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Review Article

Electron-Phonon Interaction in the High-T_C Cuprates in the Framework of the Van Hove Scenario

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Electron-lattice interaction was the original idea of Müller and Berdnorz who chose copper oxides, because of the strong Jahn-Teller effect of the Cu ion leading to the formation of bipolarons. Later several experimental features led to theoretical models based on strong electronic correlations. The high-T_C superconductors cuprates are quasi-bidimensional (2D) and thus lead to the existence of Van Hove singularities (VHs) in the band structure, that is, a peak in the electronic density of states. The presence of VHs near the Fermi-level in the cuprates is now well established. In this context we show that many physical properties of these materials can be explained using electron-phonon interaction, in particular the high critical temperature T_C, the anomalous isotope effect, the superconducting gap and its anisotropy, and the marginal Fermi-liquid properties. These compounds present a topological transition for a critical hole doping $p \approx 0.21$ hole per CuO_2 plane.

1. Introduction

Twenty three years after the discovery of the high temperature superconductivity in cuprates compounds [1], the exact mechanism of superconductivity is still not yet understood. Müller and Berdnorz stressed that superconductivity occurs because of the Jahn-Teller effect of the Cu ion. But all these compounds are also strongly anisotropic and almost two dimensional, due to their CuO_2 planes, where superconductivity mainly occurs. It is well known that electrons, in a periodic system in one or two dimensions, lead to divergences in the density of states (DOS), named Van Hove singularities (VHs) [2]. The Van Hove scenario is based on the assumption that in some superconductors the Fermi level lies close to such a singularity. Labbé and Friedel [3] applied this scenario for the first time to the A15 compounds, where the Nb chains give an almost 1D behaviour. Hirsch and Scalapino [4] examined the 2D situation (logarithmic singularity) and applied it to excitonic superconductivity. Labbé and Bok [5] proposed the Van Hove scenario for the cuprates, using electron-phonon interaction and predicted an anomalous isotope effect. The presence of saddle points (or VHs) near the Fermi level has been confirmed by many experiments, in particular by Angular Resolved Photoemission Spectroscopy (ARPES) [6, 7] in different compounds.

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 VHs in the band structure has already explained a certain number of experimental facts.

We know that several experimental features led to theoretical models based on electron-electron interaction [8, 9] (strong correlations between electrons). These feature are the following:

(i) the anomalous isotope effect,

(ii) the observation of antiferromagnetic (AF) fluctuations,

(iii) the marginal Fermi-liquid behaviour in the normal phase,

(iv) the d-wave symetry of the superconducting gap.

The strong correlations are surely very important in the underdoped regime but we shall show that electron-phonon interaction coupled with the Van Hove scenario may explain must of the properties in the region of optimum doping and the overdoped region.

In this paper, we give a rapid description of the band structure of the CuO_2 planes. We give the results of our calculations for the critical temperature T_C [5, 10, 11], the anisotropic superconducting gap [10]. We show the importance of screening and Coulomb repulsion [10, 12]. We explain the anomalous isotope effect [5], the very small values of the coherence length [13, 14].

The variation with the doping is linked to the distance of the FL from the singularity level (E_F-E_S), so does the variation with the temperature due to the Fermi-Dirac distribution [11]. We show that E_F-E_S is critical for these properties, leading to Fermi-liquid or marginal Fermi-liquid behaviour [15, 16].

We explain how the occurrence of a lattice deformation could place the Fermi level in an optimum situation of high DOS, leading to a high critical temperature for the superconducting phase.

In conclusion we show that taking into account both the electron-phonon interaction and the existence of the VHs, we obtain a model that fits with experiments in the optimum and overdoped regime of the cuprates. We hope that such an approach can help chemists to improve the HTSC.

2. Electronic Structure of the Cuprates and Van Hove Scenario

Van Hove singularities are general features of periodic system [2]. A one electron calculation is easy to perform [5]. A general feature of a 2D model is the presence of Van Hove singularity [5] (VHs) with logarithmic divergence of the DOS at an energy $E = E_S$. A simple calculation [17] gives the result shown in Figure 1 for the constant energy surfaces (CES) in k-space. This is very well confirmed by the results of Ino et al. [6] using angular resolved photoemission spectroscopy (ARPES) (see [6, Figure 7]).

A topological transition is well seen for a doping value $p_c = 0.21$ hole per Cu atom. The CES are hole-like for $p < p_c$ and electron-like for $p > p_c$. The resulting VHs gives a peak in the DOS, see Figure 2, and thus increases the transition temperature whatever the pairing mechanism. The main consequences of this Van Hove scenario are given in [17].

