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The van Hove scenario of high T_c superconductors : the effect of doping

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The van Hove scenario explains many physical properties of high T_c superconductors [1-5]. We have previously established that the B.C.S. gap equation, using an electron-phonon interaction with weak screening and a 2D electronic band structure showing saddle points (vHs) leads to an anisotropic gap Δ_k [2]. We examine the consequences of doping on the superconducting properties of the cuprates in the framework of this model. We compute, the gap anisotropy $\alpha = \Delta_{Max}/\Delta_{min}$, T_c, the density of state (D.O.S.) of quasiparticle excitations and the specific heat. Our approach neglects magnetic fluctuations and is thus not applicable to underdoped material.

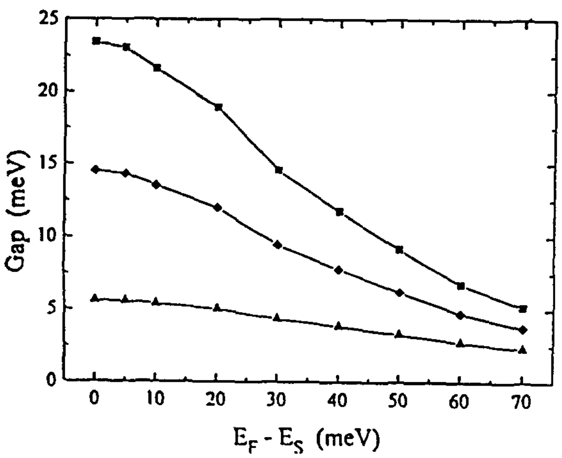

Figure 1 : Variation of the various gaps Δ_{Max}, Δ_{min}, Δ_{av} versus the doping, $D = E_F - E_s$, at T = 0K, square symbol = Δ_{Max}, diamond symbol = Δ_{av}, up triangle symbol = Δ_{min}

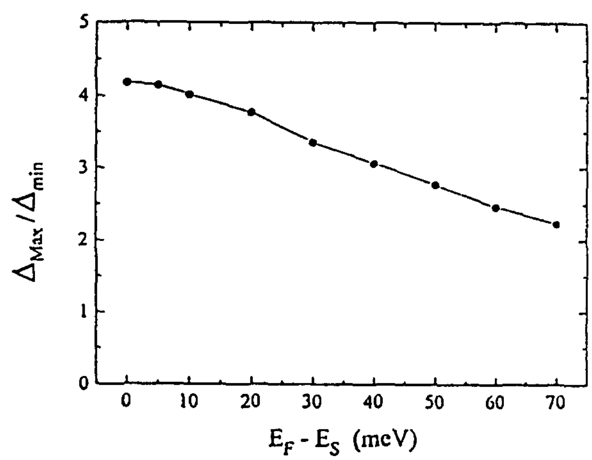

Figure 2 : Variation of the anisotropy ratio $\alpha = \Delta_{Max}/\Delta_{min}$, versus the doping, $D = E_F - E_s$

1. T_c AND GAP ANISOTROPY AS A FUNCTION OF DOPING

We use a rigid band model, the doping is represented by a shift $D = E_F - E_s$ of the Fermi level:

$$\xi_k = -2t\left[\cos k_x a + \cos k_y a\right] - D \qquad (1)$$

We use the same procedure as in our previous paper [2] to compute the various gaps. In figure (1) we present the results for Δ_{Max}, Δ_{min}, Δ_{av}, and in figure (2) the variation of the anisotropy ratio $\alpha = \Delta_{Max}/\Delta_{min}$ versus D. We observe of course that the gaps and T_c decrease with D. The agreement with experiment [5-6] is very good.

We have a maximum and a minimum value of the ratio $2\Delta(0)/k_BT_c$, for example for D=0, 6 and 1.4. We obtain a new and interesting result which is the decrease of the anisotropy ratio α with doping. This is confirmed by recent results on photoemission [7].

