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High Tc superconductors : the van Hove scenario, a review

J. Bok, J. Bouvier

Laboratoire de Physique du Solide, CNRS-ESPCI, 10, rue Vauquelin - 75231 Paris cedex 05 , France

We shall review 1/ the calculation of T_c in the framework of the v H scenario, 2/ the influence of the Coulomb repulsion which decreases T_c strongly in narrow band cuprates, 3/ the calculation of the gap anisotropy using a weakly screened electron-phonon interaction and the effect of doping, 5/ its application to tunneling spectroscopy and 6/ its application to the specific heat of HTCS.

1. CALCULATION OF Tc, THE LABBE BOK FORMULA

This 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 Δ.
- 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, ω_0 is a typical phonon frequency.

In that case, the critical temperature is given by

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

where $\lambda = \frac{1}{2} n_1 V_p$

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) is an electronic energy much larger than a typical phonon energy $\hbar\omega_0$.

2- λ is replaced by $\sqrt{\lambda}$ in formula (1) 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[1].

- The isotope effect

Labbé and Bok [2] showed using formula (1), that the isotope effect is strongly reduced for high T_c cuprates. Tsuei *et al* [3] 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 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 [3]. Experimental evidence of marginal Fermi liquid behaviour has been seen in angle resolved photoemission [4], infrared data [5] and temperature dependence of electrical resistivity [6]. 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 [6]. 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

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2. INFLUENCE OF THE COULOMB REPULSION

As soon as 1962 Anderson and Morel [7] have shown that the electron-electron repulsion plays a central role in superconductivity. Assuming a constant repulsive potential $V_{(k,k')} = V_c$ 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 (2)

$$\mu^* = \frac{\mu}{1 + \mu \ln E_F / \omega_0}$$

Cohen and Anderson [8] assumed that for stability reasons μ is always greater than λ. Ginzburg [9] gave arguments that in some special circumstances μ can be smaller than λ. Nevertheless if we take $\mu \geq \lambda$, superconductivity only exists because μ^* 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 λ and μ vary simultaneously and μ^* 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 [10] 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 $n(\varepsilon) = n_1 \ln\left|\frac{D}{\varepsilon}\right| + n_0$ between -D and +D we find for T_c, the following formula :

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

where

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

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

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. This calculations are illustrated by figure (1).

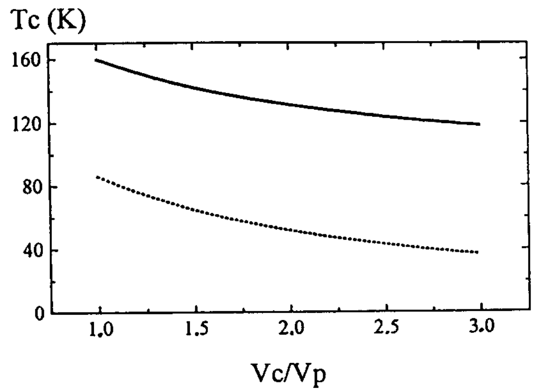

Fig.1 : Effect of Coulomb repulsion on T_c. The following numerical values have been used :
(solid line) D = 0.9 eV, n_0 = 0.3 states/eV/Cu atom, W = 2 eV, n_1 = 0.2
(dotted line) D = 0.3 eV, n_0 = 0.3 states/eV/Cu atom, W = 3 eV, n_1 = 0.16

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 μ.

3. GAP ANISOTROPY

Bouvier and Bok [11] 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. For the superconducting gap, Δ_k, the B.C.S. integral equation (at T = 0K)

$$\Delta_{\vec{k}} = -\frac{1}{2}\sum_{\vec{k}'} \frac{V_{\vec{k}\vec{k}'}\Delta_{\vec{k}'}}{\sqrt{\varepsilon_{\vec{k}'}^2 + \Delta_{\vec{k}'}^2}} \quad (4)$$

where $V_{kk'}$ is the electron-electron attraction mediated by phonons and ε_k the band structure given by

$$\varepsilon_k = -2t(\cos k_x a + \cos k_y a)$$

where t is a transfer integral between nearest neighbours. This corresponds to the case where the Fermi level E_F lies exactly at the singularity E_s ($E_F = E_s$). We take for $V_{kk'}$ a weakly screened attractive interaction :

$$V_{\vec{k}\vec{k}'} = \frac{-V}{q^2 + q_0^2}$$

$V > 0$ when $|\varepsilon_{kk'}| < \hbar\omega_0$, ω_0 being a typical phonon frequency. To solve eq (4) we use a Fourier expansion of $\Delta(\phi)$, where ϕ is the angle between $\vec{k}$ and the k_x axis :

$$\Delta(\phi) = \Delta_0 + \Delta_1 \cos 4\phi + \Delta_2 \cos(8\phi + \theta) + \ldots \quad (5)$$

We have computed numerically the first two terms Δ_0 and Δ_1, by iteration. The results of Δ versus ϕ are presented in figure (2) for two sets of parameters. We insist that most of the parameters t, ω_0 are known experimentally. We have estimated the screening parameter q_0a, in a Thomas Fermi approximation, of the order of 0.2.

