International Journal of Modern Physics B Vol. 13 Nos. 29, 30 & 31 (1999) 3425–3430

SUPERCONDUCTIVITY IN CUPRATES, THE VAN HOVE SCENARIO

J. Bok, J. Bouvier
Laboratoire de Physique Statistique
ESPCI, 10, rue Vauquelin - 75231 Paris cedex 05

The existence of van Hove singularities close to the Fermi level in all high T_c cuprates has been experimentally established. We develop a theory using these singularities which enables us to compute the main physical properties : T_c, gap and gap anisotropy, specific heat and magnetic susceptibility. All these results agree well with the experimental data in the optimal and overdoped regime. In the underdoped regime, we use the theory of electron-electron interaction in disordered conductors to explain the pseudo-gap behaviour.

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 (F.L.) in five different copper oxide compounds[1-3]. These experiments establish a general feature : in all 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[4]. 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.s. in the band structure has already explained a certain number of experimental facts.
We have developed a calculation for the anisotropy of the superconducting gap[5], using a weakly screening electron-phonon interaction in the BCS equation. This anisotropy is directly related to the presence of saddle points (vHs) in four directions of the BZ; and the value of the anisotropy ratio, i. e. $\alpha = \Delta_{Max}/\Delta_{min}$, depends on the strength of the screening parameter q_0, inverse of the screening length .

From the expression of the gap and its anisotropy, we calculated the density of states (DOS) of the quasiparticle excitations and the tunneling characteristics dI/dV for SIN and SIS junctions, the specific heat $C_s(T)$ in the superconducting and normal states and the Pauli susceptibility $X_p(T)$ in the normal state[6-8]. These calculations agree very well with experimental results. We have also taken into account the influence of doping in a rigid band model; i.e. the effect of doping is to vary the distance between the F.L. E_F and the singularity E_S[6-8]. The effect of doping is applied to Δ_k , T_c , α, dI/dV, C_s, X_p. We obtain several interesting results, among them the appearance of a dip in the DOS which is observed both by ARPES and by tunneling spectroscopy. We find interesting results for the jump of the specific heat at T_c , $\Delta C/C|_{Tc}$, it is higher that the BCS ratio (with constant DOS), for optimum doping (E_F=E_S), and goes back to the BCS value at high doping ($E_F - E_S > 70$ meV).

Some improvements of the model , taking into account the doping dependence of the screening parameter q_0, are made[6]. We thus explain why the maximum T_c is not exactly

observed when $E_F - E_S = 0$. Several experiments show the presence of a pseudo-gap in the normal state of the cuprates. We show that in the metallic state, this gap corresponds to the distance between the peak in the density of states and the Fermi level[9]. In the underdoped regime the material is a disorder metal. If electron-electron interaction is taken into account, as shown by Altshuler and Aronov[10], a dip in the DOS appears and this explains the appearance of a Coulomb pseudo-gap which has the anisotropy of the band structure. When the density of carriers in the CuO_2 plane is further decreased, and the material becomes an insulator, a Coulomb gap appears at the Fermi level as shown by Efrös and Shklovskii[11].

CALCULATION OF T_c

Labbé-Bok[4] have computed the band structure for the bidimensional CuO_2 planes of the cuprates, considered as a square lattice (quadratic phase). This approach already explains many of the properties of the high T_c cuprates near optimum doping :

- High values of T_c

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[7].

- The isotope effect

Labbé and Bok[4] showed using their formula, that the isotope effect is strongly reduced for high T_c cuprates. Tsuei *et al*[12] 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 of energy ε. goes as ε^2. The marginal Fermi liquid situation is the case where $1/\tau$ goes as ε. 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[12]. Experimental evidence of marginal Fermi liquid behaviour has been seen in angle resolved photoemission[13], infrared data[14] and temperature dependence of electrical resistivity[15]. 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[15]. 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.

GAP ANISOTROPY

Bouvier and Bok[5] have shown that using a weakly screening electron-phonon interaction, and the band structure of the CuO_2 planes leading to four saddle points , an anisotropic superconducting gap is found.

