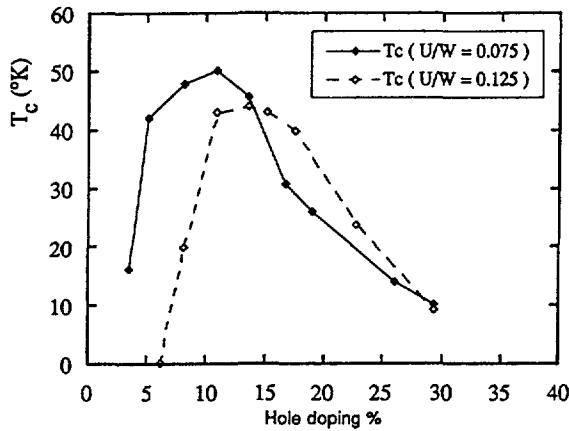


Fig. 2. — Phase diagram for superconductivity with a coupling constant g equal to $W/6$ and a Debye energy of 0.1 eV for the ratios $U/W = 0.07$ and 0.125 ($W = 4$ eV).

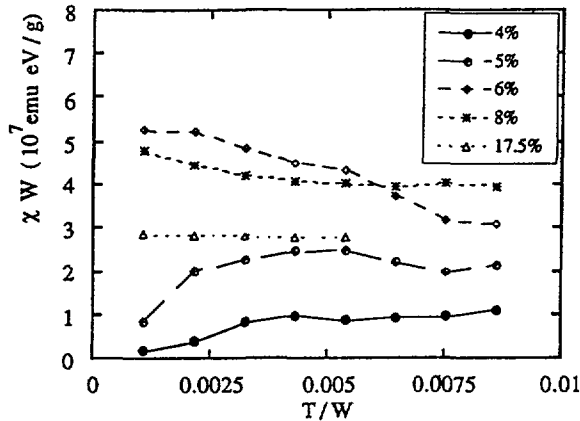


Fig. 3. — Temperature dependence of the Pauli susceptibility for various hole content x per unit cell with $U/W = 0.125$.

4.3.2 *Neutron scattering.* — Inelastic neutron scattering experiments carried out on YBCO_{6+x} show a magnetic pseudogap in the spin excitation spectrum observed at the nesting vector with a pseudogap energy increasing as x increases [15]. We propose that this crossover is related to the chemical potential as a consequence of the nesting property relationship which is $\epsilon_{k+Q} = -\epsilon_k - 2\mu$. Besides, the spin excitation spectra display at low temperature a feature with two characteristic energies. We propose that, while the lowest one is related to -2μ , the departure from perfect nesting, the highest one is a consequence of the pseudogap in the density of states and of the same order of magnitude. We can reproduce the experimental results by calculating the imaginary part of the susceptibility using the Green functions dressed by spin fluctuation. We carry out the calculation beyond the RPA approximation by taking into account the density of states of the correlated system. This correction to RPA is important, especially at small chemical potential because of the deep pseudogap (unfortunately, it has not been possible to take into account this correction for the calculation of the transport properties given below because of computation problems). The results are shown in figure 4 for different

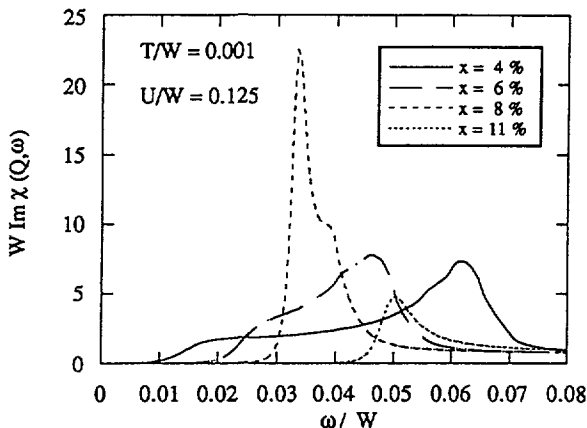


Fig. 4. — $\text{Im } \chi(Q, \omega)$ as a function of the energy (in the bandwidth units) at different temperatures calculated with $U/W = 0.125$ at $T/W = 0.001$ for different hole doping concentrations $x = 4\%$, 6% , 8% and 11% .

chemical potentials at relatively low temperature. We can see that the highest peak energy decreases for increasing μ as the width of density of states pseudogap decreases. For the highest doping, the pseudogap width is smaller than -2μ . We propose that, even though this structure has been observed for $T < T_c$, it has no relation with the superconducting gap.

