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 Berdnoz 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 Berdnoz 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 symmetry 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 most 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.

### 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,
3. (i) the electron-phonon interaction is isotropic and so is the superconducting gap $\Delta$,
4. (ii) the attractive interaction $V_p$ between electrons is nonzero only in an interval of energy $\pm h\omega_0$ around the Fermi level where it is constant. When this attraction is mediated by emission and absorption of phonons, $\omega_0$ is a typical phonon frequency.
In that case, the critical temperature is given by

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

(1a)

where $\lambda$ 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

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

(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. $\lambda$ 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 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

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

(2)

where $t'$ is an integral representing the interaction with s.n.n., where $D_x = E_F - E_S + (4t')$ 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$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ using different substitution of cations with different valences, obtaining different systems, that is

$$\text{Bi}_2\text{Sr}_2\text{Ca}_{1-x}\text{Lu}_x\text{Cu}_2\text{Cu}_8\_{\delta}, \text{Bi}_2\text{Sr}_2\text{Ca}_{1-x}\text{Na}_x\text{Cu}_2\text{Cu}_8\_{\delta},$$

$$\text{Bi}_2\text{Sr}_2\text{Ca}_{1-x}\text{K}_x\text{CaCu}_2\text{Cu}_8\_{\delta}.$$  

(3)

In Figure 3 our model account for the variation of the holes in the CuO$_2$ plane, from an optimum doping, here $\rho \approx 0.20$, 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

$$T_c \equiv \text{To exp} \left[-\frac{1}{\lambda} \mu^*\right].$$  

(4)

with $\mu = NoV_c$ and $\mu^* = \mu/(1 + \mu \ln E_F/\omega_0)$.

Cohen and Anderson [21] assumed that for stability reasons $\mu$ is always greater than $\lambda$. Ginzburg [22] gave arguments that in some special circumstances $\mu$ can be smaller than $\lambda$. Nevertheless if we take $\mu \geq \lambda$, superconductivity only exists because $\mu^*$ 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 $\lambda$ and $\mu$ vary simultaneously and $\mu^*$ 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 $\mu$, 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) $\mu^*$ is reduced compared to $\mu$ 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 $(W, \omega_0)$ 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 $^{18}O$ was substituted to $^{16}O$ 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
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 $\omega_0$. 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 coefficient $\alpha$ defined as $T_C \propto M^{-\alpha} (\alpha = 0.5$ for usual superconductors). Tsuei et al. \[26\], using the VH scenario, have calculated the variation of $\alpha$ 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 $\varepsilon^2$ and the resistivity $\rho$ varies as $T^2$. The marginal Fermi-liquid situation is the case where $1/\tau$ goes as $\varepsilon$ (electronic energy) and $\rho$ 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 $E_C$. This calculation was however contradicted by hlubina and rice \[27\].

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 framework 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 Coefficient. 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 $T$, $R_H \approx 1/p_{\text{ho}} e$, where $p_{\text{ho}}$ 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 $p_{\text{ho}} = 0.10$ to $p_{\text{ho}} = 0.27$).
We can explain [33], following the approach given by Ong [34], these results by using the band structure for carriers in the CuO2 planes. In particular, the existence of hole-like and electron-like constant energy curves, see Figure 1, which give contributions of opposite sign to RT. The transport properties explore a range of energy kBT around the Fermi level, when T is increased more and more carriers are on the electron like orbits, resulting in a decrease of RT. 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 CuO2 planes, an anisotropic superconducting gap is found.

We use the BCS equation for an anisotropic gap

$$\Delta_k = \sum_{k'} \frac{V_{kk'} \Delta_{k'}}{\xi_k^2 + \Delta_{k'}^2},$$

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

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

where g(q) is the electron phonon interaction matrix element for $\vec{q} = \vec{k} - \vec{k}'$ and q0 is the inverse of the screening length. We compute $\Delta_k$ for two values of $\vec{k}$:

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

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

We solve (5) by iteration for these two specific points of the Fermi surface, the saddle point A (π,0) or (1,0) direction, and point B (π/2,π/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 $\Delta_k$ has the same symmetry, so we may use the angle $\Phi$ between the 0 axis and the $\vec{k}$ vector as a variable and expand $\Delta(\Phi)$ in Fourier series:

$$\Delta(\Phi) = \Delta_0 + \Delta_1 \cos(4\Phi + \varphi_1) + \Delta_2 \cos(8\Phi + \varphi_2) + \cdots \quad (8)$$

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

$$\Delta_A = \Delta_{\text{max}} = \Delta_0 + \Delta_1, \quad \Delta_B = \Delta_{\text{min}} = \Delta_0 - \Delta_1 \quad (9)$$

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 $\lambda_{\text{eff}}$ 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 $\Phi = \pi/4.$](image)

![Figure 8: Variation of the various gaps $\Delta_{\text{max}}, \Delta_{\text{min}},$ and $\Delta_{\text{av}}$ versus temperature, at the optimum doping, with the following parameters, $t = 0.2$ eV, $\hbar\omega_o = 60$ meV, $q_{\text{eff}} = 0.12$, $\lambda_{\text{eff}} = 0.665$, red square symbol = $\Delta_{\text{max}}$, blue up triangle symbol = $\Delta_{\text{min}}$, black diamond symbol = $\Delta_{\text{av}}$.](image)
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 $\pi$ phase shift of the order parameter [36].

In Figure 8, we present the variation of the various gaps $\Delta_{\text{max}}, \Delta_{\text{min}}, \Delta_{\text{av}}$, and $\Delta_0$ 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 $\alpha = \Delta_{\text{max}}/\Delta_{\text{min}} = 4.2$ and for the ratios of 2$\Delta/k_BT_C$ the following values:

\[
\frac{2\Delta_{\text{max}}}{k_BT_C} = 6, \quad \frac{2\Delta_{\text{av}}}{k_BT_C} = 3.7, \quad \frac{2\Delta_{\text{min}}}{k_BT_C} = 1.4.
\] (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$_2$Sr$_2$CaCu$_2$O$_8$ (Bi 2212), YBa$_2$Cu$_3$O$_{7-\delta}$ (Y123).

In Figure 9, we present the same results, $\Delta_{\text{max}}, \Delta_{\text{min}}, \Delta_{\text{av}}$ 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 $\alpha = \Delta_{\text{max}}/\Delta_{\text{min}}$. 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 $\alpha = \Delta_{\text{max}}/\Delta_{\text{min}}$ versus the screening parameter $q_0a$.

In Figure 10, we present $T_C$ versus the screening parameter $q_0a$, Details calculations are done in [37].
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 $q_{0a}$ 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 $V_3X$ ($X = \text{Si, Ga, Ge, \ldots}$) or $\text{Nb}_3\text{Sn}$. 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

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

Using the twofold degenerate electronic dispersion, see (11), where $\beta t$ represents the difference in the interaction with the first neighbours 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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### References


