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Van Hove Scenario for High T_c Superconductors

J. Bok (✉) · J. Bouvier

Solid State Physics Laboratory, ESPCI, 10, rue Vauquelin, 75231 Paris Cedex 05, France
julien.bok@espci.fr

Abstract All the high T_c cuprates (HTSC) have a lamellar structure and hence almost two dimensional properties. This 2D character leads to the existence of Van Hove singularities (VHs) or saddle points in their electronic band structure. These VHs have been observed experimentally in all the HTSC and we show that they explain many physical properties of these compounds, both in the normal and superconducting states. This feature induces a topological transition for a hole doping of $p_o \simeq 0.20$ hole/copper atom. The constant energy curves going from hole-like to electron-like.

The discovery of high temperature superconductivity in cuprates compounds in 1986 [1] has been a great sensation in the physics community and has raised great expectations, which, we hope, will one day be fulfilled. Twenty years after this discovery, the exact mechanism of HTSC is still not yet understood and remains a great challenge for solid-state physicists ... All these compounds are strongly anisotropic and almost two dimensional, due to their CuO_2 planes, where superconductivity mainly occurs. It is well known that in 2 dimensions, electrons in a periodic potential show a logarithmic density of states (DOS), named Van Hove singularity (VHs) (Van Hove (1953) [2]). The Van Hove scenario is based on the assumption that, in high critical temperature superconductors (HTSC), the Fermi Level (FL) lies close to such a singularity (Labbé-Bok 1987) [3]. The constant energy curves are hole-like for a doping less than 0.20 and become electron-like when the doping is increased. This topological transition occurs for a hole doping around 0.20, 0.21 hole/copper atom (Fig. 1). This hypothesis has been confirmed by many experiments, in particular by Angular Resolved Photoemission Spectroscopy in different compounds [4].

We want to stress that the model of 2D itinerant electrons in presence of VHs in the band structure has already explained a great number of experimental facts. Detailed calculations are presented in a review paper [5]:

- **critical temperature and gap anisotropy**
  We have computed the critical temperature T_c and its variation with doping. The optimum T_c is obtained for a hole doping of $p = 0.16$ and not $p = 0.20$ (when $E_{Fs} = Es$) as predicted in our first simple model. This is because we did not take into account the screening in the beginning. By

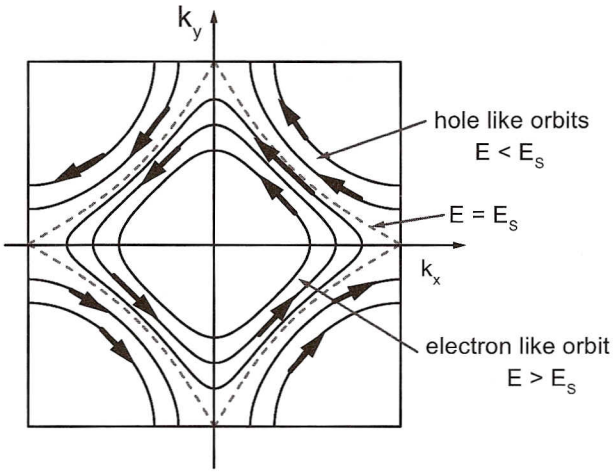

Fig. 1 Constant energy curves in the first Brillouin zone, in CuO_2 planes, representation of hole and electron like orbits

taking into account this screening and its variation with doping, our new results agree completely with the experimental results (Figs. 2, 3).

The superconducting gap is strongly anisotropic [6, 7]. It takes a high value in the directions of the saddle points (0,1) or (1,0), where the DOS is high and a low value in the (1,1) direction, where the DOS is low. It becomes negative if a repulsive interaction between electrons is included.

It has also been shown that the singularity is in the middle of a large band and that, in these circumstances, the Coulomb repulsion μ is renormalized and replaced by a smaller value [8]. This is important, because it shows that in the case of a VHs, Coulomb repulsion does not lower T_c as it does in a narrow band.

- **anomalous isotope effect and coherence length**

  Due to the peak in the DOS at the VHs, we have shown that the isotope effect should be very small at optimum doping, even if the electron-phonon interaction is responsible for the pairing of electrons [3, 5].This results from the fact that the cut-off in the BCS formula is mainly the width of the singularity and not the phonon frequency. The isotope effect reappears at low doping; this was observed experimentally [3]. We also were able to explain the very small values of the coherence length ξ [8, 9]. This is due to the fact that ξ is proportional to the Fermi velocity and that this velocity is zero at a saddle point.

- **tunnelling conductance**

  We have computed the conductance of tunnelling junctions with our calculated DOS and compared the results to the experimental curves obtained with various types of superconducting junctions. The results are satisfactory [10].

