*Journal of Superconductivity: Incorporating Novel Magnetism, Vol. 13, No. 5, 2000*

# Superconductivity in Cuprates, the van Hove Scenario

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We review the consequences of the presence of van Hove singularities close to the Fermi level in the HTCS cuprates. We show that it may explain the properties of these materials such as the high $T_c$, anomalous isotope effect, marginal Fermi liquid properties, gap anisotropy, etc. We show that the pseudogap observed in the normal state can be attributed to the Coulomb interaction between carriers in these disordered compounds.

**KEY WORDS:** Cuprates; Van Hove singularities.

## 1. INTRODUCTION

van Hove singularities (v.H.s.) are a general feature of periodic systems. They appear in one and two dimensions as divergences of the density of states. In 1987, Labbé and Bok (LB) [1] postulated that in the cuprates these v.H.s. lie close to the Fermi level (FL) and may explain some of the properties of high-$T_c$ superconductors (HTCS). Many experiments of angular resolved photoemission spectroscopy (ARPES) have confirmed the existence of saddle points (v.H.s.) close to the FL in five copper oxide compounds by three different groups, in Stanford [2], in Argonne [3], and in Wisconsin [4]. These observations have been made in the following compounds: Bi 2201, Bi 2212, Y123, Y124, and NCCO. In LSCO, experiments by Shen *et al.* have shown that the FL crosses the v.H.s. as the doping is increased; the Fermi surfaces (FS) are hole-like for underdoped samples and electron-like for overdoped ones. These experiments establish a general feature: in very high-$T_c$ superconductors cuprates ($T_c \sim 90$ K) v.H.s. are present close to the FL. The origin of the 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 the presence of v.H.s. in the band structure has already explained a certain number of experimental facts, i.e., high $T_c$'s, the anomalous isotope effect [1], and marginal Fermi liquid effects [5]. It has also been shown that the singularity is near 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 $\lambda_{\text{eff}} = \lambda - \mu^*$ and remains positive [6]. 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 [7]. We have shown by using a weakly screened electron–phonon interaction that we obtain a strong gap anisotropy [8]. We then compute the density of states (DOS) of quasiparticle excitations in the superconducting state, in the framework of this model. We also study the effect of doping, i.e., of the distance between the FL $E_F$ and the singularity $E_s$ [9]. We apply this result to the calculation of tunneling characteristics and of the electronic specific heat $C_s$ [9,10]. The influence of doping on the screening length and on the calculation of $T_c$ is also examined [11]. We thus explain why the maximum $T_c$ is not observed when $E_F - E_S = 0$.

We finally propose an explanation for the "pseudogap" observed mainly in underdoped samples. We relate the pseudogap to disorder, which gives very low diffusion coefficients. Under these conditions, the Coulomb repulsion becomes important as shown by Altshuler and Aronov [12]. We find an anisotropic pseudogap related to the shape of the FS.

## 2. CALCULATION OF $T_c$

LB [1] have calculated $T_c$ for a 2D conductor having logarithmic singularities near the FL, a simple

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0896-1107/00/1000-0781$18.00/0 

model for the $CuO_2$ planes in HTCS. The DOS is given by

$$n(\xi) = n_1 \ln|D/(\xi - \xi_s)|$$

where $D$ is the width of the singularity and $\xi_s$ the singularity energy level.

Formula (1) was obtained using the following assumptions.

(1) The Fermi level lies near the van Hove singularity.
(2) Regarding the BCS approximations:
   - The electron–phonon interaction is isotropic and so is the superconducting gap $\Delta$.
   - The attractive interaction $V_p$ between electrons is nonzero 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. It can be any other intermediate boson.

In that case, the critical temperature is given by

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

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

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

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

The two main effects enhancing $T_c$ in formula (1) are as follows.

(1) The prefactor is an electronic energy much larger than a typical phonon energy $\hbar\omega_0$.
(2) $\lambda$ is replaced by $\sqrt{\lambda}$ in comparison 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.

(1) *The variation of* $T_c$ *with doping.* The highest $T_c$ is obtained when the Fermi level is at the v.H.s.

