# SUPERCONDUCTIVITY IN CUPRATES, THE VAN HOVE SCENARIO : A REVIEW

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## INTRODUCTION

Many recent experiments of angular resolved photoemission spectroscopy (ARPES) have confirmed the existence of saddle points (van Hove singularity or v.H.s.) close to the Fermi level in five different copper oxide compounds by three different groups, in Stanford[1], in Argonne[2] and in Wisconsin[3]. These observations have been made in the following compounds : $Bi_2Sr_2CuO_6$ (Bi 2201), $Bi_2Sr_2CaCu_2O_8$ (Bi 2212), $YBa_2Cu_3O_7$ (Y123), $YBa_2Cu_4O_8$ (Y124) and $Nd_{2-x}Ce_xCuO_{4+\delta}$ (NCCO). These experiments establish a general feature : in very high $T_c$ superconductors cuprates ($T_c \sim 90$ K) van Hove singularities are present close to the Fermi level. This is probably not purely accidental and we think that any theoretical model must take into account these experimental facts. The origin of high $T_c$ in the cuprates is still controversial and the role of these singularities in the mechanism of high $T_c$ superconductivity is not yet established, but we want to stress that the model of 2D itinerant electrons in presence of v.H. singularities in the band structure has already explained a certain number of experimental facts, i.e. high $T_c$'s, anomalous isotope effect[4], marginal Fermi liquid effects[5] and the very small values of the coherence length[6]. It was also been shown that the singularity is in the middle of a wide band and that in these circumstances, the Coulomb repulsion $\mu$ is renormalized and $\mu$ is replaced by a smaller number, the effective electron-phonon coupling is $\lambda_{eff} = \lambda - \mu^*$ and remains positive[7]. We think that this fact explains the very low $T_c$ observed in $Sr_2RuO_4$, where a very narrow band has been determined by ARPES[8].

We have shown by using a weakly screened electron-phonon interaction that we obtain a strong gap anisotropy[9].

We then compute the density of states (D.O.S.) of quasiparticle excitations in the superconducting state, in the frame work of this model. We also study the effect of doping, i.e. of the distance between the Fermi level $E_F$ and the singularity $E_S$[10].

We apply this result to the calculation of tunneling characteristics and of the electronic specific heat $C_S$[10,11].

We also study the influence of doping on the screening length and on the calculation of $T_c$. We thus explain why the maximum $T_c$ is not observed when $E_F - E_S = 0$.

We finally study the influence of doping, i.e. $E_F - E_S$, on the normal state properties and interpret some properties of the so-called pseudogap[12].

*The Gap Symmetry and Fluctuations in High - $T_c$ Superconductors*
Edited by Bok *et al.*, Plenum Press, New York, 1998

## CALCULATION OF $T_c$, THE LABBE BOK FORMULA

Labbé-Bok[4] have computed the band structure for the bidimensional $CuO_2$ planes of the cuprates, considered as a square lattice (quadratic phase). The simplest band structure we can take for a square lattice is :

$$\xi_k = -2t\left[\cos k_x a + \cos k_y a\right]$$

where t is an interaction with nearest neighbours. This gives a square Fermi surface with saddle points, or v.H.s., at [ 0 , $|\pi|$ ] positions of the Brillouin zone, and a logarithmic D.O.S. with a singularity : $n(\xi) = n_1 \ln|D/(\xi-\xi_S)|$ , where D = 16t is the width of the singularity and $\xi_S$ the singularity energy level. The v.H.s. corresponds to half filling. We know that is not a good representation of the high $T_c$ cuprates because for half filling (one electron per copper site) they are antiferromagnetic insulators. We think that the Fermi level is at v.H.s. for a doping level corresponding to 20 % of holes in each $CuO_2$ plane or 0.40 filling of the first Brillouin zone (B.Z.). This can be achieved by taking into account the repulsive interaction between second nearest neighbours (s.n.n.) and the effect of the rhomboedric distorsion. For the repulsive interaction with s.n.n. the band structure becomes:

$$\xi_k = -2t\left[\cos k_x a + \cos k_y a\right] + 4\alpha t \cos k_x a \cos k_y a$$

where $\alpha t$ is an integral representing the interaction with s.n.n.. The singularity occurs for $\xi = -4\alpha t$, there is a shift towards lower energy. The Fermi surface at the v.H.s. is no longer a square but is rather diamond-shaped. More detailed calculations can be obtained in reference 6, taking also into account the rhomboedric distorsion.

The Labbé-Bok[4] formula was obtained using the following assumptions :

1- the Fermi level lies at the van Hove singularity

2- the B.C.S. approximations :

- The electron-phonon interaction is isotropic and so is the superconducting gap $\Delta$.
- The attractive interaction $V_p$ between electrons is non zero only in an interval of energy $\pm\hbar\omega_0$ around the Fermi level where it is constant. When this attraction is mediated by emission and absorption of phonons, $\omega_0$ is a typical phonon frequency.

In that case, the critical temperature is given by

$$k_B T_c = 1.13 D \exp\left[-\left(\frac{1}{\lambda} + \ln^2\left(\frac{\hbar\omega_0}{D}\right) - 1.3\right)^{1/2}\right] \qquad (1)$$

where $\lambda = (1/2) n_1 V_p$ is equivalent to the coupling constant.

A simplified version of formula (1), when $\hbar\omega_0$ is not too small compared to D, is :

$$k_B T_c = 1.13 D \exp(-1/\sqrt{\lambda})$$

The two main effects enhancing $T_c$ are

1- the prefactor in formula (1) which is an electronic energy much larger than a typical phonon energy $\hbar\omega_0$.

2- $\lambda$ is replaced by $\sqrt{\lambda}$ in formula (1) in comparaison with the BCS formula, so that in the weak coupling limit when $\lambda<1$, the critical temperature is increased. In fact it gives too high values of $T_c$, we shall see later that this is due to the fact that we have neglected Coulomb repulsion between electrons. Taking this repulsion into account we shall obtain values for $T_c$ which are very close to the observed one.

As it is however, this approach already explains many of the properties of the high $T_c$ cuprates near optimum doping.

- The variation of $T_c$ with doping

The highest $T_c$ is obtained when the Fermi level is exactly at the v.H.s.. For lower or higher doping the critical temperature decreases. That is what is observed experimentally[10].

- The isotope effect

Labbé and Bok[4] showed using formula (1), that the isotope effect is strongly reduced for high $T_c$ cuprates. Tsuei *et al*[13] have calculated the variation of the isotope effect with doping and shown that it explains the experimental observations.