This approach is not valid for the underdoped region. The strong Coulomb repulsion U between two electrons on a same site is responsible for the fact that with $p = 0$ the cuprates are Mott-insulators with antiferromagnetic (AF) order. The AF order disappears rather rapidly with doping, but AF fluctuations remain, and decrease, until the optimum doping. This region of strong correlations is present and the valid approach is that of a doped Mott-insulator [8]. This is also seen in ARPES; some points of the Fermi surface disappear for underdoped samples.

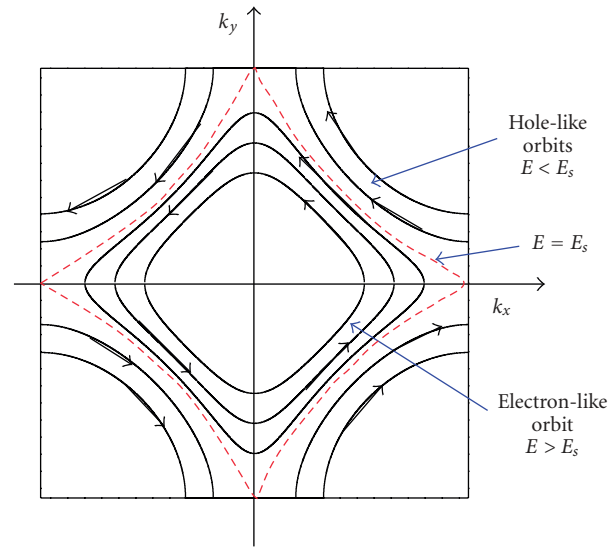

Figure 1: Constant energy surfaces.

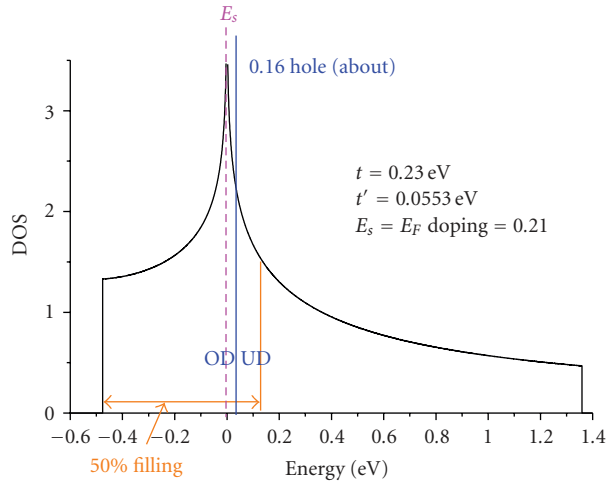

Figure 2: Density of States (DOS).

3. Calculation of T_C with Electron-Phonon Interaction

3.1. Calculation of T_C Using the BCS Approach. Labbé and Bok [5] have computed the band structure for the bidimensional CuO_2 planes of the cuprates, considered as a square lattice (quadratic phase). They obtained a formula for T_C using the following assumptions:

(1) the Fermi level lies at the Van Hove singularity,

(2) the BCS approach is valid,

(i) the electron-phonon interaction is isotropic and so is the superconducting gap Δ,

(ii) the attractive interaction V_p between electrons is nonzero 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

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

where λ is an electron-phonon coupling constant [3].

A simplified version of Formula (1a), when $\hbar\omega_0$ is not too small compared to D, is

$$k_B T_c = 1.13D \exp\left(-\frac{1}{\sqrt{\lambda}}\right). \quad (1b)$$

The two main effects enhancing T_C are the following.

(1) The prefactor in Formula (1b) is an electronic energy that is much larger than a typical phonon energy $\hbar\omega_0$.

(2) λ is replaced by $\sqrt{\lambda}$ in Formula (1b) in comparison with the BCS formula, so that in the weak coupling limit when $\lambda < 1$, the critical temperature is increased.

As it is however, this approach already explains many of the properties of the high-T_C cuprates near optimum doping.

