SUPERCONDUCTIVITY IN 2 DIMENSIONS: APPLICATION TO CuO_2 PLANES AND MgB_2.

Julien BOK and Jacqueline BOUVIER

Solid State Physics Laboratory - ESPCI. 10, rue Vauquelin. 75231 PARIS Cedex 05, FRANCE.

We recall the van Hove scenario[1,2] developed since 1987. It explains high Tc, anomalous isotope effect, gap anisotropy etc . We apply this scenario to the superconductive surface layer, obtained by field effect on $CaCuO_2$ by J. H. Schön et al[3,4]. We show that the variation of resistivity and Hall effect with temperature can be understood by the presence of a van Hove singularity (v.H.s.) in the band structure. The doping by field effect changes the distance between the Fermi level and the v.H.s.. In MgB_2, two gaps are observed. The large gap is related to a portion of the Fermi surface which is almost bidimensional.

1. INTRODUCTION

All experiments of angular resolved photoemission spectroscopy (ARPES) have confirmed the existence of saddle points (v.H.s.) close to the Fermi level in high Tc copper oxide compounds[5]. This is probably not purely accidental and we think that any theoritical model must take into account these experimental facts. We have developed a model using itinerant electrons in the presence of a v.H.s. in the band structure[1,2] since many years and we have explained a certain number of experimental facts : high Tc[1,2], anomalous isotope effect[1], gap anisotropy, specific heat, magnetic susceptibility and tunneling conductance, see for more details and more references the review paper[2]. Here we shall apply this model to explain the results obtained by J. H. Schon et al[4] on a conducting layer of the infinite phase $CaCuO_2$, obtained by field effect, and to explain the large gap of MgB_2.

2. SUPERCONDUCTOR FIELD EFFECT TRANSISTOR

A recent paper by J. Schon et al[4] reports experimental results on transport properties of electrons and holes in one plane of CuO_2 in a layered cuprate ($CaCuO_2$) where the carriers are created employing a field effect device (FET). This device allows to vary the carrier concentration from 0.26 hole per CuO_2 to 0.24 electron per CuO_2 by applying a voltage on the gate of the FET. The results reported are the variation of the resistivity and Hall cœfficient with temperature in this wide range of carriers concentration. This method allows a large variation of carriers concentration without introducing additional disorder linked to the inhomogeneous distribution of chemical dopants and to crystallographic defects. The variation of the hole or electron doping and the exploration of all the phase diagram can be performed also using one single sample. The existence of hole and electron bands can be explained following theoretical band structure calculations made by D. M. Newns et al[6]. These calculations use an Hamiltonian containing the p type orbitals of the oxygen atom, the d type orbital of the copper atom, and a large intra-atomic Coulomb repulsion U on the Cu atom. They find that the effect of U is to split the p band in two subbands. The lower Hubbard band can be doped with holes and the upper Hubbard band with electrons. In two dimensions, both bands possess a van Hove singularity. The Fermi level lies close to the v.H.s. for doping levels of the order of 0.20 hole or 0.18 electron per unit cell.

We present a model[7] that explains all the observed experimental features of $\rho(T)$ and $R_H(T)$ using the band structure for holes in a CuO_2. The Fermi surfaces of CuO_2 planes, and their variation with the doping as YBCO and the BiSCCO compounds have been studied intensively[2,5,8], they are well described by the following formula :

$$\varepsilon_k = -2\,t\,(\cos k_x a + \cos k_y a) + 4\,t'\cos k_x a \cos k_y a + (E_F - E_S) \qquad (1)$$

where t is the transfer integral between the first nearest neighbors, t' between the second nearest neighbors, a is the lattice parameter (Cu-Cu distance), E_S is the position of the saddle point (v.H.s.) and E_F the Fermi level (FL). t and t' have been determined by ARPES in Bi(2212) samples[8]. To fit the observed Fermi surface and its variation with hole doping, the following range values have been proposed: t = 0.25 to 0.18 eV and t' = 0.10 to 0.09 eV. The variation of $E_F - E_S$ with doping has been calculated by J. Bouvier and J. Bok[2,9] using the same values for t and t'.

