

Properties of the Coherence Length and Van Hove Singularity in High- T_c Superconductors

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Abstract: High- T_c superconductors are characterized by a short coherence length ξ_0 . From the quasi-2D structure of these compounds, we calculate the density of states $n(\epsilon)$, the Fermi velocity v_F and the gap energy $\Delta(0)$. From these parameters, we deduce a formula of the coherence length ξ_0 . We study the effect of the phonon-interaction V_p , the effective mass of carriers m^* and the Coulomb repulsion V_C on the coherence length ξ_0 . We show that when the coupling constant λ_p is in the range 0.06 – 0.30 and the effective mass m^* is between $2m_0$ and $6m_0$ (m_0 is the free electron mass), the values obtained of the coherence length and the gap energy are in a good agreement with experimental results.

Keywords: Superconductivity, Density of states, Coherence length, Fermi velocity, Fermi energy, Gap energy, Van Hove singularity, Phonon-interaction, Effective mass, Coulomb repulsion.

1. INTRODUCTION

The short coherence length is one of the key parameters describing the superconducting state. In the conventional superconductors, the coherence length ξ is about ($\approx 10^3 - 10^4$ Å), but in high- T_c superconductors, ξ is in the range (9 – 40 Å). Experimental results show that short coherence lengths have been obtained for of high- T_c Cu oxide superconductors: 16 Å for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ [1, 2], 13.6 Å for Tl-2223 [3], 9.7 Å for Bi-2223 and 9 ± 1 Å for Bi-2212 [4]. For lanthanum compound $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, if we estimate the coherence length between 20 Å and 40 Å, the ratio ξ/a is about $\approx 5 - 10$ and about 2.5 – 4 for other cuprate superconductors (the lattice parameter is about $a \approx 4$ Å). Several other exotic superconductors have nearly the same ratios $\xi/a \approx 2.5 - 3.5$ [5]. These results are very smaller than the typical ratios ξ/a of 10^3 for the conventional superconductors. In BCS theory, the coherence length can be calculated from the expression $\xi_0 = \hbar v_F / \pi \Delta(0)$ where v_F is the Fermi velocity and $\Delta(0)$ the gap energy which is directly related to the superconducting transition temperature T_c ($2\Delta(0) = Rk_B T_c$).

In conventional superconductors $R_{BCS} = 3.53$, but for the new superconductors, the parameter R increases with the superconducting transition temperature T_c . The coherence length can be also

evaluated from the formula $\xi_0 = \hbar v_F / \pi R T_c$ where $b = 2\hbar / \pi k_B$. From this formula, we can see that the small values of the Fermi velocity v_F , the large value of R and T_c contribute to the decrease in ξ_0 . The coherence length ξ_0 depends strongly on the Fermi velocity, on the superconducting gap ratio R and on T_c . To describe the coherence length, it is important to know the experimental values of $\Delta(0)$ or R and T_c . Experimental results show that high- T_c superconductors have large gap energy $\Delta(0)$ which leads to large superconducting gap ratio $R = 2\Delta(0) / k_B T_c$ [6-13]. These values show that the parameter R increases with the superconducting transition T_c and reaches its maximum $R = 13$ at $T_c = 135$ K for mercury compound Hg-1223. The experimental values of the gap energy of the electron-doped cuprates are summarized in Table 1.

The large value of $\Delta(0)$ or R leads to the decrease in coherence length ξ_0 . In the van Hove scenario, many works, sometimes for isotropic s-wave and other times for d-wave pairing, have been proposed to explain the large value of R [14-20]. In all these works, R is around 3.64 – 3.96 for isotropic s-wave and is in the range 4 – 5 for d-wave pairing. The deviation of R from the BCS value ($R_{BCS} = 3.53$) is still not understood. For this reason, we deduce the expression of the coherence length by using the gap energy $\Delta(0)$ instead of the superconducting gap ratio R .

