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Influence of Disorder in Superconductor Compounds

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We consider underdoped or overdoped cuprates as disordered conductors. The diffusion coefficient D can be as low as 10^{-5} m^2 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 (DOS) near the Fermi level (FL). 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.

KEY WORDS: superconductivity; pseudogap; disorder; susceptibility.

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 ARPES (angle resolved photoemission spectroscopy) 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. We propose another explanation for the pseudogap 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 Altshuler and Aronov [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 $k_F L_D \lesssim 1$ 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 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_2 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 ε_k in the CuO_2 planes (bidimensional):

$$\varepsilon_k = -2t(\cos X + \cos Y) + 4t' \cos X \cos Y + E_F - E_s \tag{1}$$

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

$$\Sigma_m = \Sigma_m^{ex} + \Sigma_m^H \tag{2}$$

where Σ_m^{ex} is the exchange part and Σ_m^H the Hartree part of the self-energy. The exchange energy is given by

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

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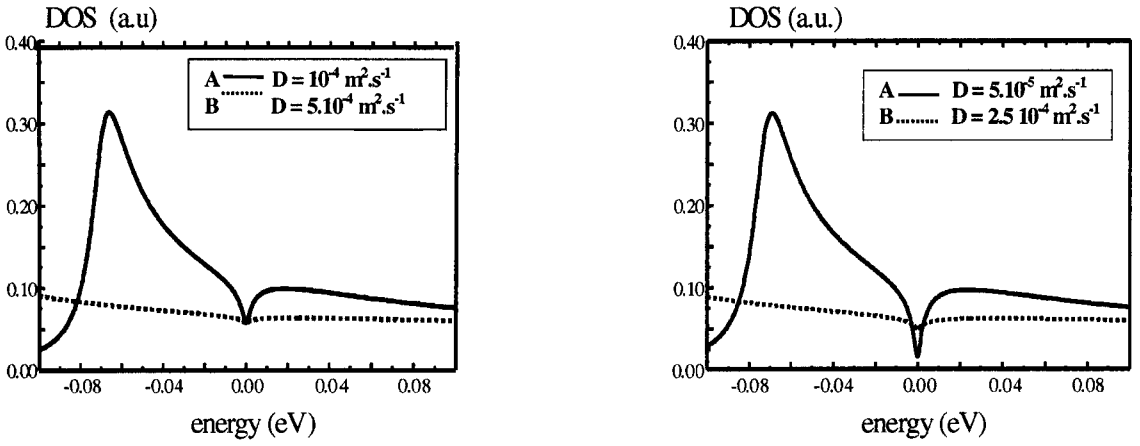

Fig. 1. Calculated DOS with Coulomb interaction with different sets of values of D, (A) in the (1, 0) direction, and equivalent directions; (B) in the (1, 1) direction.

with $\vec{q} = \vec{k} - \vec{k}$, D the diffusion coefficient. $U(\vec{q})$ 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 $U(\vec{q})$ we take a screened Coulomb potential (the screening is tridimensional):

$$U(\vec{q}) = \frac{C}{(q^2 + q_0^2)} \tag{4}$$

where q_o^{-1} is the screening length. We then compute the DOS in the two directions (1, 0) and (1, 1) within a small angle $d\phi$, 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 $(\pm\pi/2, \pm\pi/2)$. 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 Fig. 1. We can see that our model explains how 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 $q_o a$, in the A direction, the result is shown in Fig. 2. The decrease of $q_o a$ 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.

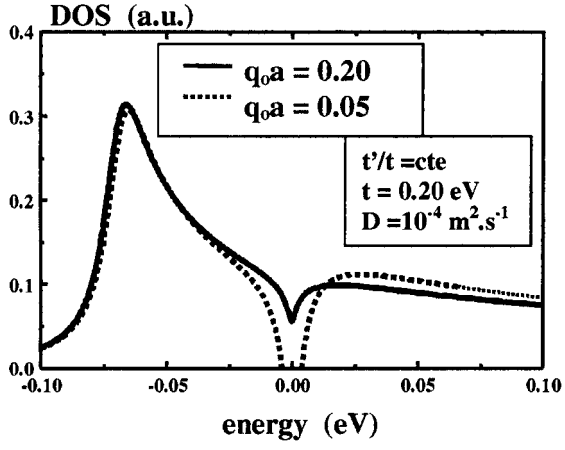

Fig. 2. Effect of the screening on the DOS calculated with the Coulomb interaction term.