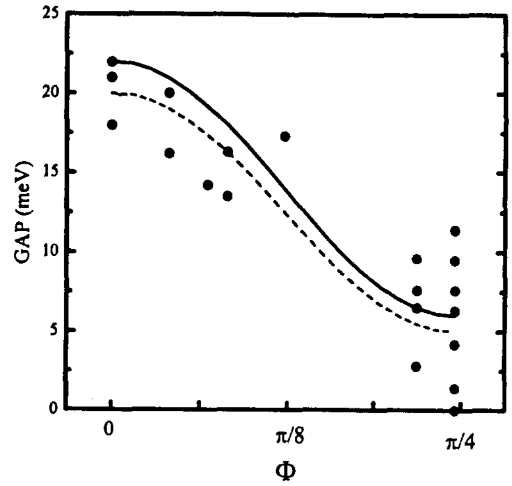

Fig. 2 : Angle-dependent calculated gap $\Delta(\phi)$ for two sets of parameters : Δ_0 = 14 meV, Δ_1 = 8 meV, for T_c= 88.5 k (solid line) and Δ_0 = 12,5 meV, Δ_1 = 7,5 meV, for T_c= 78.5 k (dashed line)

We also have computed the variation of Δ_k with temperature. On fig. (3) we have represented $\Delta_{Max} = \Delta_0 + \Delta_1$, $\Delta_{min} = \Delta_0 - \Delta_1$ and $\Delta_{AV} = \Delta_0$ as a function of temperature. We see that at zero temperature $2\Delta_{Max}/k_BT_c = 6$, $2\Delta_{min}/k_BT_c = 2.6$ and the B.C.S.value of the ration is obtained for Δ_{AV}. This may explain the various values $2\Delta/k_BT_c$ observed in experiments. Tunneling spectroscopy gives the maximum ratio and thermodynamic properties such as $\lambda(T)$ (penetration depth) gives the minimum gap.

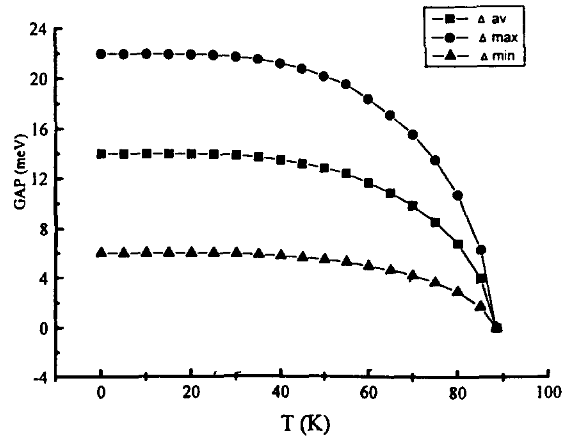

Fig. 3 : Temperature-dependent maximum (full circle), average (full square) and minimum (full triangle) gaps; for T = 0 K, for $\Delta_{av} = \Delta_0$ = 14 meV, Δ_1 = 8 meV , and for a Tc = 88.5 K.

4. TUNNELING SPECTROSCOPY

We have calculated the density of states (D.O.S) of quasiparticle excitations in the superconducting state of high T_c [12] cuprates using the model of anisotropic gap that we have recently developed [11]. We use a gap of the form given by equation (5) and the B.C.S. theory for the energies E_k of the excited states :

$$E_k^2 = \varepsilon_k^2 + \Delta_k^2$$

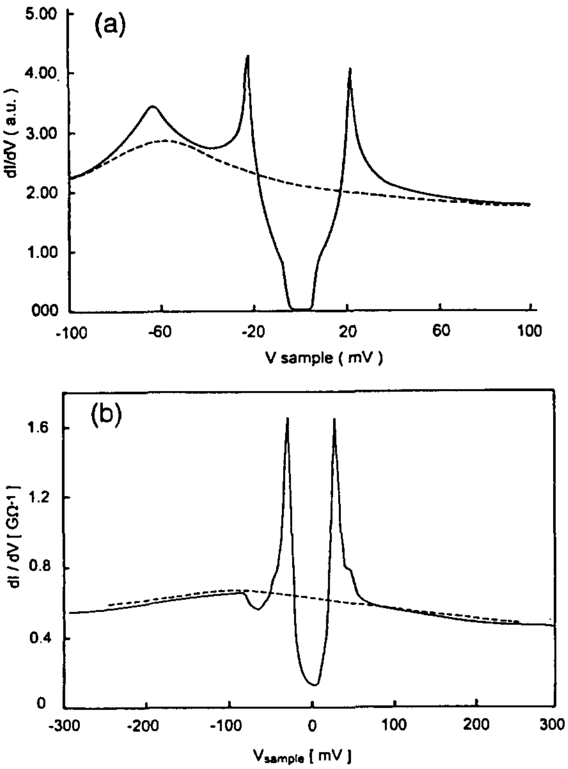

Fig. 4 : (a) Curves of the conductance calculated for a N-I-S junction. Solid line: in the superconducting state at T = 5 K with $\Delta_M = 22$ meV, $\Delta_m = 6$ meV, $\Gamma = 0.1$ meV, $t = 0.2$ eV and $\delta = -60$ meV, $\Gamma' = 5$ meV. Dashed line : in the normal state at T = 100 K with $\Delta_M = \Delta_m = 0$ meV, $\Gamma = 0.1$ meV, $t = 0.2$ eV and $\delta = -60$ meV, $\Gamma' = 5$ meV. (b) For comparison we show Fig. 7 of Ref. [13]. The maximum of the normal state conductance (or D.O.S.) at negative sample bias is well reproduced.