- Marginal Fermi liquid behaviour

In a classical Fermi liquid, the lifetime broadening $1/\tau$ of an excited quasiparticle goes as $\varepsilon^2$. The marginal Fermi liquid situation is the case where $1/\tau$ goes as $\varepsilon$. Theoretically marginal behaviour has been established in two situations (a) the half-filled nearest-neighbour coupled Hubbard model on a square lattice and (b) the Fermi level lies at a v.H. singularity[13]. Experimental evidence of marginal Fermi liquid behaviour has been seen in angle resolved photoemission[14], infrared data[15] and temperature dependence of electrical resistivity[16]. Marginal Fermi liquid theory, in the frame work of v.H.s. predicts a resistivity linear with temperature T. This was observed by Kubo et al[16]. They also observe that the dependence of resistivity goes from T for high $T_c$ material to $T^2$ as the system is doped away from the $T_c$ maximum, which is consistent with our picture; in lower $T_c$ material the Fermi level is pushed away from the singularity

## INFLUENCE OF THE COULOMB REPULSION

As soon as 1959 Bogolubov et al[17] have shown that the electron-electron repulsion plays a central role in superconductivity. Assuming a constant repulsive potential $V_{kk'} = V_c$ from 0 to $E_F$ they find that $T_c$ is given by :

$$T_c \cong To \exp\left[\frac{-1}{\lambda - \mu^*}\right]$$

With $\mu = NoV_c$ and $\mu^* = \dfrac{\mu}{1 + \mu \ln E_F / \omega_o}$ (2)

Cohen and Anderson[18] assumed that for stability reasons $\mu$ is always greater than $\lambda$. Ginzburg[19] gave arguments that in some special circumstances $\mu$ can be smaller than $\lambda$. Nevertheless if we take $\mu \geq \lambda$, superconductivity only exists because $\mu^*$ is of the order of $\mu/3$ to $\mu/5$ for a Fermi energy of the order of 100 $\hbar\omega_0$. It is useless to reduce the width of the band W ($E_F$ = W/2 for a half-filled band) because $\lambda$ and $\mu$ vary simultaneously and $\mu^*$ becomes greater if $E_F$ is reduced, thus giving a lower $T_c$. Superconductivity can even disappear in a very narrow band if $\lambda - \mu^*$ becomes negative.

We have shown[7] that nevertheless high $T_c$ can be achieved in a metal containing almost free electrons (Fermi liquid) in a broad band, with a peak in the D.O.S. near the middle of the band.

Taking a D.O.S., which is a constant $n_0$ between energies - W/2 and W/2, (the zero of energy is at the Fermi level) and is $n(\xi) = n_1 \ln|D/\xi| + n_0$ between -D and +D we find for $T_c$, the following formula :

$$k_B T_c = \frac{D}{2} \exp\left[0.819 + \frac{n_0}{n_1} - \sqrt{F}\right] \qquad \text{where}$$

$$F = \left(\frac{n_0}{n_1} + 0.819\right)^2 + \left(\ln\frac{\hbar\omega_0}{D}\right)^2 - 2 - \frac{2}{n_1}\left(n_0 \ln\frac{2.28\hbar\omega_0}{D} - \frac{1}{V_p - V_c^*}\right) \qquad (3)$$

$$V_c^* = \frac{V_c}{1 + V_c\left[\frac{n_1}{2}\left(\ln\frac{D}{\hbar\omega_0}\right)^2 + n_0 \ln\frac{W}{2\hbar\omega_0}\right]}$$

We can have a few limiting cases for this formula : $n_1 = 0$ : no singularity. We find the Anderson-Morel formula. $V_C = 0$ and $n_0 = 0$ : this gives the Labbé-Bok formula.

There are many effects enhancing $T_C$

$\lambda - \mu^*$ is reduced by the square root, down to $\sqrt{\lambda_1 - \mu_1{}^*}$ when $n_1$ is large enough.

As $\lambda - \mu^* < 1$ the critical temperature is strongly increased because this factor appears in an exponential. The prefactor before the exponential is D, the singularity width instead of $\hbar\omega_0$. We expect $D > \hbar\omega_0$. For instance D may be of the order of 0.5 eV and $\hbar\omega_0$ about a few 10 meV ($D/\hbar\omega_0$ of the order of 5 to 10).

We have made some numerical calculations using formula (3) to illustrate the effect of Coulomb repulsion. We used two values of D : D = 0.9 eV corresponding to t = 0.25 eV and a much more smaller value D = 0.3 eV. These calculations show that the Coulomb repulsion does not kill superconductivity in the framework of the L.B. model. The general rule for high $T_c$ in this model is to have a peak in the density of states near the middle of a broad band to renormalize the effective repulsion $\mu$. For a narrow band, W, or D, is small, $T_c$ decreases very rapidly as seen in figure (1). A recent case has been observed in $Sr_2RuO_4$ with a narrow band and $T_c$ is small[8].

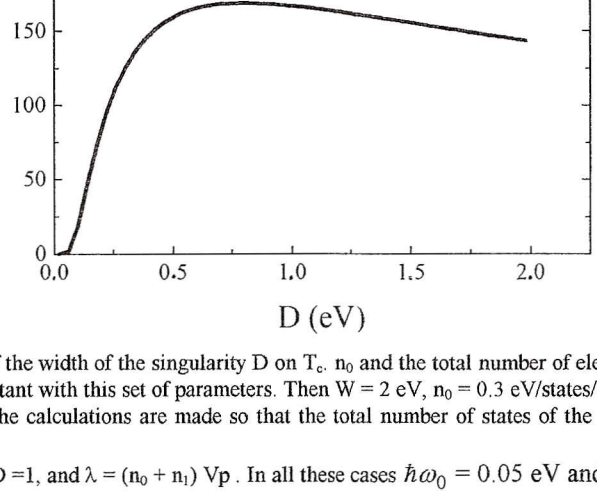


**Figure 1** : Effect of the width of the singularity D on $T_c$. $n_0$ and the total number of electrons per unit cell are maintened constant with this set of parameters. Then W = 2 eV, $n_0$ = 0.3 eV/states/Cu, $n_1$ = 0.2/D. In all these cases the calculations are made so that the total number of states of the band is one by Cu atom.

Then $n_0 W + 2 n_1 D = 1$, and $\lambda = (n_0 + n_1) Vp$. In all these cases $\hbar\omega_0 = 0.05$ eV and $\lambda = 0.5$.

## GAP ANISOTROPY

Bouvier and Bok[9] have shown that using a weakly screening electron-phonon interaction, and the band structure of the $CuO_2$ planes four saddle points: an anisotropic superconducting gap is found.

## 1. Model and basic equations

We use the rigid band model, the doping is represented by a shift $D_e = E_F - E_s$ of the Fermi level. This band structure is

$$\xi_k = -2t\left[\cos k_x a + \cos k_y a\right] - D_e \qquad (4)$$

The Fermi level is taken at $\xi_k = 0$.

We use a weakly screened attractive electron-phonon interaction potential :

$$V_{kk'} = \frac{-|g_q|^2}{q^2 + q_0^2} < 0$$

where g(q) is the electron phonon interaction matrix element for $\vec{q} = \vec{k}' - \vec{k}$ and $q_0$ is the inverse of the screening length.

We use reduced units: $X = k_x a$, $Y = k_y a$, $Q = qa$, $u = \frac{\xi}{2t}$, $\delta = \frac{D_e}{2t}$

We use the B.C.S. equation for an anisotropic gap :

$$\Delta_{\vec{k}} = \sum_{k'} \frac{V_{kk'}\,\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}} \qquad (5)$$

We compute $\Delta_{\vec{k}}$ for two values of $\vec{k}$ : $\Delta_A$ for $k_x a = \pi$, $k_y a = 0$ (6)

$\Delta_B$ for $k_x a = k_y a = \frac{\pi}{2}$

We solve equation (5) by iteration. We know from group theory considerations, that $V_{kk'}$ having a four-fold symmetry, the solution $\Delta_k$ has the same symmetry. We then may use the angle $\Phi$ between the 0 axis and the $\vec{k}$ vector as a variable and expand $\Delta(\Phi)$ in Fourrier series

$$\Delta(\Phi) = \Delta_0 + \Delta_1 \cos(4\Phi + \varphi_1) + \Delta_2 \cos(8\Phi + \varphi_2) + \ldots \qquad (7)$$