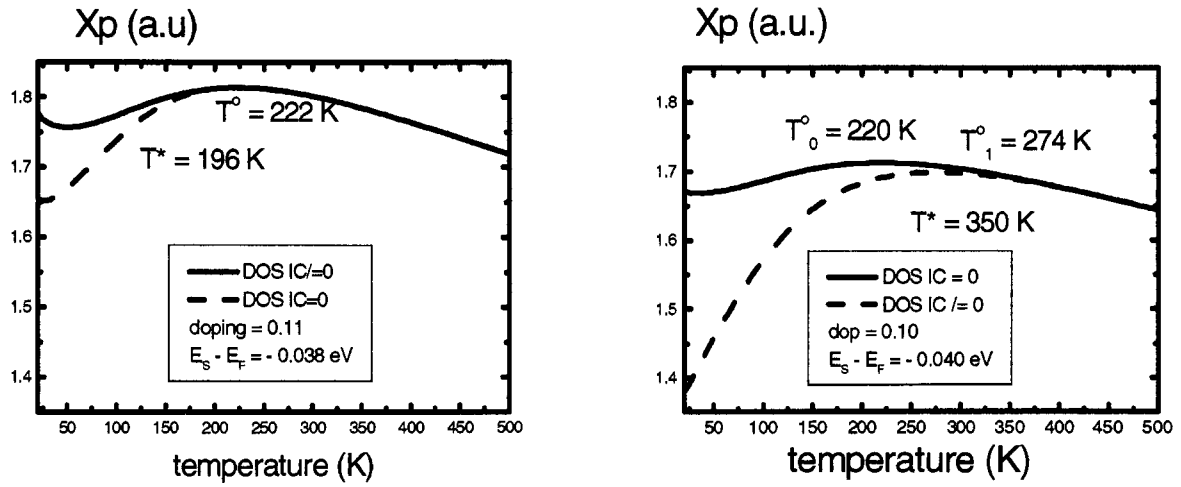

Fig. 3. Calculated Pauli susceptibilities. (A) For 0.11 hole doping; (B) for 0.10 hole, lower doping, with a deeper and broader dip, leading to a smaller $Xp(T)$, to a more pronounced decrease, and to $T^* > T^\circ$. Full line – without disorder effect; dashed line – with disorder effect.

5. SUSCEPTIBILITY AND DISORDER

Now we are able to calculate the total DOS, the dip created at FL by the disorder effect can be more or less deep or broad, depending for a given bandwidth of the coefficient of diffusion or the screening strength values. We study some cases and calculate the corresponding Pauli susceptibility, as already made but without disorder effect [3], where the maxima in the $Xp(T)$ curves were related to the high DOS at E_S. In Fig. 3 we present our theoretical results for two different pseudogaps, in Fig. 3B it is deeper and broader. At T^*, where these pseudogaps open, $Xp(T)$ (dashed line) begins to be lower than $Xp(T)$ (full line) without pseudogap. As the temperature decreases in Fig. 3A this opening occurs after the temperature T°, where the high DOS at E_S begins to be filled, but in Fig. 3B this opening occurs before this event. The consequence of these mixing effects give an effective T_1° in our initial theory [3] and $T^* > T^\circ$. This is a theoretical result to be discussed as all experimental results seem to give $T^\circ > T^*$. Such bigger pseudogap probably occurs for lower doping, leading to $T^* < T^\circ$, the lower dopings are in study. Anyway this atypical case has to be presented.

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 [4]. As we can 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]. 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 nonsuperconducting region in scanning tunneling spectroscopy measurements made by Cren *et al* [6]. 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 [7,8], where we know it is due to disorder, confirms that disorder can be at the origin of the pseudogap.

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