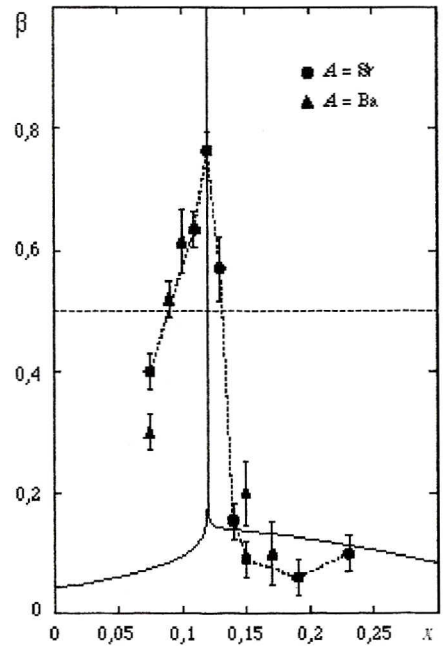


**Fig. 1.** $\beta = d\ln T_c/d\ln M$. Symbols: experimental results from measurements [13b] on $La_{2-x}A_xCuO_4$ with variation of $x$. Full line: theoretical curve [13a].

This first calculation was made neglecting the effect of screening. For lower or higher doping the critical temperature decreases. That is what is observed experimentally [9].

(2) *The isotope effect.* LB showed, using formula (1), that the isotope effect is strongly reduced for high-$T_c$ cuprates. More recently, Hocquet *et al.* [13] showed that the v.H.s. model can explain the anomalous variations of the isotope effect with doping (see Fig. 1).

(3) *Marginal Fermi liquid behavior.* 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 $\varepsilon$. Experimental evidence of marginal Fermi liquid behavior has been seen in angle-resolved photoemission [14], infrared data [15], and temperature dependence of electrical resistivity [16]. Marginal Fermi liquid theory, in the framework of v.H.s., predicts a resistivity linear with temperature $T$. This was observed by Kubo *et al.* [16]. They also observed 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 FL is pushed away from the singularity.

## 3. INFLUENCE OF THE COULOMB REPULSION

As early as 1959 Bogolubov *et al.* [17] had shown that electron–electron repulsion plays a central role in superconductivity. Assuming a constant repulsive potential $V_{kk} = V_c$ from 0 to $E_F$, they found that $T_c$ is given by

$$T_c \cong T_0 \exp\left[\frac{-1}{\lambda - \mu^*}\right]$$

with

$$\mu = N_0 V_c \qquad \text{and} \qquad \mu^* = \frac{\mu}{1 + \mu \ln E_F/\omega_0} \tag{2}$$

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 exists only 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 $W$ ($E_F \cong W/2$ 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 [6] 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 DOS near the middle of the band.

We have made some numerical calculations to illustrate the effect of Coulomb repulsion. These calculations show that the Coulomb repulsion does not kill superconductivity in the framework of the LB 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, and $T_c$ decreases very rapidly as shown in Fig. 2. A recent case has been observed in $Sr_2RuO_4$ with a narrow band and $T_c$ is small [7].

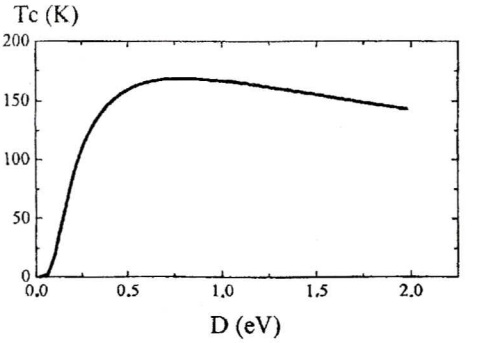


**Fig. 2.** Effect of the width of the singularity $D$ on $T_c$ [6].

## 4. GAP ANISOTROPY

Bouvier and Bok (BB) [8] have shown that, using a weakly screening electron–phonon interaction and the band structure of the $CuO_2$ plane four saddle points, an anisotropic superconducting gap is found.