2.1 RESISTIVITY

D. M. Newns[10] has shown that the van Hove singularity gives « marginal Fermi liquid » properties when E_F (FL) is very close to E_S (vHs). The lifetime ($1/\tau$) of a quasiparticle is shown to vary as ε (the energy measured from E_F) when the FL lies at the vHs[6,10], and when E_F (FL) is far from E_S (vHs) (more than k_bT) the dependence is $1/\tau \alpha \varepsilon^2$. This variation is observed experimentally in infrared reflection and in photoemission[6,10]. We have computed the resistivity in the reference[7] and we found:

$$\rho = \rho_o + b\,T^2 \quad \text{for} \quad k_bT < E_F - E_S$$

$$\rho = \rho_o + a\,T \quad \text{for} \quad k_bT > E_F - E_S$$

In our model the temperature T* is the temperature where $\rho(T)$ changes its variation going from T^2 to T, so T* is directly related to the distance between E_F (FL) and E_S (v.H.s.). In our theoretical result we find: $E_F - E_S = 1.85\ k_bT^*$. The numerical factor is due to an optimal filling of the DOS at E_S at this temperature. In Figure 1, we show the fit of experimental curves $\rho(T)$ for various hole doping, and in Figure 2 our calculated T*, reported with the experimental values of reference[4]. We can see that the agreement is remarkably good.

2.2 Hall effect

For hole energies (opposite in sign to electron energies) $E < E_S$, the orbits of carriers in a magnetic field are hole like; they give a positive Hall cœfficient R_H. For the hole energies $E > E_S$, the orbits are electron like and give a negative contribution to R_H. At very low temperature, the only important orbits are at $E \approx E_F$. The sign of R_H is positive for the hole doping $p < p_o$, and negative for $p > p_o$. The calculated value of p_o is 0.21 hole, corresponding to the experimental value where the resistivity is perfectly linear in T. The opposite signs are true in the electron band. As the temperature increases, i.e. $k_bT \geq E_F - E_S$, the electron orbits contribute to the Hall effect with a negative sign, then R_H decreases. In Figure 3 we plot R_H / R_H^* versus T/T^* and find a universal curve, as found experimentally[4]. This is natural because our only variable is $E_F - E_S$ when we change the doping.

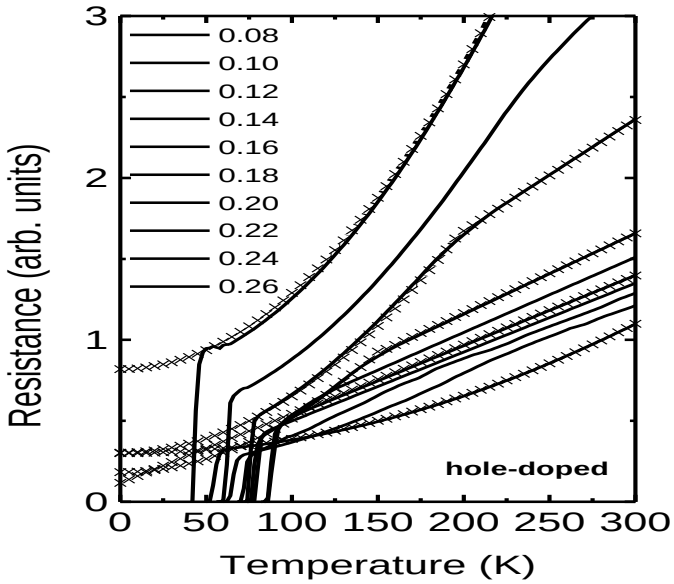

FIGURE 1

ρ(T) for hole doping, from the underdoping top curve to the overdoping bottom curve
full lines : experimental curves (4)
dashed crossed lines : fit for some curves

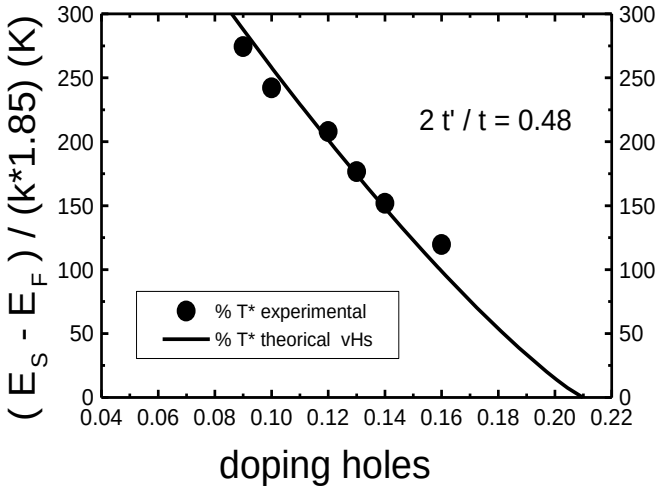

FIGURE 2

Full line: our calculated T* compared with the experimental values (dots).