In figure (1), we present the variation of the various gaps Δ_{Max}, Δ_{min} and Δ_{av} with temperature at optimum doping, i.e. for a density of holes of the order of 0.20 per CuO_2 plane, as seen before[16]. In this model the effect of doping is represented by $D_e = E_F - E_S$. In that figure $D_e = 0$ 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:

$$2\,\Delta_{MAX} / k_B\,T_c = 6\,, \quad 2\,\Delta_{av} / k_B\,T_c = 3.7, \quad 2\,\Delta_{min} / k_B\,T_c = 1.4\,.$$

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

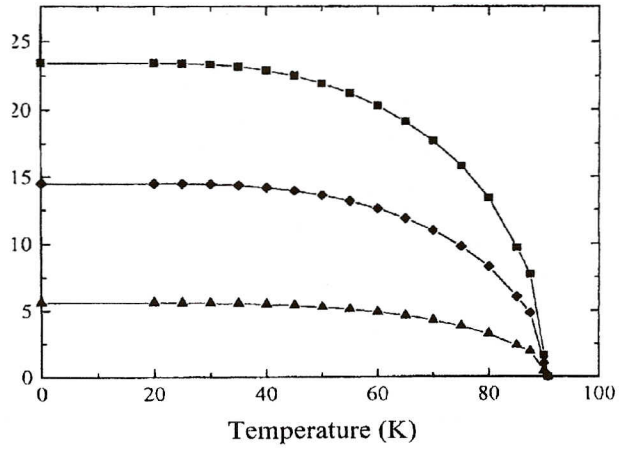

Figure 1 : Variation of the various gaps Δ_{Max}, Δ_{min} and Δ_{av} versus temperature, at the optimum doping, i.e. $D_e = E_F - E_s = 0$. We use the following parameters, $t = 0.2$ eV, $\hbar\omega_c = 60$ meV, $q_0a = 0.12$, $\lambda_{eff} = 0.665$. The critical temperature found is $T_c = 90.75$ K (square = Δ_{Max}, diamond = Δ_{av}, triangle = Δ_{min})

DENSITY OF STATES AND TUNNELING SPECTROSCOPY

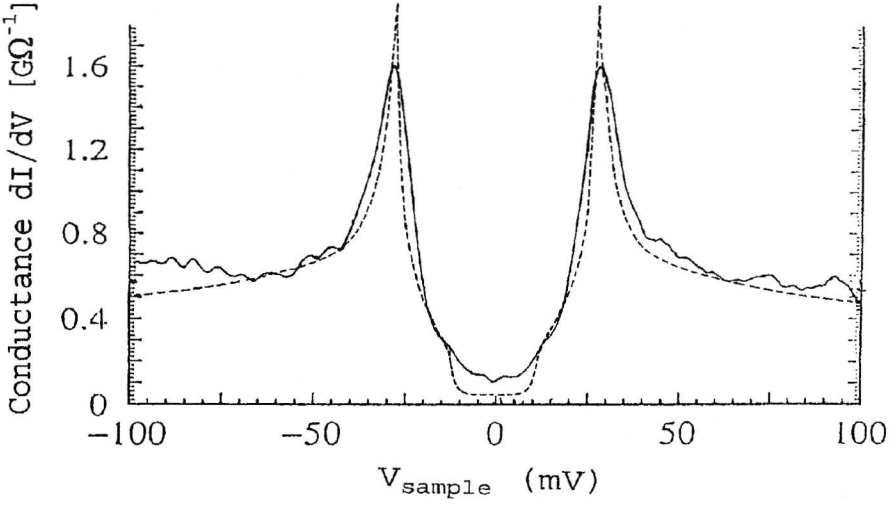

Figure 2 : The best fit of the conductance measured by tunneling spectroscopy on BSCCO, N-I-S junction, by Renner and Fischer (fig. (10) of ref. [17]). solid line : fitted curve with $\Delta_{Max} = 27$ meV, $\Delta_{min} = 11$ meV, $t = 0.18$ eV, $\Gamma = 0.5$ meV at $T = 5$ K, dashed line : experimental curve.

We have calculated the density of states of quasiparticle excitations in the superconducting state of high T_c[7,8] cuprates using the model of gap anisotropy that we have developed[5,7]. This gives the conductance of a NIS junction. Some results are given in figure (2).

SPECIFIC HEAT

The calculations are made in reference [7]. Some results are presented in figure (3) where we plot $\Delta C/C|_{Tc}$ versus T for various doping levels D_e.

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.. 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. With doping, the v.H.s moves away from E_F and $\Delta C/C|_{Tc}$ decreases toward its B.C.S. value.