We know that $\varphi_1 = 0$, because the maximum gap is in the directions of the saddle points. We use the first two terms. The first step in the iteration is obtained by replacing $\Delta_k$ by $\Delta_{av} = \Delta_0$ in the integral of equation (5). We thus obtain, for the two computed values : $\Delta_A = \Delta_{Max} = \Delta_0 + \Delta_1$ and $\Delta_B = \Delta_{min} = \Delta_0 - \Delta_1$, the following expression :

$$\Delta_{A,B}(T) = \lambda_{eff} \int_{u_{min}}^{u_{max}} \frac{\Delta_{av}(T)}{\sqrt{u^2 + u_{av}^2(T)}}\, I_{(A,B)}(u)\, \tanh\left(\frac{\sqrt{u^2 + u_{av}^2(T)}}{k_B T / t}\right) du \qquad (8)$$

with $$I_{A,B}(u) = \int_0^{x_o'} \frac{dx'}{\left[1 - \left[(\delta - u) - \cos x'\right]^2\right]^{1/2}} \frac{(q_o a)^2}{Q_{A,B}^2 + (q_o a)^2} \qquad (9)$$

where $u_{min} = -\frac{\hbar\omega_c}{2t}$, $u_{Max} = +\frac{\hbar\omega_c}{2t}$, $u_{av}(T) = \frac{\Delta_{av}(T)}{2t}$, $x_o' = a\cos\left(\frac{\delta - u}{2}\right)$

$\omega_c$ is the cut off frequency. For the following part of this work we will keep the value of $\hbar\omega_c = 60$ meV for the Bi2212 compound, a characteristic experimental phonon energy. This choice respects our approximation for $V_{kk'}$.

- For the choice of t, the transfer integral comes from the photoemission experiments and is t = 0.2 eV as explained in reference[9].
- $q_0a$ is adjusted, it is the Thomas Fermi approximation for small q's,
- $\lambda_{eff}$ is adjusted so as to find the experimental value of $\Delta_{Max}$ and $\Delta_{min}$ and we find a reasonable value of about 0.5. $\lambda_{eff}$ is the equivalent of $\lambda$-$\mu^*$ in the isotropic 3D, BCS model.

In fact the values of $q_0a$ and $\lambda_{eff}$ must depend of the doping level $D_e$. This calculation will be done later. Here $q_0a = 0.12$ and $\lambda_{eff} = 0.665$.

## 2. Results

In figure (2), we present the variation of the various gaps $\Delta_{Max}$, $\Delta_{min}$ and $\Delta_{av}$ with temperature at optimum doping, i.e. for a density of holes of the order of 0.20 per CuO plane, as seen before[6]. We take in that case $D_e = 0$ and we find $T_c = 91$ K and an anisotropy ratio $\alpha = \Delta_{Max}/\Delta_{min} = 4.2$ and for the ratios of $2\Delta/k_BT_c$ the following values :

$$\frac{2\Delta_{Max}}{k_BT_c} = 6.\,, \quad \frac{2\Delta_{av}}{k_BT_c} = 3.7\,, \quad \frac{2\Delta_{min}}{k_BT_c} = 1.4$$

This may explain the various values of $2\Delta/k_BT_c$ observed in experiments. Tunneling spectroscopy gives the maximum ratio and thermodynamic properties such as $\lambda(T)$ (penetration depth) gives the minimum gap.

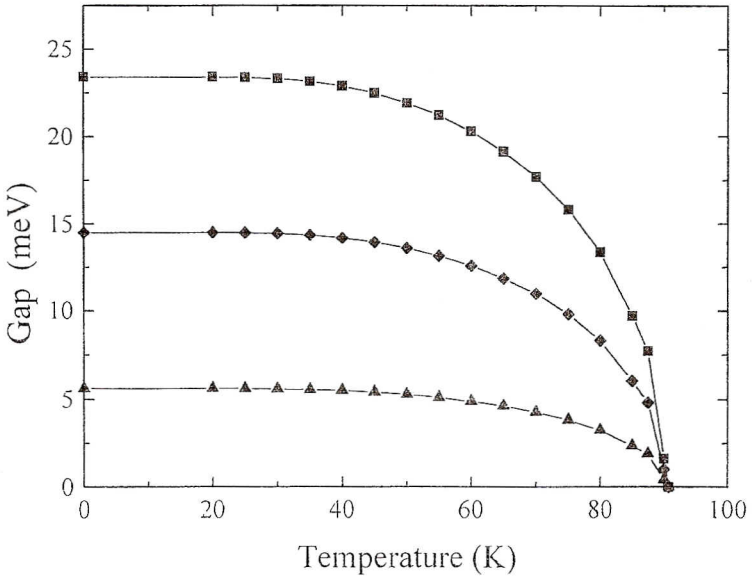


**Figure 2** : Variation of the various gaps $\Delta_{Max}$, $\Delta_{min}$ and $\Delta_{av}$ versus the temperature, at the optimum doping, i.e $D_e = E_F - E_s = 0$ in our model. With the following parameters, $t = 0.2$ eV, $\hbar\omega_c = 60$ meV, $q_0a = 0.12$, $\lambda_{eff} = 0.665$. The critical temperature found is $T_c = 90.75$ K.
square symbol = $\Delta_{Max}$ diamond symbol = $\Delta_{av}$ up triangle symbol = $\Delta_{min}$

In figure (3) we present the same results, $\Delta_{Max}$, $\Delta_{min}$, $\Delta_{av}$ as a function of $D_e = E_F - E_s$ (in meV).

In figure (4) we plot the variation of the anisotropy ratio $\alpha = \Delta_{Max}/\Delta_{min}$ versus D. In figure (5) the critical temperature $T_c$ versus $D_e$ and in figure (6) the various ratio $2\Delta/k_BT_c$ versus $D_e$.

We observe of course that $T_c$ and the gaps decrease with $D_e$ or dx. The agreement with experiment[20] is very good figure (7). We obtain a new and interesting result which is the decrease of the anisotropy ratio $\alpha$ with doping. This is confirmed by recent results on photoemission[21,22] where a maximum gap ratio $2\Delta_{Max}/k_BT_c = 7$ is observed at optimum doping with $T_c = 83$ K and $2\Delta_{Max}/k_BT_c = 3$ for an overdoped sample with $T_c = 56$ K, with a small gap $\Delta_{min} = 0$-2 meV for the both $T_c$, for a Bi2212 compound.

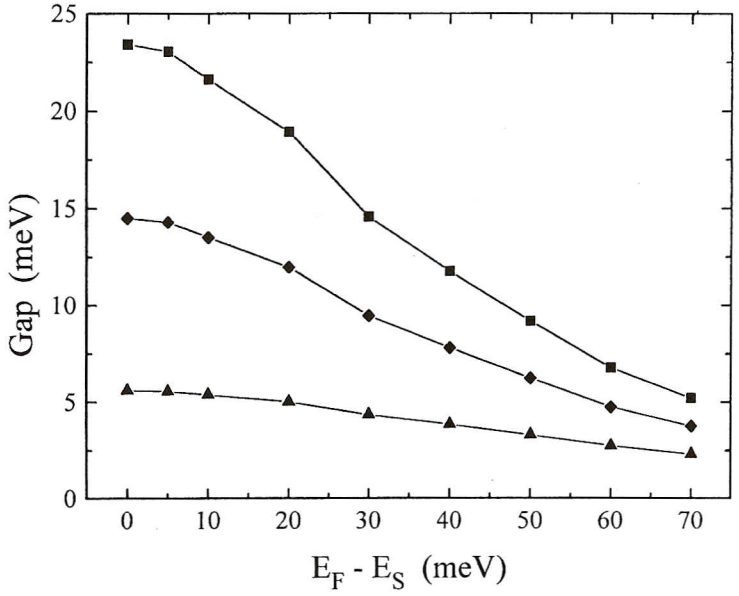


**Figure 3** : Variation of the various gaps $\Delta_{Max}$, $\Delta_{min}$, $\Delta_{av}$ versus the doping, $D_e = E_F$-$E_s$, at T = 0K
square symbol = $\Delta_{Max}$ diamond symbol = $\Delta_{av}$ up triangle symbol = $\Delta_{min}$