From these expressions of the D.O.S., we have computed the tunneling conductance dI/dV of tunnel junctions, both normal-insulator-superconductor (N.I.S.) and S-I-S junctions. We have also taken into account a possible finite lifetime of quasiparticle states, by introducing a phenomenological broadening Γ. The results are given in detail in ref [12].

Figure (4) represents the computed curve of a dI/dV versus V characteristic of a NIS junction and an experimental curve done by Renner and Fisher [13] on a BSSCO sample. We also give results corresponding to the case of a sample which is not at optimal doping, i.e. E_F-$E_S \neq 0$. In that case a dip is found is the D.O.S. Such a dip has been seen experimentally, both in photoemission [14]. and in the dI/dV characteristic [13].

5. SPECIFIC HEAT

We have also computed the specific heat of a superconductor in the framework of the van Hove scenario, i.e. using the D.OS. of excited states obtained before. Our calculations are detailed in another presentation in this conference (Bouvier, Bok). The main results are the following :

- the specific heat jump at T_c, $\Delta C/C$, is greater than the universal B.C.S. value 1.43, obtained with a constant density of state.

It varies from the value 3.5 when $E_F = E_S$ to the B.C.S. value for heavy doping E_F - E_S > 70 meV

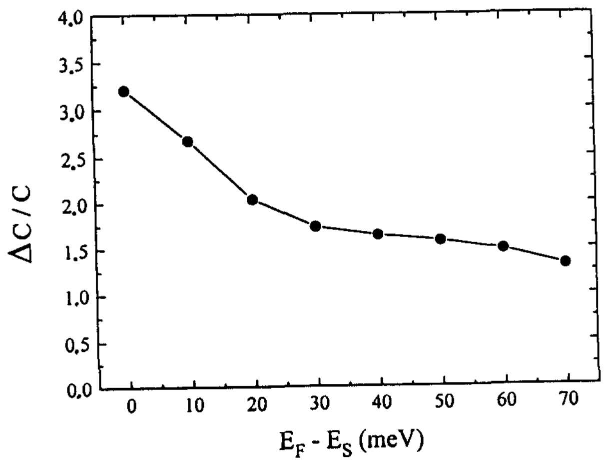

Fig. 5 : Variation of the jump in the specific heat at T = T_c, $\Delta C/C$, versus the doping D = E_F-E_s

CONCLUSION

In conclusion, we have shown that the van Hove scenario explains many properties of the high T_c cuprates.

- high T_c and anomalous isotope effect
- great variation of T_c, from 0 to 160 K, with band parameters
- the observed gap anisotropy for optimum, and overdoped samples (Bouvier, Bok, same conference).
- the observed tunneling conductance and its variation with doping
- the observed specific heat anomalies.

We want to stress that our approach neglects completely magnetic fluctuations, so that it does not apply to underdoped samples. It should apply to optimally and overdoped samples where magnetic fluctuations are very weak and even disappear.

REFERENCES

[1] Y. Koike et al, Physica C, **159**, 105 (1989)
[2] J. Labbé, J. Bok, Europhysics Letters, **3**, 1225 (1987)
[3] C.C. Tsuei, D.M. Newns, C.C. Chi et P.C. Pattnaik, Phys. Rev. Lett., **65**, 2724 (1990)
D.M. Newns, C.C. Tsuei, P.C. Pattnaik and C.L. Kane, Comments Cond. Mat. Physics, **15**, 273 (1992)
[4] G.G. Olson et al, Phys. Rev. B, **42**, 381 (1990)
[5] Z. Schlesinger et al, Phys. Rev. Lett., **67**, 1657 (1991)
[6] Y. Kubo et al, Phys. Rev. B, **43**, 7875 (1991)
[7] P. W. Anderson and P. Morel, Phys. Rev. **125**, 4, (1962)
[8] M.L. Cohen and P.W. Anderson in Superconductivity in d and f band Metals, edited by D.H. Douglass (A.I.P. New York) (1972)
[9] V. Ginzburg, Comtemporary Physics, **33**, 1, 15-23 (1992)
[10] L. Force et J. Bok, Solid State Comm., **85**, 975 (1993)
[11]J. Bouvier, J. Bok, Physica C, **249** (1995) 117
[12] J. Bok, J. Bouvier, Physica C, **274** (1997) 1
[13] Ch. Renner and O. Fisher, Phys. Rev. **B51** (1995) 9208
[14] Y. Huri et al, Phys. Rev. Lett. **67** (1991) 2573