2. DENSITY OF STATE

The D.O.S. is computed using the same procedure as in reference [4]. Figure (3) represents the variation of the D.O.S. as a function of ε for T = 0 K. This is similar to the conductance of a NIS junction. But for different values of D, we see a new maximum emerging, which is a signature of the vHs. This is seen experimentally in the STM tunneling experiments of Renner et al [8].

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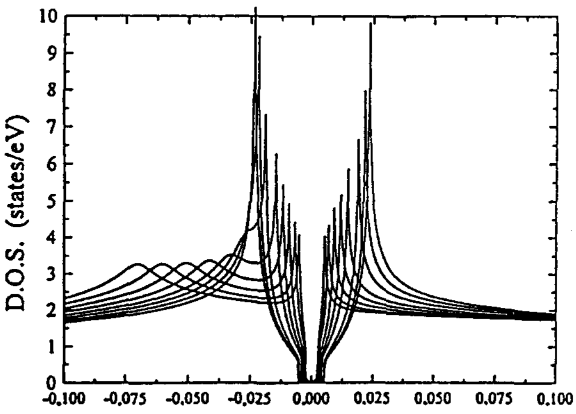

Figure 3 : Variation of the D.O.S. versus the energy ε, for T = 0 K, for different values of the doping $D = E_F - E_s$, i.e. 0, 10,20, 30, 40, 60 and 70 meV.

3. SPECIFIC HEAT

We shall now use this calculated D.O.S. to evaluate the specific heat. We use the values of ξ_k and Δ_k, $\Delta_{Max}(T, D)$ and $\Delta_{min}(T, D)$, given by formula (1) and in references [2] [5] to evaluate C_s. The results are presented in figure (4). We can make the following observations:

i - The jump in specific heat at T_c varies with doping, $(\Delta C/C)_{Tc}$ is 3.2 for D = 0 and 1.48 for D = 60 meV compared to 1.41, the B.C.S. value for an isotropic superconductor with a constant D.O.S., N_0, in the normal state. The high value of $(\Delta C/C)_{Tc}$ is essentially due to the v.H.s. when it coincides with the Fermi level and the highest value of the gap Δ_k.

ii - For a usual metal with $N_0, \gamma_N = C_N / T$ is constant, proportional to N_0. The specific heat $C_N(T)$ explores a domain of width k_BT around the Fermi level E_F. So for $D << k_BT_c$, the variation of γ_N above T_c is logarithmic, we find $\gamma_N = a (\ln 1/T) + b$ for $0 \leq D \leq 30$ meV. For D = 0 this behaviour has already been predicted by Bok and Labbé [9]. For D > 30 meV, at high temperature $T - T_c > D$, the B. L. law is observed, but for lower temperatures γ_N increases with T and passes through a maximum at T* as the law T* (K) = 2.9 D (meV).

iii - Our model,neglecting magnetic fluctuations, gives an Arrhenius law for C_s at low temperature with a caracteristic energy which is Δ_{min}.

We can compare our results on the effect of doping on C_s with experiments, for example the $Tl_2Ba_2CuO_{6+\delta}$ compounds, studied by Loram et al [10], because they are overdoped samples, with only one CuO_2 plane.

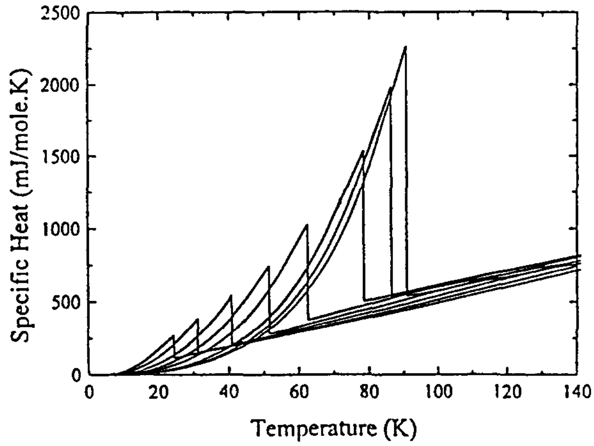

Figure 4 : The calculated specific heat versus the temperature for the different value of the doping $D = E_F - E_s = 0$, 10, 20, 30, 40, 50, 60 and 70 meV.

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