For the conventional superconductors, the Fermi velocity is large and of order $(1 - 2) 10^8$ cm.s⁻¹, but it is

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Table 1: Experimental Values of the Gap Energy for Different Copper Oxide Based Superconductors

| Compounds | T_c (K) | $\Delta(0)$ (meV) | R | References |
|---|-----------|-------------------|----------------|------------|
| $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ | 33 | 12.5 ± 0.5 | 8.9 ± 0.2 | 6 |
| | 39 | 17.5 ± 1.5 | 10.3 ± 0.9 | 7 |
| $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ | 89 | 39.5 ± 1.5 | 10.6 | 8 |
| $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ | 86 | 41 ± 4 | 11 ± 1.0 | 9 |
| | 92 | 36 ± 2 | 9.0 ± 0.5 | 10 |
| | 91 | 32 ± 3 | 8.1 ± 0.8 | 11 |
| $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+x}$ | 110 | 48 ± 5 | 10 ± 1.0 | 9 |
| | 110 | 43 ± 5 | 9.1 ± 1.0 | 12 |
| $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+x}$ | 92.5 | 43 ± 4 | 10.7 ± 1.0 | 8 |
| | 90 | 37 | 9.5 | |
| $\text{HgBa}_2\text{CuO}_{6+x}$ | 96 | 44 ± 4 | 10.6 ± 1.0 | 8 |
| | 97 | 33 | 7.9 | 13 |
| $\text{HgBa}_2\text{CaCu}_2\text{O}_{8+x}$ | 123 | 50 | 9.5 | 13 |
| $\text{HgBa}_2\text{Ca}_2\text{CuO}_{8+x}$ | 130 | 60 | 10.6 | 8 |
| | 135 | 75 | 13 | 13 |

very small for the cuprates. Using experimental values of R , T_c and ξ_0 in BCS expression, we obtain the Fermi velocity v_F in the range $(1 - 2) 10^7 \text{ cm.s}^{-1}$. For the lanthanum compound $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ with the gap energy $\Delta(0) = 17.5 \text{ meV}$ and the Fermi velocity $v_F = 2 10^7 \text{ cm.s}^{-1}$, we obtain $\xi_0 = 23.977 \text{ \AA}$. Since the lattice parameter a in CuO_2 plane, is about 4 \AA and the experimental values of the gap energy $\Delta(0)$ about $\approx 15 - 19 \text{ meV}$, the ratio ξ/a is in the range $5.52 - 6.99$.

In BCS theory, the Fermi surface is spherical and the density of states has been considered constant. For the new compounds, the Fermi surface is square and the density of states diverges at the singularity. We can see that the short coherence length in these new compounds is essentially due to a small value of the Fermi velocity, although the large value of $\Delta(0)$ or R , contributes to the decrease in the coherence length ξ_0 ($\xi_0 \propto v_F / RT_c$).

These new compounds are doped materials, with superconducting transition temperature T_c depending strongly on the hole concentration x . The critical temperature T_c increases with x and reaches its maximum at optimum doping x_{op} while the coherence length ξ_0 decreases with x and reaches its minimum at x_{op} . All the known high- T_c superconductors have conducting CuO_2 planes separated by insulating layers.

Many experimental results [21-24] have identified the presence of saddle point (SP) in the band structure energy. These saddle points produce a van Hove singularity in the density of states. At optimum doping, when the Fermi level lies to the van Hove singularity, the gap energy $\Delta(0)$ and the superconducting gap ratio R are maximum [20] while the coherence length ξ_0 is minimal. When the van Hove singularity is displaced from the Fermi level, R and T_c decrease while ξ_0 increases. The origin of high- T_c superconductors is still controversial and the role of these singularities in the mechanism of high- T_c superconductivity is not yet established. Near the singularity, the density of states diverges and even weak interaction can produce a large effect on T_c . The van Hove singularity leads to the magnetic excitations [25] which play a fundamental role both in normal and superconducting states [26].