3.2. The Variation of T_C with Doping. Then we did more accurate calculations (1995–1997) [10, 11]. By taking into account the repulsive interaction between second nearest neighbours (s.n.n.) and the variation of hole doping [11], the band structure becomes

$$E_k = -2t(\cos X + \cos Y) + 4t' \cos X \cos Y + D_e, \quad (2)$$

where t' is an integral representing the interaction with s.n.n., where $D_e = E_F - E_S + (4t')$ represents the doping in hole p. The Fermi surface at the VHs is no longer a square but is rather diamond shaped, see Figure 1, and we obtain the DOS of Figure 2. For lower or higher doping the critical temperature decreases. We adjusted the experimental results of Koike et al. [18]; see Figure 3 [11]. In this case the authors varied the hole concentration in the CuO_2 planes of $Bi_2Sr_2CaCu_2O_{8+\delta}$ using different substitution of cations with different valences, obtening different systems, that is

$$Bi_2Sr_2Ca_{1-x}Lu_xCu_2O_{8+\delta}, Bi_2Sr_2Ca_{1-x}Na_xCu_2O_{8+\delta},$$
$$Bi_2Sr_{2-x}Ca_{1-x}La_xCaCu_2O_{8+\delta}, Bi_2Sr_{2-x}K_xCaCu_2O_{8+\delta}. \quad (3)$$

In Figure 3 our model account for the variation of the holes in the CuO_2 plane, from an optimum doping, here $p \approx 0.20$, of this group of compounds, and we calculate the corresponding T_C when E_F shift from E_S.

3.3. Influence of the Coulomb Repulsion. Although BCS theory [19] neglects Coulomb repulsion, Morel and Anderson [20] showed very early that it plays a central role in superconductivity. Assuming a constant repulsive potential V_C from 0 to E_F, they found that T_C is given by

$$T_C \cong \text{To} \exp\left[-\frac{1}{\lambda - \mu^*}\right] \quad (4)$$

with $\mu = \text{No}V_c$ and $\mu^* = \mu/(1 + \mu \ln E_F/\omega_0)$.

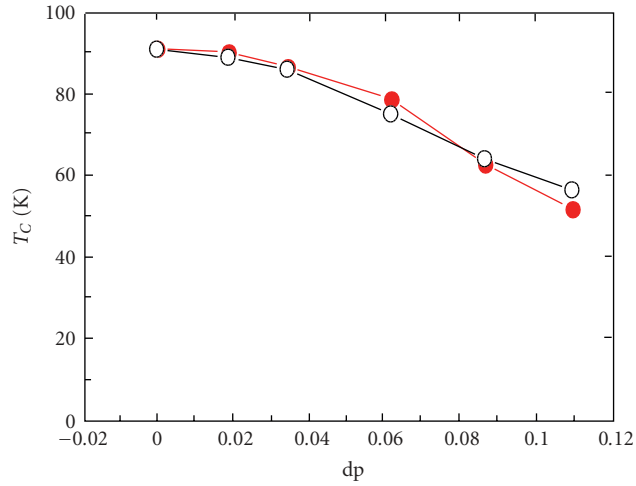

Figure 3: Comparison of the variation of T_C with the variation of the doping dp from the optimum doping at dp = 0, calculated in our model (red filled circles) and the experimental results of Koike et al. (black open circles) [18].

Cohen and Anderson [21] assumed that for stability reasons μ is always greater than λ. Ginzburg [22] 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 E_F of the order of 100 $\hbar\omega_0$. It is useless to reduce the width of the band W, 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.

Force and Bok studied the renormalization of μ, in the case of a peak in the DOS in the middle of a broad band [14]. They predict a high-T_C in this case due to three main effects.

(i) $(\lambda - \mu^*)$ is replaced by the square root $(\lambda - \mu^*)^{1/2}$.

(ii) μ^* is reduced compared to μ because the renormalization is controlled by the width W of the broad band and not the singularity.

(iii) The prefactor before the exponential in the formula giving T_C is the width of the singularity D instead of the phonon energy $\hbar\omega_0$.

In Figure 4, we show the variation of T_C with the width of the singularity D, with all other parameters (W, ω_o) remaining constant.

