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# Coulomb interaction in disordered metals and HTSC

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## Abstract

We consider underdoped or overdoped cuprates as disordered conductors. The diffusion coefficient  $D$  can be as low as  $10^{-5} \text{ m}^2 \text{ s}^{-1}$ . Under these conditions Coulomb interaction between electrons must be taken into account. The main effect is to open a dip in the density of state near the Fermi level. We show that this model explains most of the observed features of the so-called “pseudogap” in the normal state including its value, anisotropy and variation with doping. Such a model applied to disordered metals explains the dips observed in conductance measurements. © 2001 Elsevier Science B.V. All rights reserved.

*Keywords:* Disordered conductors; HTSC; Coulomb interaction; Cuprates

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## 1. Introduction

Many experiments made in the normal state of high  $T_c$  superconductors (HTSC) have revealed a so-called pseudogap. This pseudogap was observed in transport, magnetic, specific heat measurements and in scanning tunneling and angle resolved photoemission spectroscopy (ARPES) measurements [1]. The pseudogap observed in the normal state seems to be a partial gap. It is related to a crossover temperature, named  $T^*$ , below which its observation is possible. Many authors relate  $T^*$  with magnetic phenomena (e.g. spin gap). We propose another explanation for the pseudo-

gap related to  $T^*$ . It is mainly observed in underdoped samples, which are disordered and in which the mean free path and thus the diffusion coefficient is very low. Under these conditions, the diffusion length ( $L_D$ ) becomes of the order of magnitude or smaller than the electron wavelength  $1/k_F$ . The materials are thus disordered conductors and the Coulomb repulsion becomes important (for a review see Ref. [2]).

## 2. Description of the model used

Altshuler and Aronov [2] have developed a theory to study the effect of the electron–electron interaction on the properties of disordered conductors. The conditions for its application  $k_F L_D \ll 1$  is also satisfied for underdoped cuprates. The theory has also shown that the interaction effects are most clearly pronounced in low-dimensionality systems. We compute the one particle density of

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state (DOS) taking into account the Coulomb interactions in the self-energy term. We show that particle repulsion produces a dip in the DOS at the Fermi energy. In the cuprates, where the Fermi surface is very anisotropic, we find that the pseudogap appears first and is more pronounced in the directions of the saddle points (1,0) and equivalent of the CuO<sub>2</sub> planes, where the Fermi velocity is smaller. This is clearly seen in the ARPES experiments.

We take an anisotropic dispersion relation for the one electron energy  $\varepsilon_k$  in the CuO<sub>2</sub> planes (bidimensional):

$$\varepsilon_k = -2t(\cos X + \cos Y) + 4t' \cos X \cos Y + E_F - E_S \quad (1)$$

$E_F$  is the Fermi level (FL) energy, we take  $E_F = 0$ , and  $E_S$  is the saddle point energy,  $X = k_x a$ ,  $Y = k_y a$ ,  $\mathbf{k}(k_x, k_y)$  is the wave vector. The self-energy is computed using the following formula [2]:

$$\Sigma_m = \Sigma_m^{\text{ex}} + \Sigma_m^{\text{H}} \quad (2)$$

where  $\Sigma_m^{\text{ex}}$  is the exchange part and  $\Sigma_m^{\text{H}}$  the Hartree part of the self-energy. The exchange energy is given by:

$$\Sigma_{m,\varepsilon}^{\text{ex}} = \frac{1}{2\pi v} \int_{\varepsilon}^{\infty} d\omega \int \frac{d^3 q}{(2\pi)^3} U(\vec{q}) \frac{Dq^2}{\omega^2 + (Dq^2)^2} \quad (3)$$

with  $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ ,  $D$  the diffusion coefficient.  $U(\mathbf{q})$  is the Fourier transform of the long range Coulomb interaction and the term in  $Dq^2$  the Fourier transform of the electron–electron correlation function. For  $U(\mathbf{q})$  we take a screened Coulomb potential (the screening is tridimensional):

$$U(\mathbf{q}) = C/(q^2 + q_0^2) \quad (4)$$

where  $q_0^{-1}$  is the screening length. We then compute the DOS in the two directions (1,0) and (1,1) within a small angle  $d\theta$ , using a self-consistent procedure.

### 3. Variation of the diffusion coefficient $D$ with doping and direction

In a simple Fermi liquid, the diffusion coefficient is given by  $D = (1/3)v_F l$ ,  $v_F$  is the Fermi velocity and  $l$  is the mean free path. For a given sample,

with doping and disordered fixed,  $l$  is constant and  $v_F$  varies with direction, it is much smaller near the saddle point A ( $0, \pm\pi$ ) than at point B ( $\pm\pi/2, \pm\pi/2$ ). When the doping varies,  $l$  changes mainly due to the disorder and may be due to the impurities. In underdoped samples there are disorder in the oxygen vacancies and crystalline defects. We assume that  $l$  is strongly reduced as the doping decreases until we reach a region where the crystalline order is restored in the insulating antiferromagnetic state.  $E_F - E_S$  varies slightly and  $v_F$  at point A is reduced,  $v_F$  at point B remains almost unchanged, so the anisotropy remains.