4.3.3 *Resistivity.* — We have studied the electron scattering contribution to the electrical resistivity due to antiferromagnetic spin fluctuations in the relaxation-time approximation : i.e. the relaxation time $\tau = \hbar/\text{Im } \Sigma$ is the lifetime of the quasi-particles reduced by the electron-electron scattering and the electronic energies are the energies E_k of the quasi-particles dressed by the spin fluctuations. The conductivity σ_{xx} is :

$$\sigma_{xx} = \frac{2 e^2}{(2 \pi)^2 \hbar^2} \int dk_x dk_y \tau(E_k) \left(\frac{\partial E_k}{\partial k_x} \right)^2 \left(- \frac{\partial f_F}{\partial E} \right)_{E = E_k} \tag{5}$$

The resistivity is plotted for two concentrations of holes 7% and 8% (Fig. 5). It exhibits a

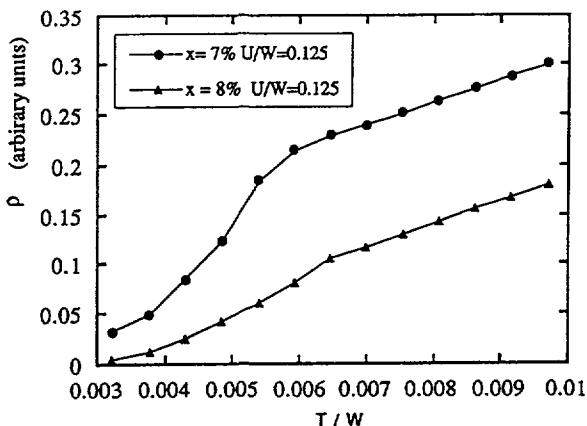


Fig. 5. — Temperature dependence of the resistivity for 7% and 8% hole per unit cell with $U/W = 0.125$.

T^2 behaviour at low temperature and linear T dependence at higher temperatures. The larger the doping concentration, the larger the crossover temperature. In fact, the temperature of the crossover is related to the chemical potential which is the amount of departure from perfect nesting. By extrapolating to the half-filled band case, we should obtain a linear T dependence of the resistivity down to 0 K. Of course, we have only calculated the spin fluctuation contribution to the resistivity. Although we expect this contribution to be dominant above the crossover, however, other mechanisms may add their contributions, which might be important especially below the crossover.

Comparing our resistivity and neutron scattering calculations, we establish a relation between the two crossover temperatures : $T_{\text{cross}}^{\text{res}}/T_{\text{cross}}^{\text{neu}} \approx 0.2$. Using inelastic neutron experiments on $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ ($x = 0.51, 0.69, 0.92$) [15], the resistivity crossover temperature for each compound is estimated (see Tab. I). It turns out that this crossover temperature for resistivity is always below the superconducting transition temperature which is consistent with the observed linear T dependence of the resistivity.

Table I. — Crossover temperatures extracted from neutron scattering experiments [16] and crossover temperatures estimations for the resistivity of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ compounds.

Compound	Crossover temperature for neutron experiment $T_{\text{cross}}^{\text{neu}}$	Crossover temperature estimation for resistivity $T_{\text{cross}}^{\text{res}}$	Superconducting transition temperature T_c
$\text{YBa}_2\text{Cu}_3\text{O}_{6.51}$	46 K	10 K	47 K
$\text{YBa}_2\text{Cu}_3\text{O}_{6.69}$	185 K	41 K	59 K
$\text{YBa}_2\text{Cu}_3\text{O}_{6.92}$	324 K	71 K	91 K

4.3.4 *Thermopower*. — The thermoelectric power provides fundamental information concerning the charge carriers. For high T_c materials, the temperature dependence of the thermopower and the sign change remain unexplained [16]. We have calculated the diffusion thermopower S :

$$S = \frac{\pi^2 k^2 T}{3 e} \left[\frac{\partial \ln \sigma(\varepsilon)}{\partial \varepsilon} \right]_{\varepsilon_F} \quad (6)$$

where σ is the conductivity. In equation (6), $\frac{\partial \ln \sigma(\varepsilon)}{\partial \varepsilon}$ is replaced by $\frac{\Delta \sigma}{\sigma \Delta E}$ for 7.5 % doping using the previous data displayed in figure 5 : the calculated S is positive and exhibits a maximum in the vicinity of the crossover temperature for the resistivity [13], as observed experimentally.

5. Conclusion.

The marginal Fermi liquid theory is very appealing because it yields a satisfactory account of many experimental data near the band half filling. However, away from half-filling, there

exists some experimental evidence for departures from the marginal behaviour. Our simple model provides a microscopic justification for such a behaviour : that of a marginal Fermi liquid near half-filling and a crossover towards a usual Fermi liquid behaviour when one departs from half-filling. Such a model seems to yield satisfactorily a qualitatively correct description of the experimental results. Of course, this model is much too simple to describe completely and quantitatively the whole complexity of real materials, but it seems to be a starting point providing a qualitatively correct basis for understanding the physics of high T_c superconductors.

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