4. Anomalous Isotope Effect

The variation of T_C with the mass M of the atom of the metal is considered as an evidence for electron-phonon interaction as the origin of pairing. In this BCS model [19] T_C varies as $M^{-1/2}$. The almost absence of isotope effect when O^{18} was substituted to O^{16} in the cuprates [23] was considered as an evidence for non phonon origin of superconductivity. But Labbé and Bok [5], using Formula (1a), have shown

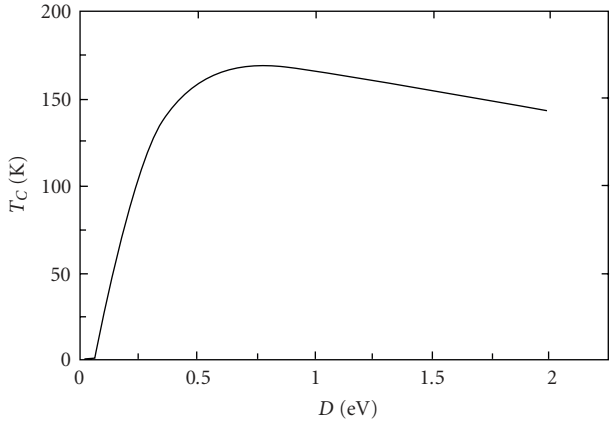

Figure 4: Effect of the band width D of the singularity on T_C.

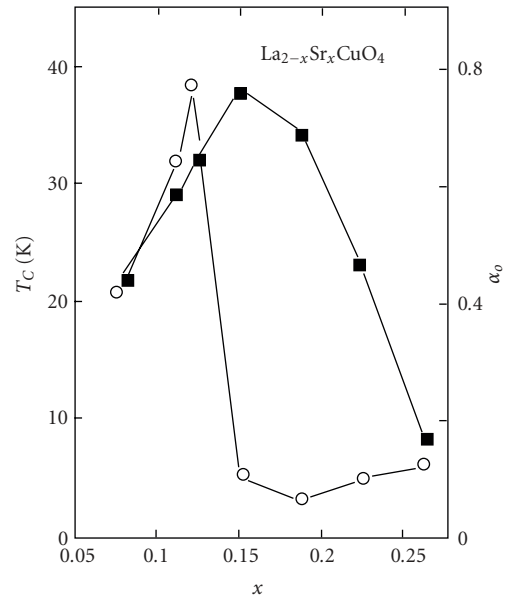

Figure 5: From [26], experimental results of T_C (■) and α_o (◯) as a function of doping concentration for $La_{2-x}Sr_xCuO_4$ (the data where taken from [24]).

that the isotope effect is strongly reduced for HTCS cuprates at optimum doping. This is due to the fact that in this situation the Fermi level lies near the VHs and then the width of the singularity D is more important than the phonon frequency ω_o. They also have predicted that the isotope effect should reappear for underdoped samples. This was later experimentally observed [24, 25]. The isotope effect may be measured by the cœfficient α defined as T_C proportional to $M^{-\alpha}$ ($\alpha = 0.5$ for usual superconductors). Tsuei et al. [26], using the VH scenario, have calculated the variation of α with doping and shown in that it explains the experimental observations, see Figure 5.

5. Non-Fermi-liquid Properties

5.1. Resistivity. In a classical Fermi-liquid, the lifetime broadening $1/\tau$ of an excited quasiparticle goes as ε^2 and the resistivity ρ varies as T^2 .The marginal Fermi-liquid situation is the case where $1/\tau$ goes as ε (electronic energy) and ρ is linear in T. In the half-filled nearest-neighbour coupled Hubbard model on a square lattice, Newns et al. [15, 16] have shown that this can also occur when E_F is close to E_S. This calculation was however contradicted by Hlubina and Rice [27].

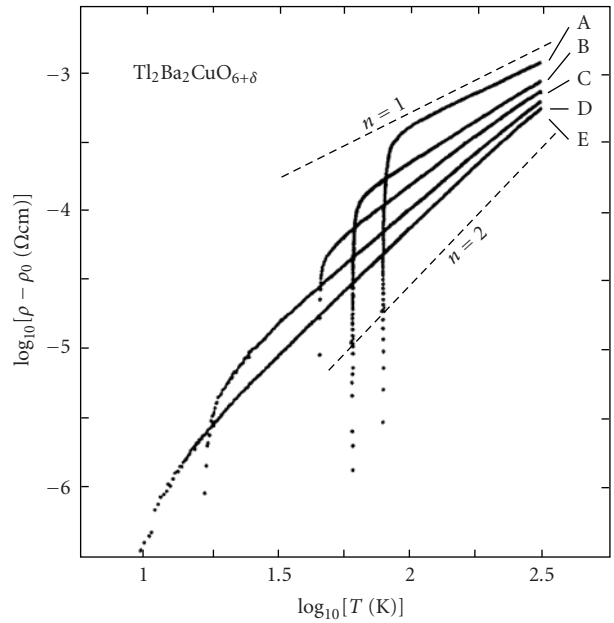

Figure 6: From [30], fit of the resistivity ρ of $Tl_2Ba_2CuO_{6+\delta}$ to a power law temperature dependence $\rho = \rho_o + AT^n$ shown on a log-log scan. The dashed lines indicate the slope for $n = 1$ and $n = 2$.