For these new superconductors, there is coexistence between superconductivity and two dimensional antiferromagnetism characterized by a short magnetic correlation length ξ_m decreasing with concentration x . For lanthanum compound $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and bismuth compounds, it has been shown that the superconducting transition temperature $T_c(x)$ and the Neel temperature $T_N(x)$ disappear together when it becomes metallic for higher x value. This suggests that magnetic excitations can give an attractive interaction between two electrons or holes [27]. It is often assumed that there is a straightforward competition between nearly antiferromagnetic models

and VHS model of superconductivity, with one excluding the other [28]. The searchers have serious problems with the two classes of phenomenological theories: the marginal Fermi liquid (MFL) and antiferromagnetic Fermi liquid (AFFL). It has been believed that these two theories have inconsistencies. MFL model could follow from the VHS theory, but only if the Fermi level coincides with the VHS. The antiferromagnetic models seem to describe well the magnetic phase (low doping regime), while the VHS model seems to work well near the optimum doping. There is no universally accepted model of the physics associated with VHS, however this model can explain main electronic properties of these compounds. The VHS model is studied in more details in Ref. 28.

In 1987, Labbé and Bok [29] suggested that a logarithmic singularity in the density of states explain the high T_c and the small isotope effect. With the tight-binding model on a two-dimensional square lattice, Bok [30] has calculated the average of the Fermi velocity and obtained an approximate formula of the coherence length ξ_0 ($\xi_0 \approx aD/\Delta(0)$, where D is the width of singularity and $\Delta(0)$ the gap energy). The coherence length depends on the ratio $\Delta(0)/D$. This ratio is very small in conventional superconductors ($\Delta(0)/\varepsilon_F \approx 10^{-4}$), but large in high- T_c superconductors. It is necessary to calculate this parameter which is not calculated in Ref. 30.

To study the properties of the coherence length of high- T_c superconductors, it is important to know the Fermi velocity v_F and the ratio $\Delta(0)/D$. These parameters are well known for the conventional superconductors.

In this paper, we develop a previous work describing the gap energy [31] to study the coherence length ξ_0 . We calculate the density of states $n(\varepsilon)$, the Fermi velocity and the ratio $\Delta(0)/D$ by using the quasi-free electron model. From these parameters, we deduce a formula of the coherence length ξ_0 . We study the effect of the phonon-interaction V_p , the effective mass of carriers m^* and the Coulomb repulsion V_C on the coherence length ξ_0 . In the weak coupling limit, we obtain short coherence length in a good agreement with experimental results.

2. CALCULATION OF THE DENSITY OF STATES

We know that pure superconductors metal such Al, In, Nb, Pb, Sn, and Zn are very described in the free electron model. For two-dimensional square lattice in this model, the density of states is constant. But for the

new superconductors, the presence of the saddle points leads to the singularity in the density of states. Near the singularity, we consider a two-dimensional electronic spectrum given by [32-34]

$$\varepsilon(\mathbf{k}) = \varepsilon_F(1-\gamma) + \frac{\hbar^2}{2m^*} k_x k_y \quad (1)$$

where ε_F is the Fermi energy and m^* is the effective mass of carriers in CuO_2 plane. The electronic spectrum described by Eq. (1) gives logarithmic singularities in the density of states at $\varepsilon_{\text{VHS}} = \varepsilon_F(1-\gamma)$. The parameter γ allows us to control the position of the VHS with respect to the Fermi level, i.e $\gamma = (\varepsilon_F - \varepsilon_{\text{VHS}})/\varepsilon_F$. The electronic spectrum given by Eq. (1) has been shown to be in a good agreement with angle-resolved photoemission spectra experiments in high- T_c superconductors and can explain main electronic properties of these new compounds [35]. From this equation, we have

$$k_y = \frac{2m^*}{\hbar^2} \frac{[\varepsilon - \varepsilon_F(1-\gamma)]}{k_x} \quad (2)$$

When $k_y = k_x$, we have

$$k_y = k_x = \sqrt{\frac{2m^*}{\hbar^2} [\varepsilon - \varepsilon_F(1-\gamma)]} \quad (3)$$

We calculate the number of states between $\varepsilon_k = 0$ and $\varepsilon_k = \varepsilon$ (see Figure 1)