To compare our results on the effect of doping on C_s with experiments, we have chosen the $Tl_2Ba_2CuO_{6+\delta}$ family, (studied by Loram et al, figure (9) of reference [18]), because they are overdoped samples, with only one CuO_2 plane. Recent results by Loram et al, (figure (2a) of reference [19] 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 $\Delta C/C|_{Tc} = \Delta\gamma/\gamma|_{Tc} = 1.67$ [18], and 1.60 [19] greater than the B.C.S. value 1.41 for a metal with a constant DOS.

For $D_e = 0$, we find that γ_N is not constant but given by a logarithmic law[20] : $\gamma_N = a\ln(1/T) + b$. When D_e increases, the behaviour changes, γ_N passes through a maximum for a value of T, T^*. This behaviour is clearly seen in the $YBCuO_{6+x}$ family[18]. 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 characteristic energy that is Δ_{min}. We see that such a law is observed in $YBaCuO_{6.92}$ and for $Tl_2Ba_2CuO_6$ at optimum doping.

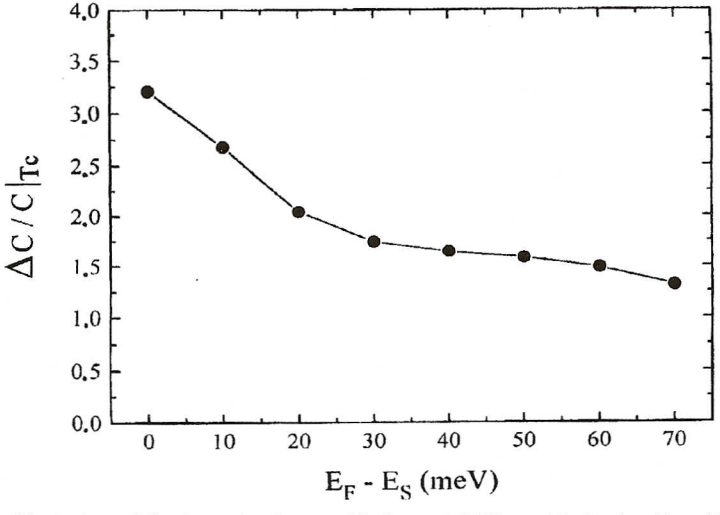

Figure 3 : Variation of the jump in the specific heat, $\Delta C/C|_{Tc}$, with doping $D_e = E_F$-E_S.

"PSEUDO-GAP" AND COULOMB INTERACTION

Several experiments on photoemission, NMR and specific heat have been analyzed using a normal state pseudo-gap[21]. 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[21] introduce a pseudogap in the normal state. This seems to us rather artificial.

Using the true band structure we have computed the Pauli spin susceptibility[9]. The results fit well the experiments. We find a characteristic temperature T* where the variation of χ_p versus T goes through a maximum. We have also computed the electronic specific heat C_s in the normal state[7] 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[22]. In figure (4) we compare our computed T* with the experimental one (reference [22]), the agreement is excellent. 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..

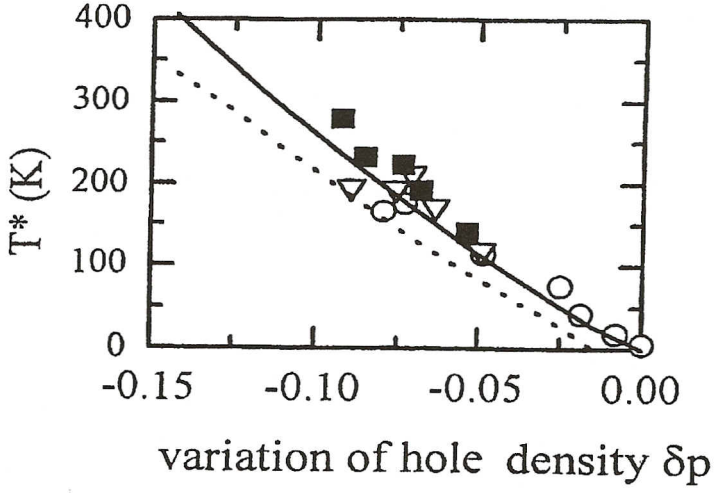

Figure 4 : The temperature, T*, where the calculated χ_p (dashed line) and the specific heat (solid line) go through a maximum, versus δp. For comparison we show the results presented in fig. (27) of ref. [22], the symbols are the same. (solid squares : from thermoelectric power, circles : from specific heat, triangles: from NMR Knight shift data).