Experimental evidence of marginal Fermi-liquid behaviour has been seen in angle resolved photoemission [28], infrared data, and temperature dependence of electrical resistivity [29]. Marginal Fermi-liquid theory, in the frame work of VHs, predicts a resistivity linear with temperature T. This was observed by Kubo et al. [30] and cited in [8]. 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 maximum T_C, see Figure 6, which is consistent with our picture; in lower T_C material the Fermi level is pushed away from the singularity.

5.2. Hall Cœfficient. Many measurements of the Hall coefficient R_H in various high-T_C cuprates have been published [31, 32]. The main results are the following

(i) At low temperature T, $R_H \approx 1/p_{h0}e$, where p_{h0} is the hole doping, when T increases R_H decreases, and for highly overdoped samples it becomes even negative.

(ii) These authors are also able to define a temperature T_0, where R_H changes its temperature behaviour, and they found that $R_H(T)/R_H(T_0)$ versus T/T_0 is a universal curve for a large doping domain (from $p_{h0} = 0.10$ to $p_{h0} = 0.27$).

We can explain [33], following the approach given by Ong [34], these results by using the band structure for carriers in the CuO_2 planes. In particular, the existence of hole-like and electron-like constant energy curves, see Figure 1, which give contributions of opposite sign to R_H. The transport properties explore a range of energy k_BT around the Fermi level, when T is increased more and more carriers are on the electron like orbits, resulting in a decrease of R_H. In [33] we present our calculations and the theoretical fits of many experimental results, and we show that it works and this supports our model.

6. Gap Anisotropy

6.1. The Calculation. Bouvier and Bok [10] have shown that using a weakly screening electron-phonon interaction, and the band structure of the CuO_2 planes, an anisotropic superconducting gap is found.

We use the BCS equation for an anisotropic gap

$$\Delta_{\vec{k}} = \sum_{k'} \frac{V_{kk'}\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}}, \tag{5}$$

and instead of a constant potential as used in BCS, we choose a weakly screened attractive electron-phonon interaction potential:

$$V_{kk'} = \frac{-\left|g_q\right|^2}{q^2 + q_0^2} < 0, \tag{6}$$

where $g(q)$ is the electron phonon interaction matrix element for $\vec{q} = \vec{k}' - \vec{k}$ and q_0 is the inverse of the screening length. We compute $\Delta_{\vec{k}}$ for two values of $\vec{k}$:

$$\Delta_A \quad \text{for } k_x a = \pi, \qquad k_y a = 0, \tag{7a}$$

$$\Delta_B \quad \text{for } k_x a = k_y a = \frac{\pi}{2}. \tag{7b}$$

We solve (5) by iteration for these two specific points of the Fermi surface, the saddle point A $(\pi,0)$ or (1,0) direction, and point B $(\pi/2,\pi/2)$ or (1,1) direction. To obtain the entire dependence in the wave vector $\vec{k}$, we know from group theory considerations that $V_{kk'}$ having a fourfold symmetry, the solution Δ_k has the same symmetry, so we may use the angle Φ between the 0 axis and the $\vec{k}$ vector as a variable and expand $\Delta(\Phi)$ in Fourrier series:

$$\Delta(\Phi) = \Delta_0 + \Delta_1\cos(4\Phi + \varphi_1) + \Delta_1\cos(8\Phi + \varphi_2) + \cdots \tag{8}$$

Further developments of the calculations and explanations about this model are done in [10]. We obtain, for the two computed values

$$\Delta_A = \Delta_{\max} = \Delta_0 + \Delta_1, \qquad \Delta_B = \Delta_{\min} = \Delta_0 - \Delta_1 \tag{9}$$

The gap anisotropy is important because the scattering is essentially forward, this is due to the weak screening in two dimensions. The wave vector explores a small region in k-space. The gap is important in the direction of the saddle point, due to its high density of states, and its effect is reinforced by the weak screening. But for the point B $(\pi/2,\pi/2)$ the DOS is smaller and the effect is reduced.

From our theoretical results, we find an effective coupling constant λ_{eff} in agreement with the hypothesis of the BCS weak electron-phonon coupling.