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 given by Eq. (3):

$$\xi_k = -2t[\cos k_x a + \cos k_y a] + 4t' \cos k_x a \cos k_y a + D_e \tag{3}$$

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 the BCS equation for an anisotropic gap:

$$\Delta_{\vec{k}} = \sum_{k'} \frac{V_{kk'}\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}} \tag{4}$$

We compute $\Delta_{\vec{k}}$ for two values of $\vec{k}$:

$$\Delta_A \quad \text{for} \quad k_x a = \pi, \quad k_y a = 0$$
$$\Delta_B \quad \text{for} \quad k_x a = k_y a = \pi/2 \tag{5}$$

For the following part of this work we keep the value of the cutoff frequency $\hbar\omega_c = 60$ 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 Ref. 8.
- $q_o a$ is adjusted, it is the Thomas Fermi approximation for small $q$'s. We find $q_o a$ of the order of 0.2. This weak screening is due to the 2D character of the material, to the low number of carriers, and to the high dielectric constant.
- $\lambda_{eff}$ 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.

We solve Eq. (4) by iteration. We find a maximum gap in the direction of the saddle points ($\Delta_{max} = \Delta_A$) and a minimum gap at 45° ($\Delta_{min} = \Delta_B$); this is related to the difference in density of states in the $(0, \pi)$ and $(\pi, \pi)$ directions and to the weak screening as also noted by Abrikosov [20].

We obtain a nonzero minimum gap (no nodes in the order parameter). This is because we have taken a pure attractive potential. If we include a repulsive term in the interaction potential, a d-wave solution may be obtained [20].

In Fig. 3, 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 $CuO_2$ plane. In that case we take $D_e = 0$, and we find $T_c = 91$ K, an anisotropy ratio $\alpha = \Delta_{max}/\Delta_{min} = 4.2$, and, for the ratios of $2\Delta/k_BT_c$, the following values: $2\Delta_{max}/k_BT_c = 6$, $2\Delta_{av}/k_BT_c = 3.7$, and $2\Delta_{min}/k_BT_c = 1.4$. 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) give the minimum gap.

In Fig. 4 we present the same results, $\Delta_{max}$, $\Delta_{min}$, and $\Delta_{av}$ as a function of $D_e = E_F - E_S$ (meV). We observe of course that $T_c$ and the gaps decrease with $D_e$ or $dx$. The agreement with experiment [21] is very good (see Fig. 5). We obtain a new and interesting result, which is a decrease in the anisotropy ratio $\alpha$ with doping. This is confirmed by recent results on photomission [22,23], 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

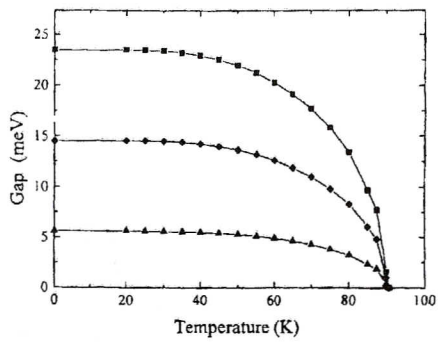


**Fig. 3.** Variation of the various gaps, $\Delta_{max}$, $\Delta_{min}$, and $\Delta_{av}$, versus the temperature, at the optimum doping, i.e., $D_e = E_F - E_S = 0$ in our model.

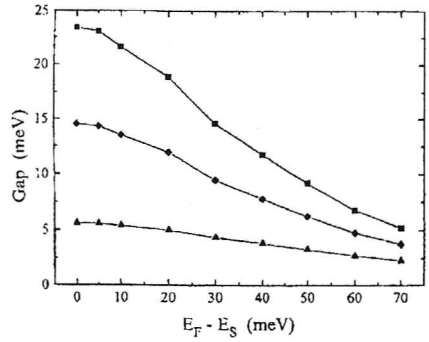


**Fig. 4.** Variation of the various gaps, $\Delta_{max}$, $\Delta_{min}$, and $\Delta_{av}$, versus the doping, $D_e = E_F - E_S$, at $T = 0$ K. Square, $\Delta_{max}$; diamond, $\Delta_{av}$; triangle, $\Delta_{min}$.

sample with $T_c = 56$ K, with a small gap $\Delta_{min} = 0$–2 meV for both $T_c$'s for a Bi2212 compound.