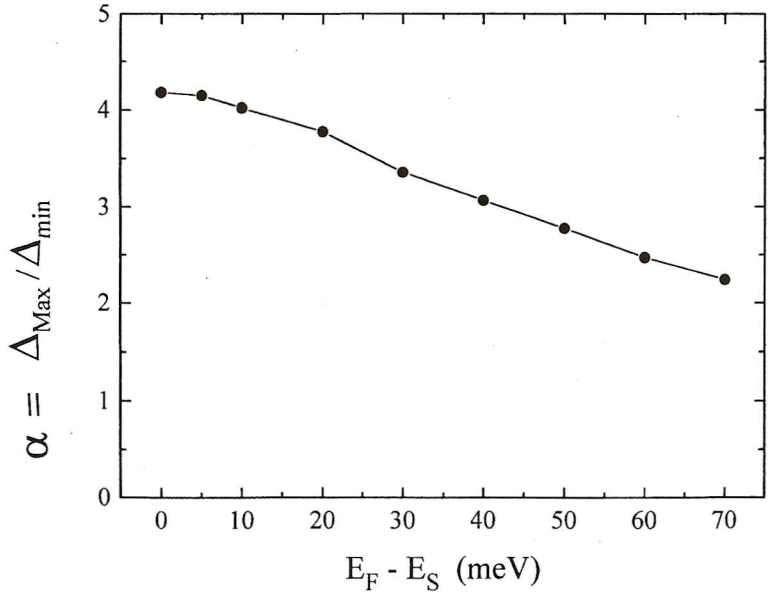


**Figure 4** : Variation of the anisotropy ratio $\alpha = \Delta_{Max}/\Delta_{min}$, versus the doping, $D_e = E_F - E_s$

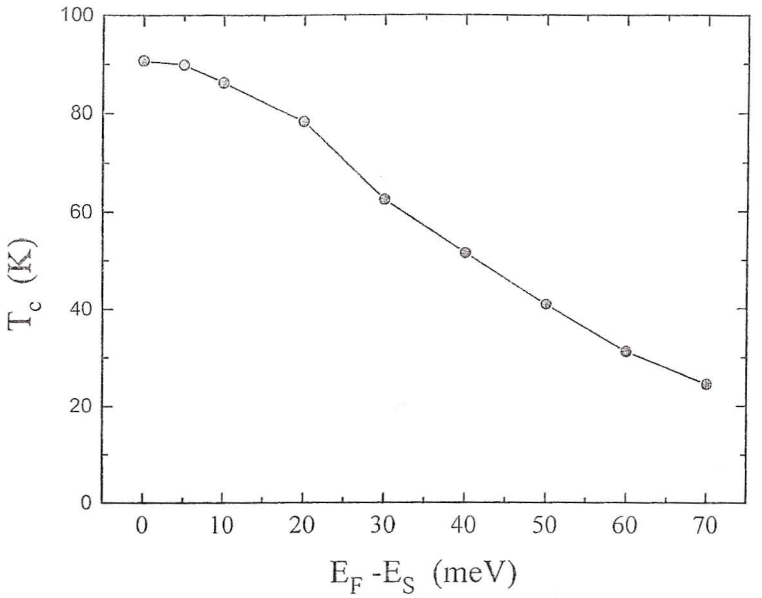


**Figure 5** : Variation of the critical temperature $T_c$ versus the doping $D_e = E_F - E_s$

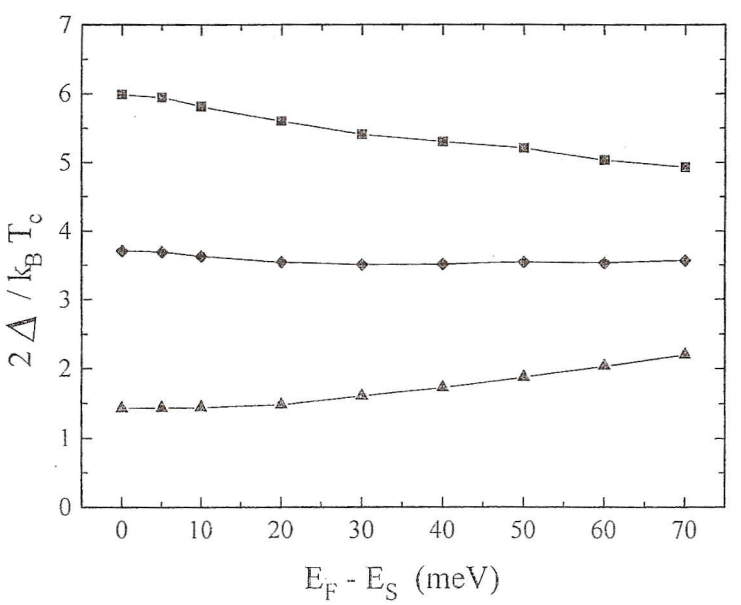


**Figure 6** : Variation of the various rations $2\Delta/k_BT_c$ versus the doping $D_e = E_F-E_s$
square symbol = $2\Delta_{Max}/k_BT_c$ diamond symbol = $2\Delta_{av}/k_BT_c$ up triangle symbol = $2\Delta_{min}/k_BT_c$

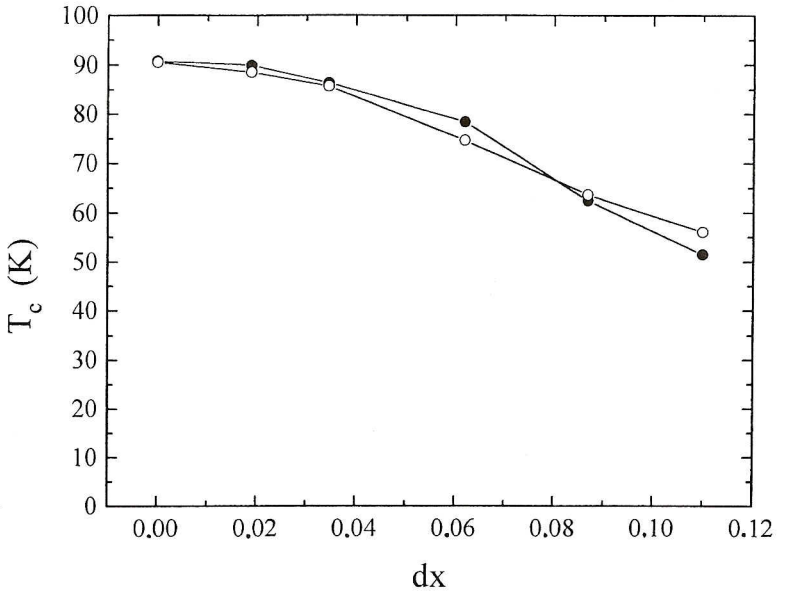


**Figure 7** : Comparison of the variation of $T_c$ versus the doping dx calculated in our model (filled circles) and the experimental results of Koïke et al ref (20) (open circles).