6.2. Results. In Figure 7, we present the result of the iterative calculation.

We thus obtain an "extended s-wave" gap and not a d-wave pair function. The order parameter is never negative in our model. Abrikosov [35] has shown, however, that if a short-range repulsive interaction (which can represent either

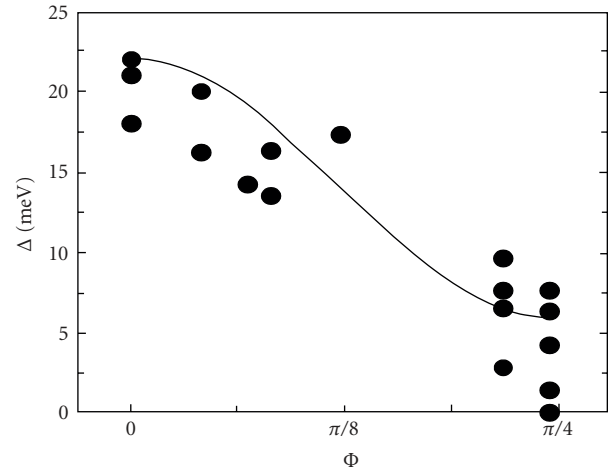

Figure 7: Anisotropic superconducting gap. Exact calculation for $\Phi = 0$ and $\pi/4$. This represents an s-wave anisotropic superconducting gap with no nodes in $\Phi = \pi/4$.

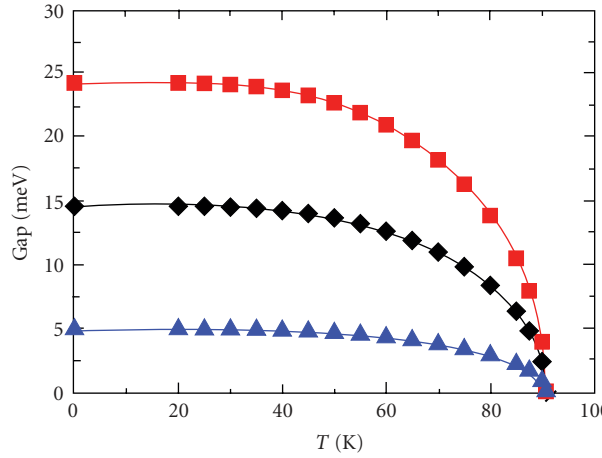

Figure 8: Variation of the various gaps $\Delta_{\max}$, $\Delta_{\min}$, and Δ_{av} versus temperature, at the optimum doping, with the following parameters, $t = 0.2$ eV, $\hbar\omega_o = 60$ meV, $q_0 a = 0.12$, $\lambda_{\text{eff}} = 0.665$, red square symbol = $\Delta_{\max}$, black diamond symbol = Δ_{av}, blue up triangle symbol = $\Delta_{\min}$.

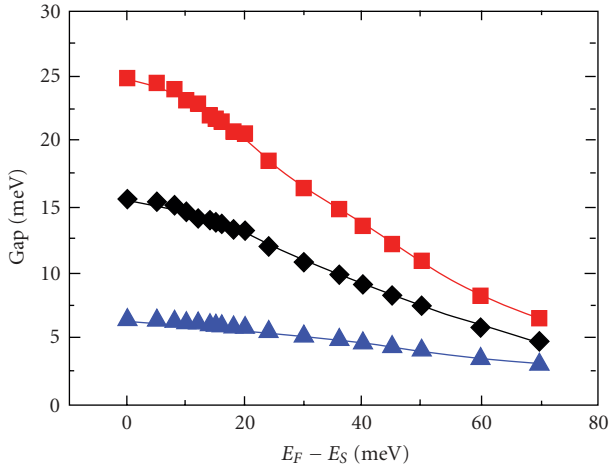

FIGURE 9: Variation of the various gaps Δ_{max}, Δ_{min}, Δ_{av} versus the doping linked to E_F-E_S at $T = 0$ K red square symbol = Δ_{max}, black diamond symbol = Δ_{av}, blue up triangle symbol = Δ_{min}.