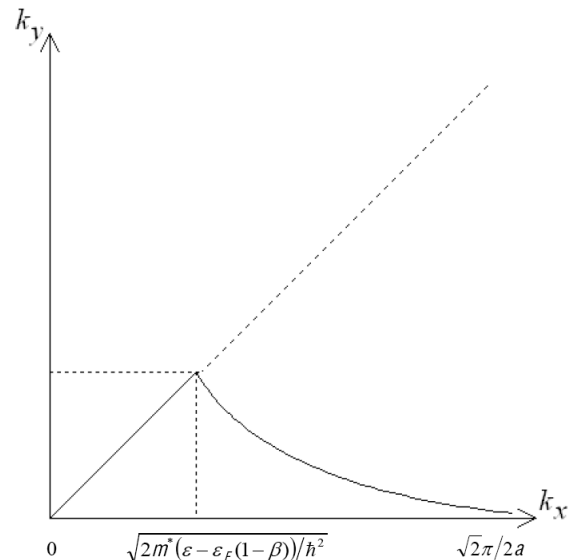


Figure 1: Calculation of the area between the curves 0 and ε (1/8 of Brillouin zone). The curve $\varepsilon_k = \varepsilon$ is the hyperbole given by Eq. (3).

$$N(\varepsilon) = 8 \frac{a^2}{(2\pi)^2} \left[\frac{1}{2} \frac{2m^*}{\hbar^2} [\varepsilon - \varepsilon_F(1-\gamma)] + \int_{\frac{\pi\sqrt{2}}{a}}^{\frac{\pi\sqrt{2}}{a}} \frac{2m^*}{\hbar^2} [\varepsilon - \varepsilon_F(1-\gamma)] \frac{dk_x}{k_x} \right] \quad (4)$$

After calculation, we obtain

$$N(\varepsilon) = \frac{a^2}{\pi^2} \frac{2m^*}{\hbar^2} [\varepsilon - \varepsilon_F(1-\gamma)] \cdot \left[1 + \ln \frac{\pi^2 \hbar^2}{4a^2 2m^* [\varepsilon - \varepsilon_F(1-\gamma)]} \right] \quad (5)$$

After differentiation of this equation, with respect to the energy ε , we obtain the expression of the density of states near the singularity.

$$n_s(\varepsilon) = \frac{dN(\varepsilon)}{d\varepsilon} = \frac{2m^* a^2}{\pi^2 \hbar^2} \ln \frac{\pi^2 \hbar^2}{4m^* a^2 |\varepsilon - \varepsilon_F(1-\gamma)|} \quad (6)$$

Near the band edge, the energy $\varepsilon(\mathbf{k})$ has the form

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m^*} \quad (7)$$

and the density of states is constant in two-dimensional square lattice

$$n_0 = \frac{m^* a^2}{2\pi \hbar^2} \quad (8)$$

The final density of states $n(\varepsilon)$ takes the form

$$n(\varepsilon) = n_s(\varepsilon) + n_0 = \frac{2m^* a^2}{\pi^2 \hbar^2} \ln \frac{\pi^2 \hbar^2}{4m^* a^2 |\varepsilon - \varepsilon_F(1-\gamma)|} + \frac{m^* a^2}{2\pi \hbar^2} \quad (9)$$

In the tight-binding model, the energy dispersion is given by $\varepsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a)$ where t is transfer integral. The Fermi surface is a perfect square and near the singularity, the density of states is $n(\varepsilon) = (1/2D) \ln(D/|\varepsilon|)$ where $D = \pi^2 t$ [36]. Near the band edge the two-dimensional electronic spectrum is developed as $\varepsilon(\mathbf{k}) = t \left((k_x a)^2 + (k_y a)^2 \right)$ which leads to a constant density of states $n_0 = 1/4\pi t$. Another work [37] shows that the density of states $n(\varepsilon)$ derived from a tight-binding model on a two dimensional square lattice contain a logarithmic term plus a constant one $n(\varepsilon) = n_1 \ln(D/|\varepsilon|) + n_0$, where $n_1 = 1/2\pi^2 t$, $D = 4t$ and $n_0 = (1/2\pi^2 t) \ln 4$. If we take into account, the

second neighbor interaction t' , the singularity is displaced towards lower energy and it occurs for $\varepsilon = -4t'$. In this work, the authors have shown that the additional constant term in $n(\varepsilon)$ enhances the isotope coefficient α . We can write the general density of states as the form

$$n(\varepsilon) = n_1 \ln \frac{D}{|\varepsilon - \varepsilon_F(1-\gamma)|} + n_0 \quad (10)$$

where $n_1 = 1/2D$ and $D = \pi^2 \hbar^2 / 4m^* a^2$. For $\gamma = 0$, the Fermi level coincides with the singularity. When the parameter γ increases from 0 to 0.9, the singularity is shifted to lower energy. With this form of the density of states ($\gamma = 0$), we have established analytical expressions of the superconducting gap ratio R [38], the critical temperature T_c and the isotope coefficient α [39, 40]. These expressions do not provide any upper limit. These equations are applicable to low as well as high temperature superconductors.