## DENSITY OF STATES AND TUNNELING SPECTROSCOPY

We have calculated the density of states of quasiparticle excitations in the superconducting state of high $T_c$[10,11] cuprates using the model of anisotropic gap that we have recently developed[9,10]

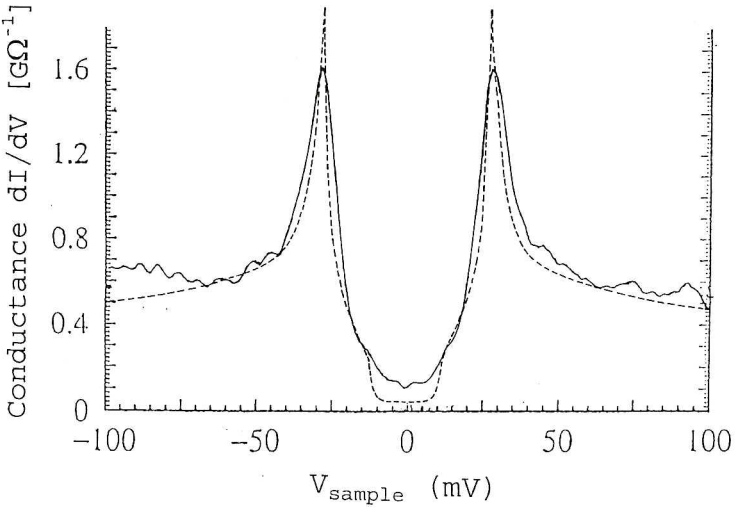


**Figure 8** : The best fit of the conductance measured by tunneling spectroscopy on BSCCO, N-I-S junction, by Renner and Fischer (Fig. (10) of Ref. [23]). solid line : fitted curve with $\Delta_{Max}$ = 27 meV, $\Delta_{min}$ = 11 meV, t = 0.18 eV, Γ = 0.5 meV at T = 5 K,dashed line : experimental curve.

Here the D.O.S. is computed using the formula :

$$n(\varepsilon) = \frac{1}{2\pi^2}\frac{\partial A}{\partial \varepsilon} \qquad (10)$$

where A is the area in k space between two curves of constant energy of the quasiparticle excitation $\varepsilon_k$ given by : $\varepsilon_k^2 = \xi_k^2 + \Delta_k^2$ (11)

where $\xi_k$ is the band structure (eq. (4)). We use the same procedure and the same expression of $\Delta_k$ as before.

Figure (8) represents the variation of the D.O.S. as a function of $\varepsilon$ for T = 0 K. This is similar to the experimental conductance (dI/dV versus the voltage V) of a N-I-S junction here we show the measurement made by Renner and Fisher[23] on a BSCCO sample. $\Delta_{Max}$ is located at the maximum peak and $\Delta_{min}$ at the first shoulder after the zero bias voltage, figure (9). But for different values of $E_F$-$E_s$, we see a new maximum emerging, which is a signature of the van Hove singularity and a dip between this maximum and the peak at $\Delta_{Max}$. This dip is seen experimentally in the STM tunneling experiments of Renner et al[23], figure (10), and in photoemission measurements[24].

For the calculation of the conductance, we use the following formula

$$\frac{dI}{dV} = CN_0 \int_{-\infty}^{+\infty} N_S(\varepsilon)\left[-\frac{\partial f_{FD}}{\partial V}(\varepsilon - V)\right]d\varepsilon \qquad (12)$$

where $f_{FD}$ is the usual Fermi-Dirac function; I and V are the current and voltage, C a constant proportional to $|T|^2$, the square of the barrier transmission, $N_0$ the D.O.S. of the normal metal that we assume constant, and $N_s(\varepsilon)$ the previously calculated D.O.S. in the anisotropic superconductor.

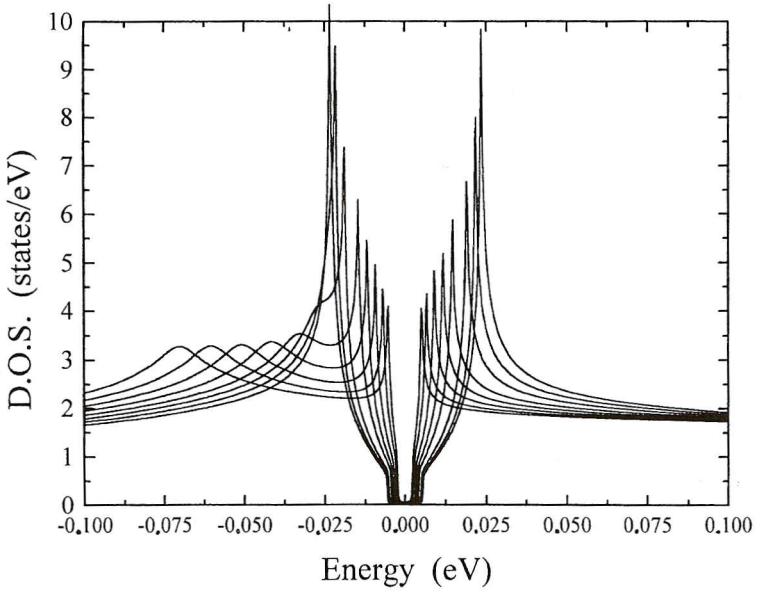


**Figure 9** : Variation of the D.O.S. versus the energy $\varepsilon$, for T = 0 K, that is similar at a NIS junction, for different values of the doping $D = E_F - E_s$, i.e. 0, 10, 20, 30, 40, 60 and 70 meV with $\Gamma$ = 0.1 meV and $\Gamma'$ = 5 meV in the model of ref [11]

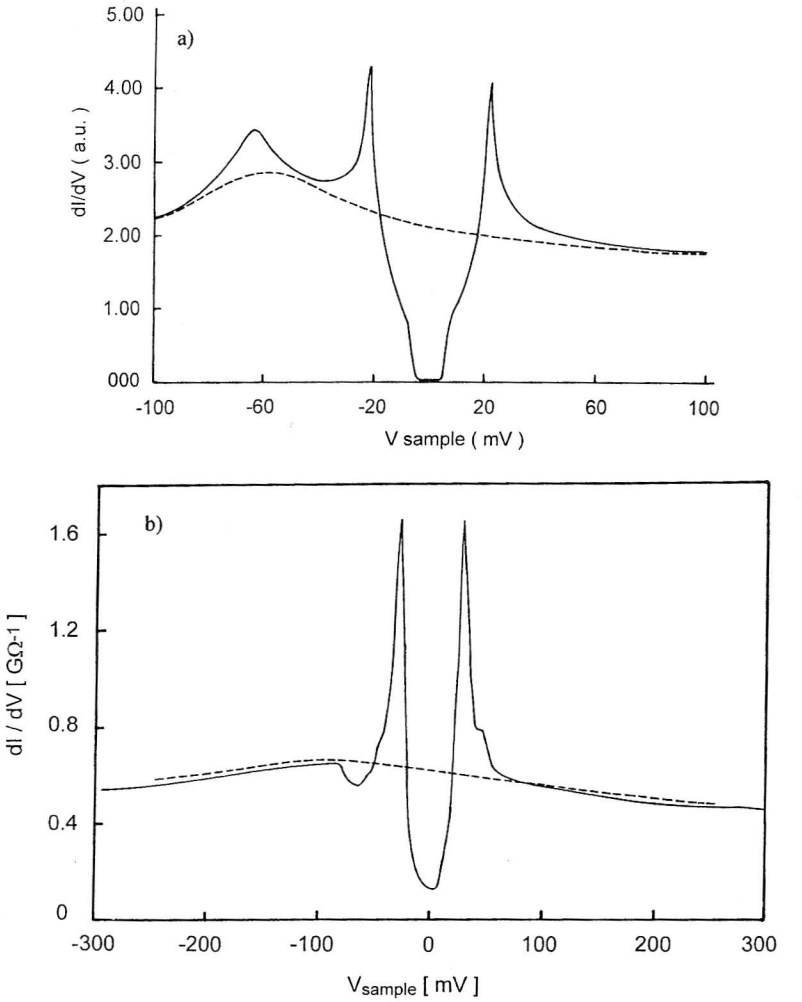


**Figure 10** : (a) Curves of the conductance calculated for a N-I-S junction. Solid line: in the superconducting state at T = 5 K with $\Delta_{Max}$ = 22 meV, $\Delta_{min}$ = 6 meV, $\Gamma$ = 0.1 meV, t = 0.2 eV and $D_e$ = -60 meV, $\Gamma'$ = 5 meV. Dashed line : in the normal state at T = 100 K with $\Delta_{Max} = \Delta_{min}$ = 0 meV, $\Gamma$ = 0.1 meV, t = 0.2 eV and $D_e$ = -60 meV, $\Gamma'$ = 5 meV. (b) For comparison we show Fig. (7) of Ref. [23]. The maximum of the normal state conductance (or D.O.S.) at negative sample bias is well reproduced.