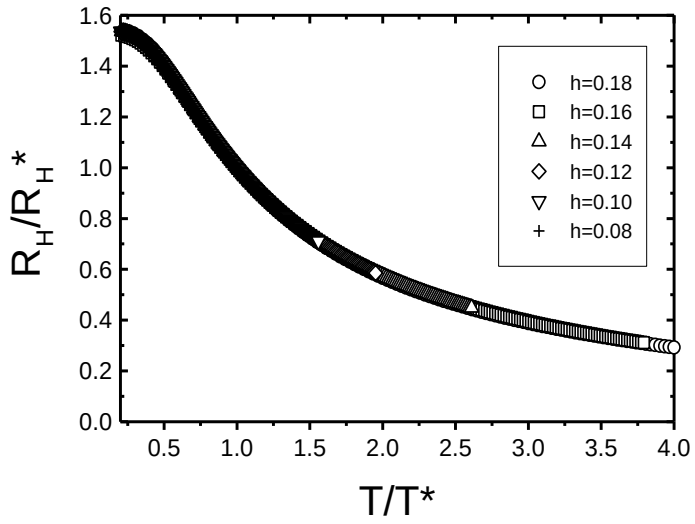

FIGURE 3
Universal curve for the ratio of R_H/R_H^*, for hole doping.

3. MgB_2

We have computed the critical temperature of MgB_2 using the Morel-Anderson approach[2,11]. We used the band structure (1), one piece of the Fermi surface is nearly 2D and gives a large gap. We have used a screened electron-phonon interaction for pairing. In this compound Tc is not so high because the Fermi level is rather far from the singularity (about 2.4 eV). We present in Table I our calculated values of the large gap Δ, using the following parameters: bandwidth W = 6 eV, and various values for the screening $q_o a$ (a is the unit cell parameter) and for the effective electron-phonon constant λ_{eff}^*, chosen to obtain Tc = 41 K.

$q_o a$	λ_{eff}*	Δ meV
0.2	0.100	6
0.2	0.140	7
0.3	0.140	6.
0.3	0.100	6.25

Table I

4. Conclusion

In conclusion, we have shown that the van Hove scenario explains many experimental results obtained in 2D superconductors. The single doped monolayer, made by J. H. Schön, is a perfect object to check the van Hove scenario in the HTSC cuprates. J. Bouvier et al (12) have already proposed the same explanation for the maxima observed in the variation with temperature of several measured quantities: Pauli susceptibility, the specific heat, the Knight shift, the thermoelectric power etc…(13). On the other hand, some experiments (14) show a pseudogap, i.e. a loss of states near the Fermi level. This pseudogap may be related to disorder introduced by doping (15). In some highly disordered samples two characteristic temperatures T° and T* are observed corresponding to these two different effects.

REFERENCES

1) J. LABBE and J. BOK, Europhys. Lett. **3** (1987) 1225.

2) J. BOUVIER and J. BOK, The Gap Symmetry and Fluctuations in HTSC, in: Superconductivity in cuprates, the van Hove scenario : a review, in: The Gap Symmetry and Fluctuations in HTSC, eds J. Bok et al., Plenum Press, New York 1998.

3) J. H. SCHON, M. DORGET, F. C. BEURAN, X. Z. XU, E. ARUSHANOV, C. DEVILLE-CAVELLIN, and M. LAGUES, Nature **414** (2001) 434.

4) J. H SCHON, M. DORGET, F. C. BEURAN, X. Z. XU, M. LAGUES, C. DEVILLE-CAVELLIN, C. M. VARMA and B. BATLOGG, Mapping the Phase Diagram of electrons and Holes in a Layered Cuprate Using Field-Effect Doping, preprint (private communication), to be published.

5) Z. X. SHEN, W. E. SPICER, D. M. KINGS, D. S. DESSAU, Science **267** (1995) 343.

6) D. M. NEWNS, P. C. PATTNAIK and C. C. TSUEI, Phys. Rev. B **43** (1991) 3075.

7) J. BOUVIER and J. BOK, cond-mat/**0203128.**

8) M. R. NORMAN et al, Nature **392** (1998) 157.

9) J. BOUVIER and J. BOK, Physica C **288** (1997) 217.

10) D. M. NEWNS, Comment Cond. Mat. Phys. **15** (1992) 273.

11) L. FORCE and J. BOK, Solid State Comm. **85** (1993) 975.

12) J. BOUVIER and J. BOK, J. of Supercond. **10** (1997) 673.

13) J. R. Cooper and J. W. Loram, J. Phys. I France **6**, (1996) 2237.

14) See for a review T. Timusk and B. Statt, *Rep. Prog. Phys.* **62**, 61 (1999).

15) J. BOUVIER and J. BOK, Physica C **364-365**, (2001) 471.

16) J. BOUVIER and J. BOK, Physica C **217-225**, (1997) 217.