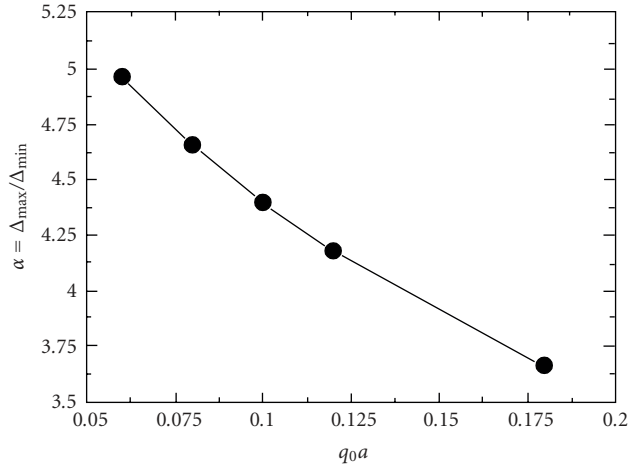

FIGURE 10: The anisotropy ratio $\alpha = \Delta_{max}/\Delta_{min}$ versus the screening parameter q_0a.

some part of the Hubbard repulsion at the copper sites or the interaction mediated by spin fluctuations) is added, then the order parameter can vary in sign and become negative at points of the Fermi surface distant from the singularity. Such an approach may reconcile all the observations leading sometimes to s-wave and other times to d-wave symmetry of the order parameter. The fact that the order parameter is negative in certain regions of the Fermi surface explains the results of experiments showing a π phase shift of the order parameter [36].

In Figure 8, we present the variation of the various gaps Δ_{max}, Δ_{min}, and Δ_{av} (or Δ_0) with temperature at optimum doping, that is, for a density of holes of the order of 0.20 per CuO_2 plane. 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:

$$\frac{2\Delta_{max}}{k_BT_C} = 6, \qquad \frac{2\Delta_{av}}{k_BT_C} = 3.7, \qquad \frac{2\Delta_{min}}{k_BT_C} = 1.4. \tag{10}$$

This may explain the various values of $2\Delta/k_BT_C$ observed in various experiments. The critical temperature found is $T_C = 90.75$ K as for HTSC cuprates as $Bi_2Sr_2CaCu_2O_8$ (Bi 2212), $YBa_2Cu_3O_{7-\delta}$ (Y123).

In Figure 9, we present the same results, Δ_{max}, Δ_{min}, Δ_{av} as a function of E_F-E_S linked to the variation of doping.

6.3. Effect of the Screening on the Gap Anisotropy and T_C. We stress the importance of q_0a, the screening parameter, in the value of T_C, and the anisotropy ratio $\alpha = \Delta_{max}/\Delta_{min}$. We give the results of our study, in the approximation of weak screening ($q_0a < 0.2$). The results are presented in Figure 10. We see that increasing q_0a, or, in other word, going towards more metallic system or 3D, the anisotropy of the gap decreases. For T_C, the results are presented in Figure 11. The effect of increasing the screening strength is to decrease T_C. An increase of the screening can be due to the proximity of E_F to E_S, where the DOS is high, and in the other side T_C is increased by the high DOS. There is a competition of the two

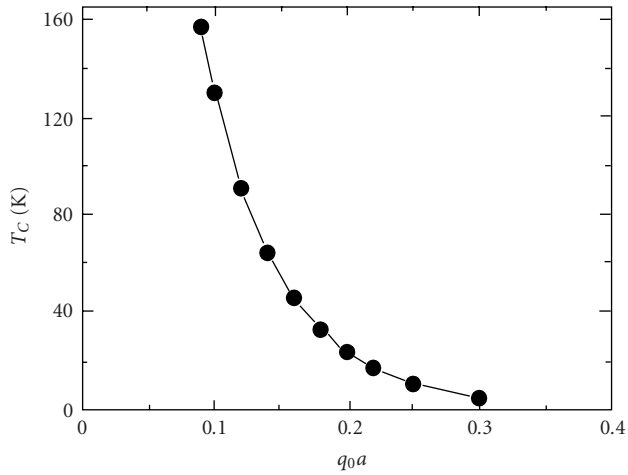

FIGURE 11: T_C versus the screening parameter q_0a, Details calculations are done in [37].