## SPECIFIC HEAT

### 1. Theoretical calculation

The purpose of this chapter is to evaluate the influence of the v.H.s. and the anisotropy of the gap on the specific heat calculated in the mean field B.C.S. approximation, i.e. we do not take into account the fluctuations near the critical temperature $T_c$. There are a great number of experiments measuring $C_s$. To compare our calculations to experiments, we must subtract the part due to fluctuations. These kind of adjustment have been made by various authors by using the fact that thermodynamic fluctuations are symmetric about $T_c$ and can be easily evaluated above $T_c$[25,26]. Also we do not take into account the magnetic fluctuations in low temperature, nor the pair-breaking which may exist in overdoped sample. By the usual way, we obtain for $C_s$ :

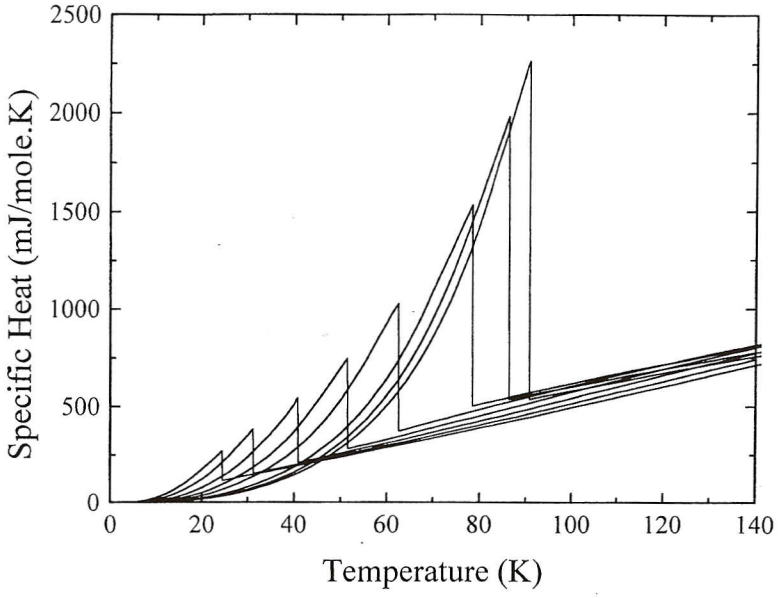


**Figure 11** : The calculated specific heat versus the temperature for the different value of the doping $D_e = E_F - E_s = 0$, 10, 20, 30, 40, 50, 60 and 70 meV.

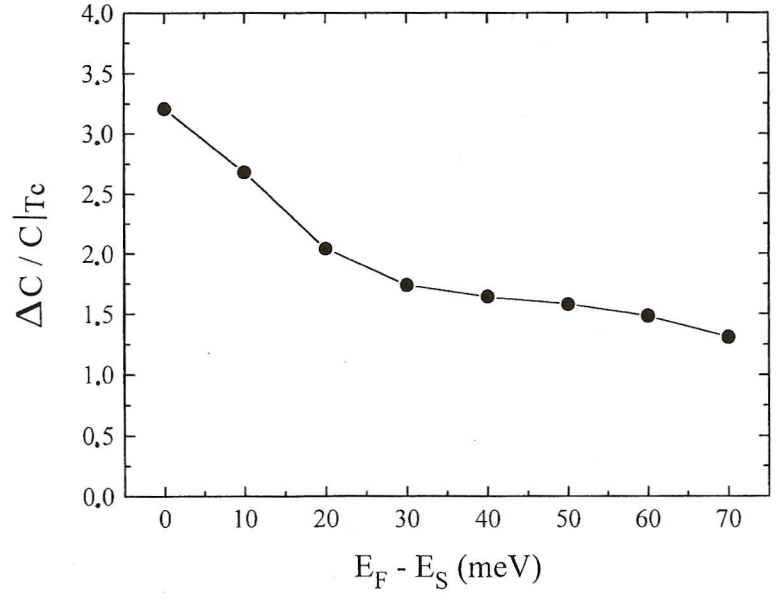


**Figure 12** : Variation of the jump in the specific heat, $\Delta C/C|_{Tc}$, versus the doping $D_e = E_F - E_S$.

$$C_s(T) = \frac{2}{k_B T^2} \sum_k \frac{\exp(\varepsilon_k / k_B T)}{\left(1+\exp(\varepsilon_k / k_B T)\right)^2} \varepsilon_k^2 - \frac{1}{k_B T} \sum_k \frac{\exp(\varepsilon_k / k_B T)}{\left(1+\exp(\varepsilon_k / k_B T)\right)^2} \frac{\partial \Delta_k^2(T)}{\partial T} \quad (13)$$

We use the values of $\varepsilon_k$ and $\Delta_k$ ($\Delta_{Max}$ (T, $D_e$) and $\Delta_{min}$ (T, $D_e$)) given by formula (8) and (4,11) to evaluate the two integrals of (13) numerically. Near $T_c$ we have a very good agreement between the calculated values and the following analytical formula :

$$\Delta_{Max,min} = \Delta_{Max,min}(T=0)\, 1.7 \left(1-(T/T_c)\right)^{1/2}$$

We see that the slopes $\partial\Delta^2 / \partial T$ do not depend on doping which simplifies the calculation of the second integral of formula (13). The results are presented in figures (11) and (12) where we plot $C_s$ and $\Delta C/C|_{Tc}$ versus T for various doping levels $D_e$.

We can make the following observations :

1- The jump in specific heat varies with doping $\Delta C/C|_{Tc}$ is 3.2 for $D_e = 0$ and 1.48 for $D_e = 60$ meV compared to 1.41, the B.C.S. value for a 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 $\Delta_k$. With doping, the v.H.s moves away from $E_F$ and $\Delta C/C|_{Tc}$ decreases toward its B.C.S. value.

2 - There is also a difference in the specific heat $C_N$ in the normal state. For a usual metal with a constant D.O.S. $N_0$, $\gamma_N = C_N / T$ is constant and proportional to $N_0$. Here we find $\gamma_N = a \ln(1/T) + b$ for $0 \le D \le 30$ meV where a and b are constant. For $D_e = 0$ this behaviour has already been predicted by Bok and Labbé in 1987[27]. The specific heat $C_N(T)$ explores a domain of width $k_BT$ around the Fermi level $E_F$. So for $D_e << k_BT_c$, the variation of $\gamma_N$ above $T_c$ is logarithmic. For $D_e > 30$ meV, at high temperature $T - T_c > D_e$, the B. L. law is observed, but for lower temperatures $\gamma_N$ increases with T and passes through a maximum at T*, following the law : T* (meV) = 0.25 $D_e$ (meV) or T* (K) = 2.9 $D_e$ (meV).