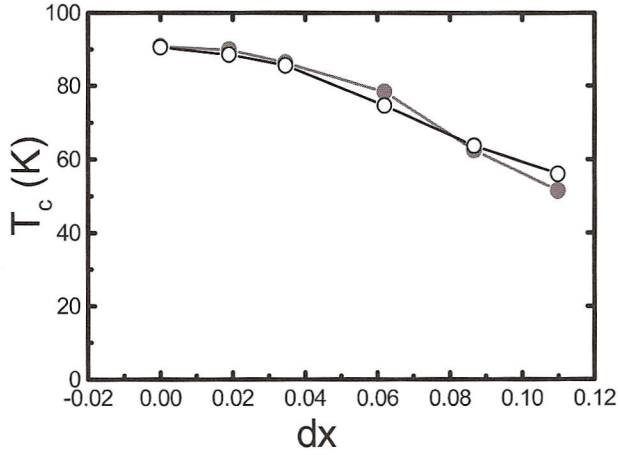

Fig. 2 Comparison of the variation of Tc versus the variation of doping dx, from the optimal doping; calculated in our model (*red filled circles*) and the experimental results of Koïke et al. (*black open circles*) [16]

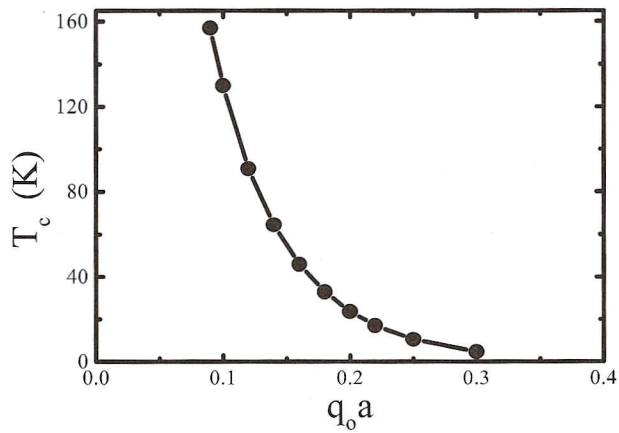

Fig. 3 Tc versus the screening parameter $q_0 a$ (cf. [11])

- **the specific heat** [7] **and the magnetic susceptibility** [11]**.**
  These two thermodynamical quantities go through a maximum as the temperature varies. The variation of all these properties with hole doping (from underdoped to overdoped samples) and temperature are obtained and compared with the experiments. The agreement is very satisfactory. The variation with the doping is linked to $(E_F - E_S)$, so does the variation with the temperature due to the Fermi-Dirac distribution. When kT becomes of the order of $E_F - E_S$, the high density of states in the singularity is populated and contributes to this maximum. The good fit between theory and experiment is shown in Fig. 4.

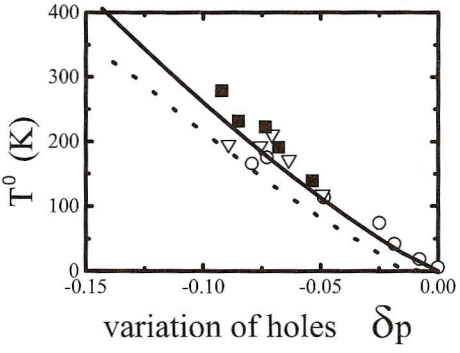

Fig. 4 The temperature, T° (directly linked to VHs), where the calculated χ_p (*dashed line*) and the specific heat (*solid line*) go through a maximum, versus δp. For comparison we show results presented in Fig. 27 of [17], the symbols are the same. (*solid squares*: from thermoelectric power, *circles*: from specific heat, *triangles*: from NMR Knight shift data)

- **transport properties**
  Transport properties in the normal state are described. We show that $E_F - E_S$ is critical for these properties, leading to Fermi liquid or marginal Fermi liquid behaviour [12]. We compute the Hall coefficient and its variation with doping and temperature [13]. We show that the experimental results may be explained by the topology of the Fermi surface (FS) which goes from hole-like to electron-like as the hole doping is increased. When the temperature is increased, the electron-like orbits start being populated. They give a negative contribution to the Hall coefficient which

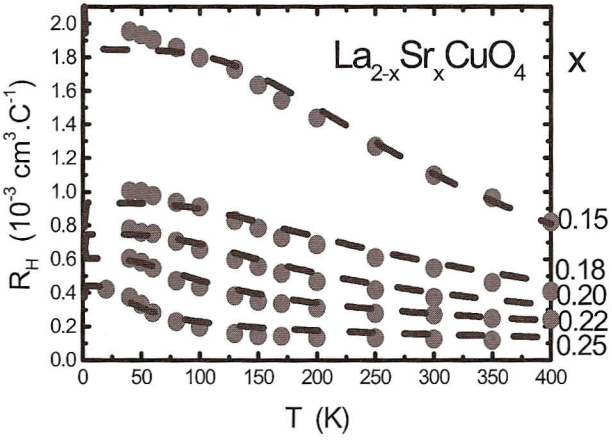

Fig. 5 *Filled circles*: experimental $R_H(T)$ given by [18]. In polycrystalline $La_{2-x}Sr_xCuO_4$, for $x = 0.15, 0.18, 0.20, 0.22, 0.25$. *Dashed lines*: theoretical fits, the theoretical hole levels as the same as the experimental. The calculations are made with: $t = 0.23$ eV, $t' = 0.06$ eV, $2t'/t = 0.52$, $\Gamma(E_S) = 0.1$ (cf. [13])