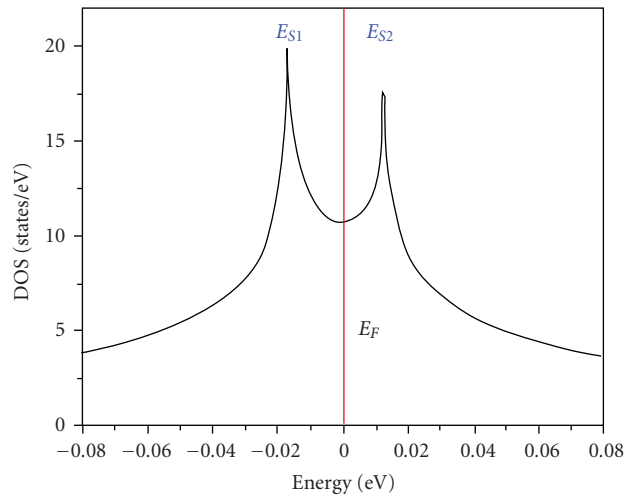

FIGURE 12: Density of States (DOS) in the orthorhombic phase.

effects to obtain the maximum T_C. It is why we have to take into account these two effects and why the experimental T_C is not maximum when $E_F = E_S$ [37].

We show that the effect of increasing $q_0 a$ is to transform the system in a metallic and more isotropic one.

7. Evidence of Lattice Involvement

Labbé and Friedel [38–40] gave an explanation for the martensitic phase transformation from the cubic to the tetragonal structure observed at low temperature in the A15 compounds of formula V_3X (X = Si, Ga, Ge, ...) or Nb_3Sn. This change of structure occurs at a temperature T_m greater than T_C. The Vanadium (V) atoms form a linear chain and an almost one-dimensional approximation can be used for the d electrons. In these conditions a VHs appears at the bottom of the band and can explain high-T_C [3, 41–43]. The electronic energy is reduced when the lattice is deformed and leads to a band type Jahn-Teller effect. This effect can explain the observed cubic to tetragonal transition at low temperature. This effect does not change very much T_C in these A15 compounds, because the role of the high DOS due to the VHs is important only for small doping (low concentration of d electrons).

The situation is more favorable in the cuprates, which are almost bidimensional and where the VHs lies near the middle of the band. Far or near T_C, lattice deformations tetragonal to orthorhombic phase transformations, deformation of the orthorhombic phase, even martensitic phase transformations, have been observed in the cuprates in function of temperature, doping, substitution, or under strained [11, 44–48]. This leads to a competition between electronic and elastic energies. Evidence of the role of phonon in the physics of cuprates has been seen experimentally; see, for example, the paper of Graf et al. [49].

When the Fermi level lies close to a VHs, of energy E_S, as it is the case for cuprates near optimum doping, the situation could be unstable and a small distortion increases the distance E_F-E_S and decreases strongly the electronic energy.

We propose a different scenario in most of these 2D compounds. When the lattice in the CuO_2 plane is quadratic, the four saddle points correspond to the same electronic energy E_S and the VHs is fourfold degenerate. Due to the doping, and then to the effect of decreasing the temperature, the lattice becomes orthorhombic (rectangular unit cell). The degeneracy is lifted and we hope to obtain two VHs at different energy E_{S1} and E_{S2} corresponding to the saddle points along k_x and k_y in reciprocal space

$$E_k = -2t(1+\beta)\cos X - 2t\cos Y + 4t'\cos X \cos Y + D_e. \tag{11}$$

Using the twofold degenerate electronic dispersion, see (11), where βt represents the difference in the interaction with the first neigbours in the x and y direction, we calculate the DOS versus energy, represented on Figure 12. In optimal conditions the Fermi level could lie between E_{S1} and E_{S2}. E_F is then between these energy levels of high DOS in a dip, itself of a smaller but sufficiently high DOS, the lattice is stabilized. No more phase transformation could be possible, at lower temperature this situation favors the BCS condensation into a superconducting phase instead of a lattice transformation, leading to high-T_C due to the high DOS.

The goal for experimentalists will be to find the optimal parameters (doping, strain, temperature, etc.) to lead the sample to such situation that it condensates when E_F is pinned in its dip in order to obtain a very high-T_C.

We want to indicate in favour of the electron-lattice interaction that Deutscher and de Gennes [50] proposed a model valid in the underdoped regime based on the idea that if two holes occupy two adjacent copper sites, a contraction of the Cu–O–Cu band occurs. This increases significantly the transfer integral between the Cu and this can lead to the formation of bound hole pairs.

8. Conclusion

Strong correlations are probably the dominant factor in the underdoped region. But in the optimum and overdoped regions, we have shown that the experimental observations may be explained by electron-phonon or electron-lattice interaction coupled with the Van Hove scenario, both in the normal and superconducting states. The existence of VHs close to the Fermi level is now well established experimentally, and this fact must be taken into account in any physical description of the properties of high-T_C superconducting cuprates.

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