## 2. Comparison with experiments

Because of the difficulty to extract exactly $C_s$ from the experimental data, we will compare only the general features to our calculation. We see that the doping has a strong influence on $T_c$ and all the superconducting properties, so we assume that its role is to increase the density of holes in the $CuO_2$ planes. To compare our results on the effect of doping on $C_s$ with experiments, we have chosen the family of the $Tl_2Ba_2CuO_{6+\delta}$ , studied by Loram et al, fig. (9) of ref. [28], because they are overdoped samples, with only one $CuO_2$ plane. The family $YBa_2Cu_3O_{6+x}$ is underdoped for $x < 0.92$ and for $x > 0.92$ the chains become metallic and play an important role. However, recent results by Loram et al, fig. (2a) of the ref. [29] on Calcium doped YBCO, $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{7-\delta}$ , which are overdoped two dimensionnal systems, show a very good agreement with our results. We notice the displacement and the decrease of the jump in specific heat $C_s$ with doping. The jump $\Delta C/C|_{Tc} = \Delta\gamma/\gamma|_{Tc} = 1.67$ [28], and 1.60 [29] greater than the B.C.S. value 1.41 for a metal with a constant DOS. We find theoretically this increase in our model due to the logarithmic v.H.s.. The symmetrical shape of the peak of $C_s$, at low doping level, is due to the critical fluctuations. A subtraction of these fluctuations[25,26] gives an asymmetrical shape. For high doping levels the classical B.C.S. shape is found.

For $D_e = 0$, we find that $\gamma_N$ is not constant but given by the logarithmic law[27] : $\gamma_N = a \ln(1/T) + b$. When $D_e$ increases, the law changes, $\gamma_N$ passes through a maximum for a value of T, T*. This behaviour is clearly seen in the $YBCuO_{6+x}$ family[28]. We explain the high value $\Delta C/C|_{Tc} = 2.5$ for $x = 0.92$ in the YBCO family, and we find also the predicted variation of T*.

Our model, neglecting magnetic fluctuations gives an Arrhenius law for $C_s$ at low temperature with a caracteristic energy which is $\Delta_{min}$. We see that such a law is observed in $YBaCuO_{6.92}$ and for $Tl_2Ba_2CuO_6$ at optimum doping.

## EFFECT OF SCREENING ON THE GAP ANISOTROPY AND THE SPECIFIC HEAT

In the preceding parts we have taken $q_0a = 0.12$ and the effective coupling constant $\lambda_{eff} = 0.665$ in order to fit the experimental values of the gap observed by ARPES and tunneling spectroscopy. We also have stressed the importance of $q_0a$ in the value of the anisotropy ratio $\alpha = \Delta_{Max}/\Delta_{min}$. We shall now study in more details the influence of $q_0a$ on $\alpha$ and on the slope :

$$R = T_c\left(\frac{d\ln \Delta C}{dT}\right)_{T=Tc} \qquad (14)$$

where $\Delta C = C_s(T) - C_s(0)$, $C_s(0)$ is computed for $\Delta_k = 0$ (normal state).
This slope R is available from many experiments for 2D superconductors.

The calculation use equation (5) where $q_0a$ is included in $V_{kk'}$.

For this study, we adjusted our values of $\lambda_{eff}$ to obtain a constant critical temperature of 90.75 K and an average gap of $\Delta_{av} = 14.50 \pm 0.15$ meV. This approximation is valid in the limit of weak screening ($q_0a < 0.2$).The results are presented in figure (13).

The specific heat is computed using formula (13). The results are presented in figures (14) and (15) for $\Delta C / C|_{Tc}$ and the slope R. The B.C.S. values for an isotropic s-wave superconductors are 1.43 for $\Delta C / C|_{Tc}$ and 2.62 for R.

Comparison with experiments :

There are no direct experiments to measure $\alpha$ as a function of $q_0a$. The photoemission experiments measure the anisotropy as a function of doping, so $q_0a$ and $E_F$-$E_s$ vary simultaneously. But there is a decrease in $\alpha$ when the doping is varying[21,22].