## 5. DENSITY OF STATES AND TUNNELING SPECTROSCOPY

We have calculated the DOS of quasiparticle excitations in the superconducting state of high-$T_c$ [9,10] cuprates using the model of anisotropic gap that we have recently developed [8,9]. We can represent the variation of the DOS 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; we can compare with the measurement made by Renner and Fisher [24] on a BSCCO sample. $\Delta_{max}$ is located at the maximum peak and $\Delta_{min}$ at the first shoulder after the zero-bias voltage. 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

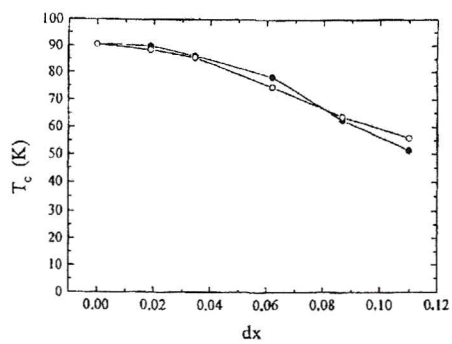


**Fig. 5.** Comparison of the variation of $T_c$ versus the doping $dx$ calculated in our model (filled circles) and the experimental results of Koike *et al.*, [21] (open circles).

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.* [24] (see Fig. 6) and in photoemission measurements [25].

## 6. SPECIFIC HEAT

We have computed the specific heat taking into account the v.H.s. and the anisotropy of the gap in the mean field BCS approximation. The detailed calculations are given in Ref. 9. We can make the following observations.

(1) The jump in specific heat varies with doping. $\Delta C/C|_{Tc}$ is 3.2 for $D_e = 0$ meV and 1.48 for $D_e = 60$ meV, compared to 1.41, the BCS value for a isotropic superconductor, with a constant DOS, $N_0$ 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 BCS value.

(2) There is also a difference in the specific heat $C_N$ in the normal state. For a usual metal with a constant DOS $N_0$, $\gamma_N = C_N/T$ is constant and proportional to $N_0$. Here we find $\gamma_N = a\ln(1/T) + b$ for $0 \leq D \leq 30$ meV, where $a$ and $b$ are constant. For $D_e = 0$ this behavior was predicted by BL in 1987 [26].

A detailed comparison with experiments by Loram *et al.* and by Junod *et al.* is given in Refs. 27 and 28. To compare our calculations with experiments, we have subtracted the contribution of fluctuations to the specific heat. Our model explains rather well the anomalous values of $\Delta C/C|_{Tc}$ and of the slope $R = T_c(d\ln\Delta C/dT)$ observed in 2D cuprates when the Fermi level is close to the v.H.s. [9,11].

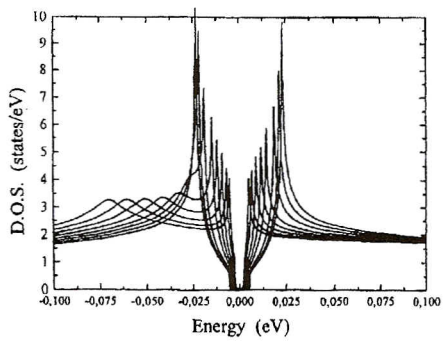


**Fig. 6.** Variation of the DOS versus the energy $\varepsilon$, for $T = 0$ K, which is similar at a N–I–S junction, for different values of doping $D_e = E_F - E_S$, i.e., 0, 10, 20, 30, 40, 60, and 70 meV, in the model of Ref. 10.

## 7. THE "PSEUDOGAP"

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 measurements [30–35]. In fact two characteristic temperatures have been observed, i.e., $T^*$ and $T^0$.

The pseudogap observed in the normal state seems to be a partial gap (i.e., a dip in the DOS). It is related to a crossover temperature, $T^*$, below which its observation is possible. Many authors relate this pseudogap with magnetic phenomena (e.g., spin gap). But we have another explanation for the pseudogap related to $T^*$. It is observed mainly in underdoped samples, which are disordered and in which the mean free path and thus the diffusion coefficient are very low. Under these conditions, the diffusion length 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. 12).

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. This dip is more pronounced in directions where the Fermi velocity is low. In the cuprates, where the Fermi surface is very anisotropic, we find that the pseudogap appears first in the directions of the saddle points $(0,\pi)$ and equivalent to the $CuO_2$ planes. This is clearly seen in the ARPES experiments. For more detailed calculations and results, see the other paper by the authors (J. Bouvier and J. Bok) in these proceedings. In Fig. 7 we present one relevant result.

