

Superconductivity and Phase Diagram in a CuO_2 Monolayer

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We recall the van Hove scenario (J. Labbe and J. Bok, *Europhys. Lett.* **3**, 1225 (1987); J. Bouvier and J. Bok, in *The Gap Symmetry and Fluctuations in HTSC*, J. Bok *et al.*, eds. (Plenum, New York, 1998)) developed since 1987. It explains high T_c , 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.* Preprint (private communication), to be published). We show that the variation of resistivity and Hall effect with temperature in the normal state 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.

KEY WORDS: phase diagram; superconductivity; resistivity.

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 T_c copper oxide compounds [1]. This is probably not purely accidental and we think that any theoretical 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 [2,3] since many years and we have explained a certain number of experimental facts: high T_c [2,3], anomalous isotope effect [2], gap anisotropy, specific heat, magnetic susceptibility, and tunneling conductance, see for more details and more references the review paper [3]. Here we compute the transport properties, resistivity, and Hall effect in a conducting CuO_2 layer.

2. SUPERCONDUCTOR FIELD EFFECT TRANSISTOR

A recent paper by Schön *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 coefficient 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 Newns *et al.* [5]. 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.

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We present a model [6] 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 [1,3,7], they are well described by the following formula:

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

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 [7]. 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 Bouvier and Bok [3,8] using the same values for t and t' .

2.1. Resistivity

Newns [9] has shown that the van Hove singularity gives “marginal Fermi liquid” properties when E_F (FL) is very close to E_S (v.H.s.). The lifetime ($1/\tau$) of a quasiparticle due to electron–electron interaction is shown to vary as ε (the energy measured from E_F) when the FL lies at the v.H.s. [5,9], and when E_F (FL) is far from E_S (v.H.s.) (more than $k_b T$) the dependence is $1/\tau \propto \varepsilon^2$. This variation is observed experimentally in infrared reflexion and in photo-emission [5,9]. We have computed the resistivity in Ref. [6] and we found:

$$\begin{aligned} \rho &= \rho_0 + bT^2 \quad \text{for } k_b T < E_F - E_S \\ \rho &= \rho_0 + aT \quad \text{for } k_b T > E_F - E_S \end{aligned}$$

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: $E_F - E_S = 1.85 k_b T^*$. The numerical factor is due to an optimal filling of the DOS at E_S at this temperature. In Fig. 1, we show the fit of experimental curves $\rho(T)$ for various hole doping, and in Fig. 2 our calculated T^* , reported with the experimental values of Ref. [4]. We can see that the agreement is remarkably good.

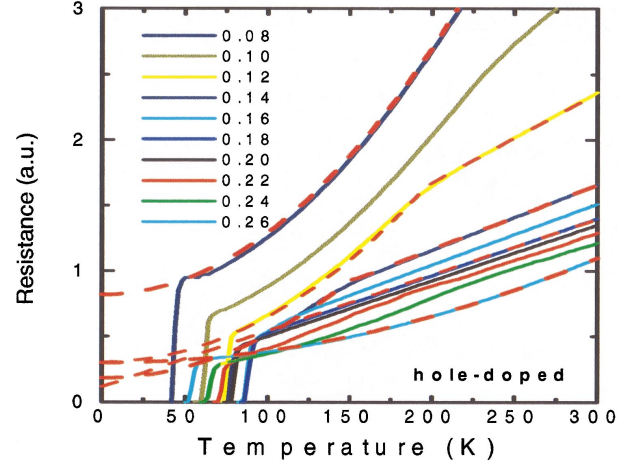


Fig. 1. $\rho(T)$ for hole doping, from the underdoping top curve to the overdoping bottom curve full lines: experimental curves [4]; dashed crossed lines: fit for some curves.

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 coefficient 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 $p < p_0$, and negative for $p > p_0$. The calculated value of p_0 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,

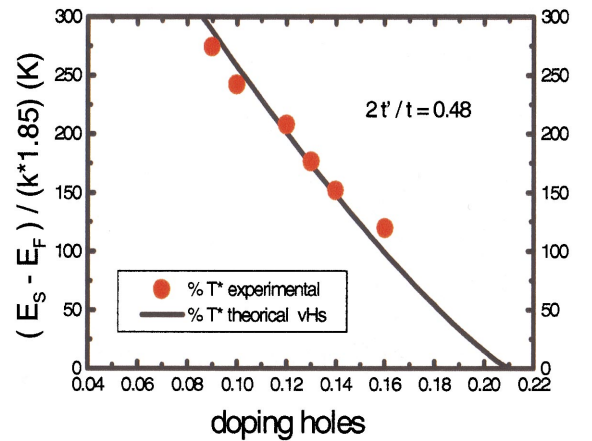


Fig. 2. Full line: our calculated T^* compared with the experimental values (dots).

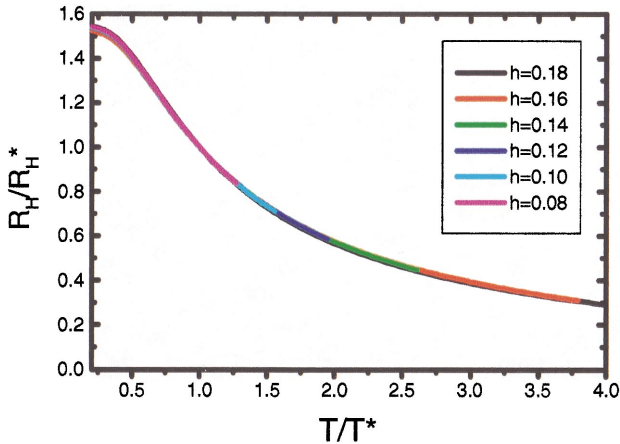


Fig. 3. Universal curve for the ratio of R_H/R_H^* , for hole doping.

i.e. $k_b T E_F - E_S$, the electron orbits contribute to the Hall effect with a negative sign, then R_H decreases. In Fig. 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.

3. 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. Bouvier *et al.* [10] 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. [11]. On the other hand, some experiments [12] show a pseudogap, i.e. a loss of states near the Fermi level. This pseudogap may be related to disorder introduced by doping [13]. In some highly disordered samples two characteristic temperatures T^0 and T^* are observed corresponding to these two different effects.

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