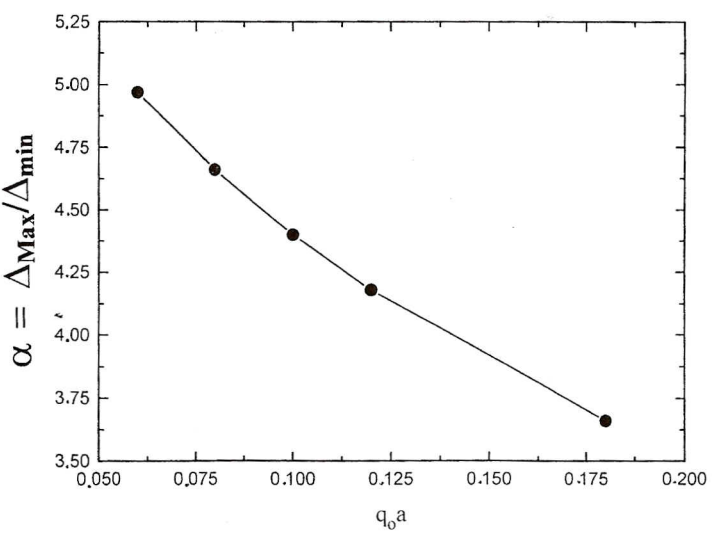


**Figure 13** : The anisotropy ratio $\alpha = \Delta_{Max}/\Delta_{min}$ versus the screening parameter $q_0a$.

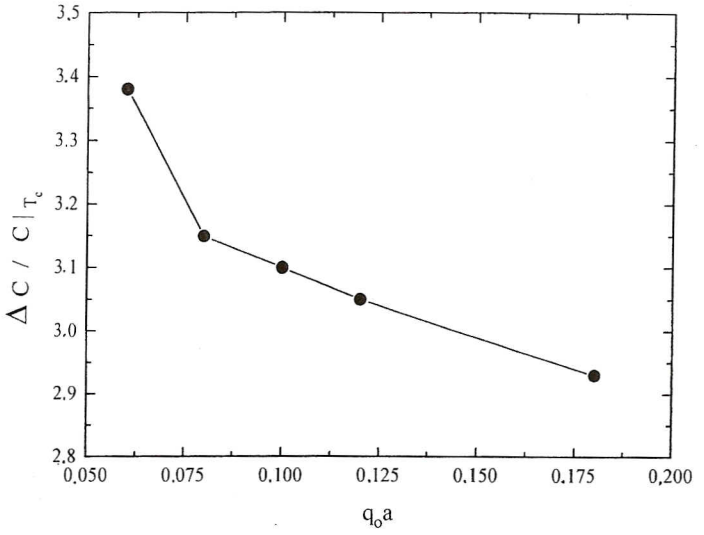


**Figure 14** : The specific heat jump at $T_c$, $\Delta C / C|_{Tc}$ versus the screening parameter $q_0a$.

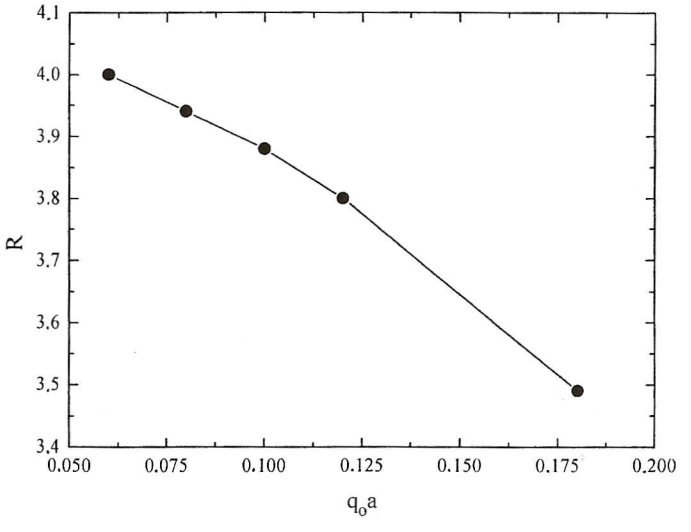


**Figure 15** : The slope R versus the screening parameter $q_0a$.

On the other hand, there are a large number of measurements of specific heat[26,28,29,30]. The extraction of the electronic contribution to the total specific heat is rather difficult. A subtraction of the phonon part and of the influence of fluctuations near $T_c$ is necessary. The slope R has been evaluated by Marcenat *et al*[26] for $YBa_2Cu_3O_{6.92}$. Experimental results have also been obtained by Junod *et al*[30] and Loram *et al*[28] for $Tl_2Ba_2CuO_6$ with a $T_c$ of 85 K. For YBCO the value obtained experimentally by is $R = 6 \pm 1$ higher than our computed value. But YBCO is a special case with chains and 3D character. $Tl_2Ba_2CuO_6$ is a 2D material and the measured R is $4 \pm 0.5$ very close to our calculated value $3.5 < R < 4$ for reasonable values of $q_0a$.

In conclusion, our model explains anomalous values of $\Delta C / C|_{Tc}$ and R observed in 2D cuprates when the Fermi level is close to the van Hove singularity.

## VAN HOVE SINGULARITY AND "PSEUDO-GAP"

Several experiments on photoemission, NMR and specific heat have been analyzed using a normal state pseudo-gap[31]. In fact, all what is needed to interpret these data is a density of state showing a peak above the Fermi energy. To obtain the desired D.O.S. several authors[31] introduce a pseudogap in the normal state. This seems to us rather artificial, the above authors themselves write that the physical origin of this pseudogap is not understood.

We have shown that by using a band structure of the form :

$$\xi_K = -2t\left[\cos k_x a + \cos k_y a\right] - D_e$$

where $D_e = E_F - E_s$, we may interpret the results obtained in the normal metallic state. We have computed the Pauli spin susceptibility[12] using the following formula :

$$\chi_p = \frac{\mu_o \mu_B}{B} \int_{-\infty}^{+\infty} n(\varepsilon)\left(f_{FD}(\varepsilon + \mu_B B) - f_{FD}(\varepsilon - \mu_B B)\right) d\varepsilon \qquad (15)$$

The results fit well the experiments. We find a characteristic temperature T* where the variation of $\chi_p$ versus T goes through a maximum. We may express $D_e$ as a variation of doping $\delta p = p - p_0$, $p_0$ being the doping for which $E_F = E_s$, $p_0 = 0.20$ hole/copper atom in the $CuO_2$ plane. Figure (16) represents the various experimental points taken from figure (5) of reference [31] where the authors plot $E_g/k_B T_{cMax}$ versus p. We see that what the authors call pseudogap is exactly our $E_F$-$E_S$, the distance from the Fermi level to the peak in the D.O.S..

We have also computed the electronic specific heat $C_s$ in the normal state[10] using the same D.O.S.. We find that $\gamma = C_s/T$ goes through a maximum with temperature T, at a value T* as found experimentally by Cooper and Loram[32]. In figure (17) we compare our computed T* with the experimental one (ref. [32]), the agreement is excellent.

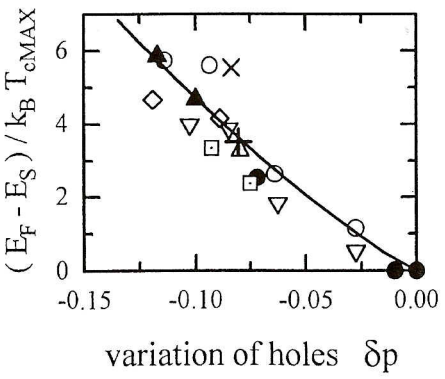


**Figure 16** : $D_e = E_F - E_S$ divided by $k_B T_{cMAX}$ ($T_{cMAX}$ = 110 K) versus the variation of the density of hole, calculated from the band structure of the formula (4) : solid line. The different symbols are the same as in the fig. (5) of the ref. [31]), they represent the values of the so-called normal pseudogap divided by $k_B T_{cMAX}$ ($E_g / k_B T_{cMAX}$) obtained from NMR on different compounds.
Our calculations are made with a transfer integral t = 0.25 eV, $\delta p$ is taken as zero for p = 0.20.

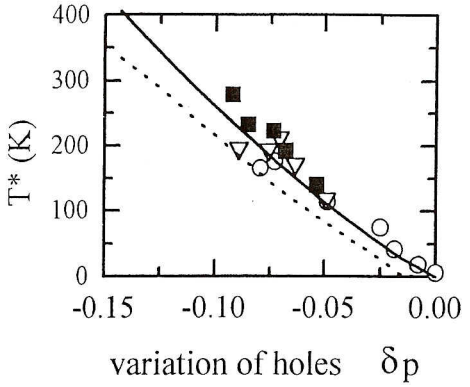


**Figure 17** : The temperature, T*, where the calculated $\chi_p$ (dashed line) and the specific heat (solid line) go through a maximum, versus δp. For comparaison we show the results presented in fig. (27) of ref. [32], the symbols are the same. (solid squares : from thermoelectric power, circles : from specific heat, triangles: from NMR Knight shift data).

In conclusion, we are able to interpret the NMR and specific heat data in the normal metallic state without invoking a pseudogap, but simply by taking into account the logarithmic singularity in the D.O.S..

We explain the shift between the observed experimental optimum $T_c$, where $p = 0.16$ instead of 0.20, and the expected optimum $T_c$ from our theory, i.e. where $D_e = 0$ , by the fact that in first time in our gaps calculations we have not taking into account the variation of the 3D screening parameter $q_0a$ in function of $D_e$. These calculations are in progress and show the competition between the effect of the position of the v.H.s. and the value of $q_0a$ for getting the optimum $T_c$, this competition depends on the compound. When the overdoping increases, i.e. the density of free carriers increases, then $q_0a$ increases too, and in our model this leads to a decrease in $T_c$. It is why for $D_e = 0$ , or $dx = 0.20$, we have not the optimum $T_c$, and why the logarithmic law for $\chi_p$ is found in the overdoped range[12]. In the underdoped range in respect of the observed optimum $T_c$, (i.e. density of free carriers decrease), $q_0a$ decrease too, but the Fermi level go too far away the singularity to obtain high $T_c$. By this way our results agree completely with the experimental observations.

## CONCLUSION

Note that our model is valid only in the metallic state. It has been shown by Boebinger *et al*[33] that LaSrCuO for example undergoes a metal-insulator transition in the underdoped regime, fonction of temperature in the normal state. Of course our model is not valid for these very low doping levels.

We have shown the importance of the van Hove singularity in the interpretation of the physical properties of the cuprates high $T_c$ superconductors (HTSC). The v.H.s. is essential to obtain high $T_c$ and therefore in the coupling mechanism. In the framework of that scenario we explain a main characteristic : the anisotropic gap. V.H.s. account for several experimental features seen in conductance, specific heat, Pauli susceptibility and so on. Last the shift of Fermi level from singularity level explains the so-called pseudogap and the behaviour of HTCS versus doping.

The physic of HTSC, seeing all these convincing results, have to take into account the v.H.s..

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