### 4. Effect of the diffusion coefficient, the screening and the bandwidth

Our results are presented in Figs. 1 and 2. We can see that our model explains why the pseudogap opens in the (1,0) direction and not in the (1,1) direction as seen in ARPES [1]. We have studied the effect of screening by varying  $q_0 a$ , in the A direction, the result is shown in Fig. 3. The decrease of  $q_0 a$  increases the number of states in the wings and deepens the dip. The effect of varying the transfer integrals,  $t$  and  $t'$ , i.e. the bandwidth, is less important.

### 5. Disordered metal

Osofsky et al. [3] measured the point-contact tunneling conductance on different Si-doped (0–

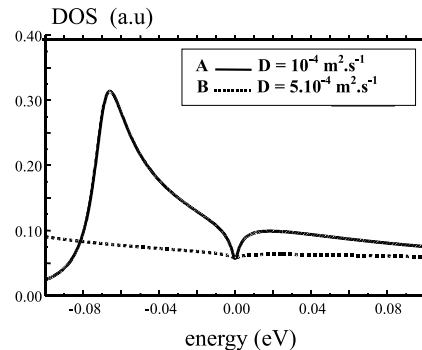


Fig. 1. Calculated DOS with Coulomb interaction – A: in the (1,0) direction, and equivalent directions; B: in the (1,1) direction.

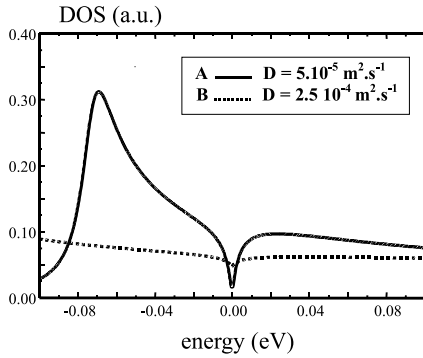


Fig. 2. Calculated DOS with Coulomb interaction – A: in the (1,0) direction, and equivalent directions; B: in the (1,1) direction.

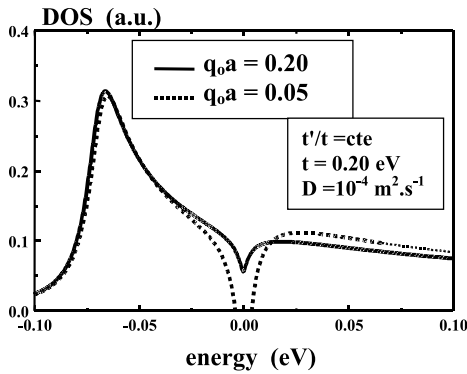


Fig. 3. Effect of the screening on the DOS calculated with the Coulomb interaction term.

30%) W (tungsten) films. The Si doping induces disorder which has been confirmed by conductivity and X-ray diffraction characterisation [3]. A more pronounced dip appears as the disorder increases. In Fig. 4 we note that our fit for  $T = 0$  K agrees very well with the experimental behaviour at 1.5 K consistent with the disorder being truly responsible for the dip.

## 6. Discussion and conclusion

Experiments reported by Vobornik et al. [4] show the possibility of having disorder-induced pseudogaps comparable to those existing in underdoped Bi2212 samples. The pseudogap can also be observed in overdoped samples [5–7]. As we can

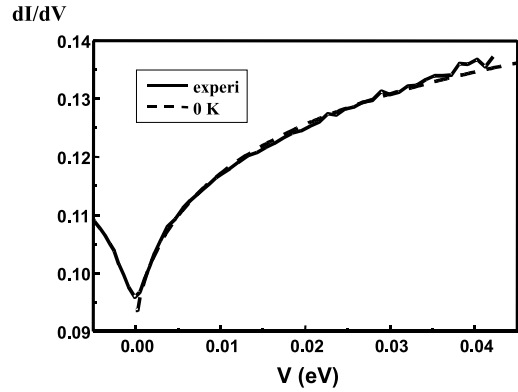


Fig. 4. Full line: experimental curve; dashed line: the fitting curve for the Si-20% doped W sample.

see in our figures, the dip is less pronounced if either the screening or the diffusion coefficient is higher. These higher values exist in the overdoped regime, leading to a lower value of  $T^*$ . Then it seems to be below  $T_c$ , so it cannot be observed in the normal state [5–7]. Therefore in varying the physical parameters in our model (screening, doping (i.e.  $E_F - E_S$ ), diffusion coefficient, bandwidth), we have a good explanation for the evolution of the pseudogap in the phase diagram. The pseudogap decreases from underdoped to overdoped region in agreement with these parameters. The pseudogap was observed in a non-superconducting region in scanning tunneling spectroscopy measurements made by Cren et al. [8]. This shows that the pseudogap is not inevitably related to superconductivity, but is an intrinsic property of the material. The existence of the “Coulomb dip” in the HTSC and the Si-doped metals, where we know it is due to disorder, confirms the origin of the pseudogap.

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