In the underdoped regime, this explanation is no longer valid[23]. The material is no longer metallic and the Fermi surface (F.S.) disappears in photoemission measurements[23]. In this underdoped regime, the material is disordered and we may apply the model of Altshuler and Aronov[10] using electron-electron interaction in disordered conductors. The Coulomb in disordered metals introduces strong corrections in the DOS near the Fermi level. Altshuler and Aronov have shown that particle repulsion produces a minimum in the DOS at the Fermi energy. As the density of carriers is reduced, the dip in the DOS at

the F.L. becomes more and more pronounced. These results have been confirmed by experiments on Gold doped Germanium, $Ge_{1-x}Au_x$ (see figure (10) in reference [10]). Altshuler and Aronov have made the calculation for an isotropic conductor. The calculation for a band structure with saddle points is under progress.

But it is easily seen that the F.S. first disappears near the saddle points where the Fermi velocity becomes very small and the electron-electron interaction is the more efficient. This is confirmed by photoemission measurements[23].

CONCLUSION

In the light of all these convincing results, we see that the physics of HTSC must take into account the v.H.s. together with the effects of doping and the electron-electron interaction.

REFERENCES

1. Z. X. Shen, W.E. Spicer, D.M. King, D.S. Dessau, B.O. Wells, *Science* **267** (1995) 343.
2. H. Ding, J. C. Campuzano, K. Gofron, C. Gu, R. Liu, B. W. Veal and G. Jennings. *Phys. Rev. B* **50** (1994) 1333.
3. Jian Ma, C. Quitmann, R.J. Kelley, P. Alméras, H. Berger, G. Margaritondoni, M. Onellion. *Phys. Rev. B* **51** (1995) 3832.
4. J. Labbé and J. Bok, *Europhys. Lett.* **3** (1987) 1225.
5. J. Bouvier and J. Bok, *Physica C* **249** (1995) 117.
6. J. Bouvier and J. Bok, 'Superconductivity in the cuprates, the van Hove scenario : a review.' published in « The Gap Symmetry and Fluctuation in High Temperature Superconductors » edited by J. Bok and G. Deutscher, Plenum Publishing Corporation (1998)
7. J. Bok and J. Bouvier, *Physica C* **288** (1997) 217.
8. J. Bok and J. Bouvier, *Physica C* **274** (1997) 1.
9. J. Bok and J. Bouvier, *J. Superc.* **10** (1997) 673.
10. B.L. Altshuler and A.G. Aronov, 'Electron-Electron Interactions in Disordered Systems', edited by A.L. Efrös and M. Pollak, Elsevier Science Publishers B.V. (1985).
11. A.L. Efrös and B.I. Shklovskii, *J. Phys. C***8** (1975) L49.
12. C.C. Tsuei, D.M. Newns, C.C. Chi et P.C. Pattnaik, *Phys. Rev. Lett.* **65** (1990) 2724. D.M. Newns, C.C. Tsuei, P.C. Pattnaik and C.L. Kane, *Comments Cond. Mat. Physics* **15** (1992) 273.
13. G.G. Olson et al, *Phys. Rev. B* **42** (1990) 381.
14. Z. Schlesinger et al, *Phys. Rev. Lett.* **67** (1991) 1657.
15. Y. Kubo et al, *Phys. Rev. B* **43** (1991) 7875.
16. J. Bok and L. Force, *Physica C* **185-189** (1991) 1449.
17. Ch. Renner and O. Fisher, *Phys. Rev.* **B 51** (1995) 9208.
18. J.W. Loram, K.A. Mirza, J.M. Wade, J.R. Cooper and W.Y. Liang, *Physica C* **235-240** (1994) 134.
19. J.W. Loram, K.A. Mirza, J.R. Cooper, J.L. Tallon. to be published in the *proceedings of M^2S-HTSC-V*, Feb 28-Mar 4, 1997, Beijing, China.
20. J. Bok and J. Labbé, *C.R. Acad. Sci Paris* **305** (1987) 555.
21. G.V.M. Williams,J.L Tallon,E.M. Haines,R. Michalak, and R. Dupree, *Phys. Rev Lett.* **78** (1997) 721.
22. J.R. Cooper and J. W. Loram, *J. Phys. I France* **6** (1996) 2237
23. H. Ding et al, *Nature* **382** (1996) 51.