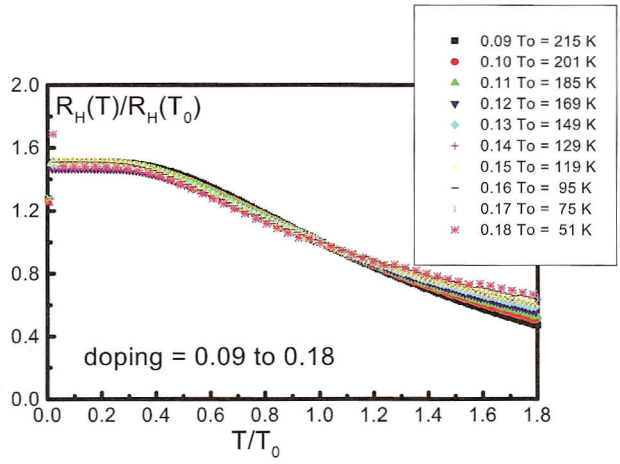

Fig. 6 Universal law $R_H(T)/R_H(T_0)$ versus T/T_0 for various hole doping levels, from 0.09 to 0.18 (cf. [13])

decreases as temperature increases as observed in all experiments (Figs. 5, 6). The critical doping, for which a topological transition is observed and calculated is $p = 0.21$ hole per CuO_2 plane.

- **effect of disorder**

  In the normal states the cuprates, especially the underdoped ones, may be considered as bad metals in the sense of Altshuler and Aronov [14], because the diffusion coefficient is very low. The diffusion coefficient is proportional to the Fermi velocity which is zero at the saddle points. The

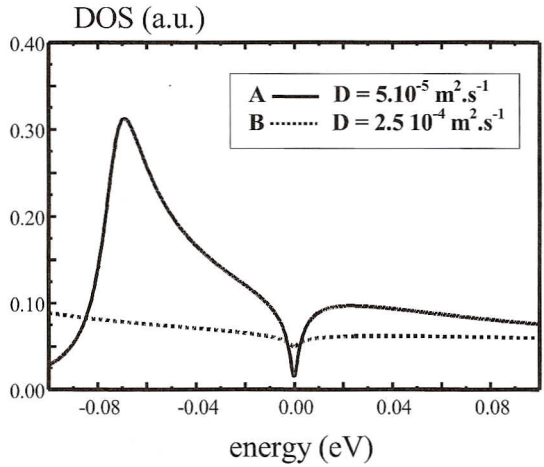

Fig. 7 Calculated DOS with Coulomb interaction with different sets of values of D: in the (1,0) direction, and equivalent directions – B: in the (1,1) direction

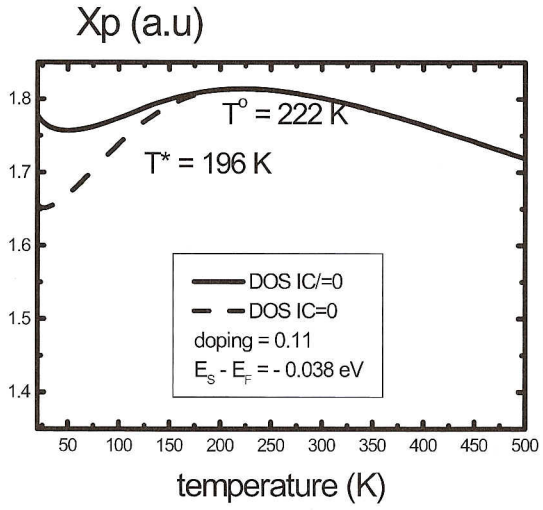

Fig. 8 Calculated Pauli Susceptibilities. *Full line* = without disorder effect – *Dashed line* = with disorder effect, for 0.11 hole doping

Coulomb interaction between electrons must then be taken into account The main effect is to open a dip in the DOS at the Fermi level [14, 15], see Fig. 7. We show that this may explain many observed features of the "pseudo-gap": its value, anisotropy and variation with doping [15]. The anisotropy is directly related to the anisotropy of the Fermi velocity. The loss of states at the Fermi level explains the decrease of thermodynamic coefficients, such as the magnetic susceptibility, at low temperature (Fig. 8).

In conclusion we have shown that Van Hove singularities play an important role in HTSC, and that by taking them into account, we may explain many of their normal and superconducting properties. We argue that the observed topological transition, occurring around p = 0.2 hole per copper atom, is a crucial feature to explain the physical properties of the cuprates, in particular the Hall effect. The presence of VHs is now well established and almost all theoretical models take them into account under various names, VHs, saddle points, hot spots, etc.

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