At higher temperatures, there is another crossover temperature, $T^0$, which corresponds to a maximum in the variation of the specific heat and the magnetic susceptibility with temperature. We explain the maximum of these physical parameters at $T^0$ by the presence of a logarithmic singularity in the DOS at a distance $E_F - E_S$ from the FL. The exact calculation is given in Ref. 36. The physical origin of this phenomenon is the following: the above physical parameters depend on the value of the DOS at the FL

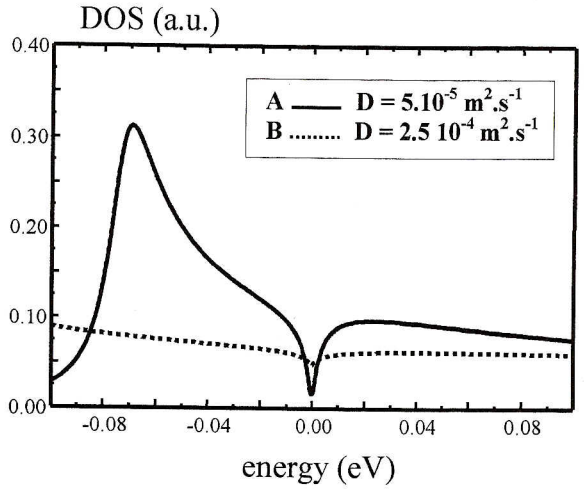


**Fig. 7.** Calculated DOS with Coulomb interaction with the values of the diffusion coefficient $D$: (A) in the (1,0) direction, and equivalent directions, $D = 5 \cdot 10^{-5}$ m$^2 \cdot$ s$^{-1}$; (B) in the (1,1) direction, $D = 2.5 \cdot 10^{-4}$ m$^2 \cdot$s$^{-1}$.

at zero temperature; when $k_B T$ is of the order of $E_F - E_S$, the peak of the DOS plays an important role and gives the observed variation of the parameters with temperature. An example of the variation of $T^0$ with doping is given in Fig. 8 and compared with experimental points [37].

## 8. CONCLUSION

We have shown the importance of the v.H.s. in the interpretation of the physical properties of the high-$T_c$ superconductor (HTSC) cuprates. The v.H.s. is essential to obtain a high $T_c$ and therefore in the coupling mechanism. In the framework of that scenario we explain a main characteristic: the anisotropic gap. The v.H.s. accounts for several experimental features seen in conductance, specific heat, Pauli susceptibility, the behavior of HTCS versus doping, and so on; the shift of the Fermi level from the singularity level explains the characteristic maximum temperature $T^0$ in some variations of physical properties with temperature. Finally, the so-called pseudogap related to $T^*$ is explained by a "Coulomb dip" due to repulsive Coulomb interaction between carriers in the disordered material.

This scenario allows us to give a tentative description of the whole phase diagram of HTCS cuprates. We start with an A. F. Mott–Hubbard insulator, and by doping with holes, we first obtain a disordered conductor, then a metal with hole-like orbits; near optimal doping we have an anormal metal with marginal Fermi liquid, with properties due to the presence of the v.H.s.; then by overdoping we obtain a metal with electron-like orbits and almost-normal FL properties. The effect of disorder is in fact observed in the whole range of doping (in other words, a pseudogap is observed [38]). But this effect is smaller in the overdoped region due to stronger screening (cf. Bouvier and Bok in these Proceedings).

In conclusion, the physics of HTCS, considering all these convincing results, have to take into account the v.H.s.

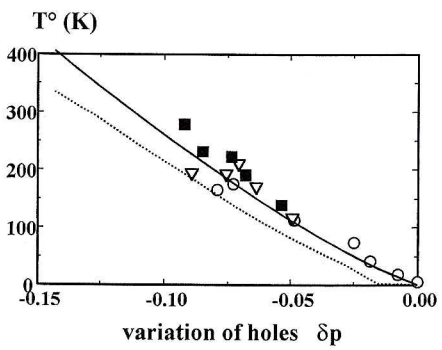


**Fig. 8.** The temperature, $T^0$, where the calculated $\chi_p$ (dashed line) and the specific heat (solid line) go through a maximum, versus $\delta p$ (variation of holes). For comparison we show the results presented in Fig. 27 of Ref. 37; the symbols are the same (filled squares, from thermoelectric power; circles, from specific heat; triangles, from NMR Knight shift data). $\delta p$ is taken as zero for $p = 0.20$.

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