For a half-filling system, the Fermi level is just on the singularity $\varepsilon_F = \varepsilon_{\text{VHS}}$. We know for half filling the high- T_c superconductors are antiferromagnetic insulators. The Fermi level is at the VHS for a doping level corresponding to 20 % of holes in each CuO_2 plane or 40 % filling of the Brillouin zone (BZ) [41]. This can be achieved by taking into account the interaction between second nearest neighbors and the effect of the orthorhombic distortion [42]. The introduction of this orthorhombic distortion increases the value of the superconducting gap ratio R , and with decreasing second neighbor hopping, R decreases [43]. The variation of R suggests that the Fermi level is shifted from the singularity. We shall mention that this model for the density of states of a two-dimensional system is unstable at half-filling in view of nesting effect [44]. We believe that instability is due to the magnetic excitations or thermodynamic fluctuations. The role of the singularity in the mechanism of high- T_c superconductivity and the stability of the system are not yet established but we want to stress that this model has already explained a certain number of experimental facts, *i.e* high T_c [14, 29, 39, 40, 45], small isotope effect [37, 39, 40, 45], linear resistivity and thermo power [33], and thermal conductivity [34]. We focus on the role of the van Hove singularity that will be present in stable situations.

3. EXPRESSION OF THE FERMI VELOCITY

The width of singularity has been chosen equal to the Fermi energy $D = \varepsilon_F$ [14, 17, 18, 20, 45]. From Eq. 9, we have.

$$\varepsilon_F = D = \frac{\pi^2 \hbar^2}{4m^* a^2}. \quad (11)$$

The Fermi velocity is calculated from the simple expression

$$\varepsilon_F = \frac{1}{2} m^* v_F^2. \quad (12)$$

From these two expressions, we have the simple form of the Fermi velocity v_F

$$v_F = \frac{\pi \hbar}{\sqrt{2m^* a}}. \quad (13)$$

The Fermi velocity decreases with the effective mass m^* . From Eq. 13, the Fermi velocity v_F is in the range $(1.072 - 3.218)10^7 \text{ cm.s}^{-1}$ when m^* is between $2m_0$ and $6m_0$ (m_0 is the free electron mass). The small value of v_F leads to small value of coherence length. For lanthanum compounds $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, ξ_0 is estimated between 20 Å and 40 Å. With experimental values of the superconducting gap ratio R and the superconducting transition temperature T_c and BCS formula of the coherence length ξ_0 , we obtain the Fermi velocity v_F in the range $(1 - 1.859) 10^7 \text{ cm.s}^{-1}$. With Eq. (13), we obtain the same values when the effective mass m^* is large. The Fermi velocity varies from zero to its maximum given by Eq (13).

The average of the Fermi velocity $\langle v_F \rangle$ and the coherence length ξ_0 deduced from $\langle v_F \rangle$ are studied in details in a previous work [46]. In the following section, we calculate the coherence length from the expression giving the maximum of the Fermi velocity.

4. EXPRESSION OF THE COHERENCE LENGTH

In the BCS theory, the coherence length is given by [47]

$$\xi_0 = \frac{\hbar V_F}{\pi \Delta(0)}. \quad (14)$$

Introducing Eqs. (11) and (13) in Eq. (14), we obtain the following expression of ξ_0

$$\xi_0 = \frac{\sqrt{2}}{\pi^2} \frac{2D}{\Delta(0)} a \quad (15)$$

This formula shows that the coherence length

depends on the ratio $\Delta(0)/D = \Delta(0)/\varepsilon_F$. The coherence length decreases when the ratio $\Delta(0)/D$ increases. This ratio estimates what fraction of the carriers which are directly involved in the pairing. A large gap energy and small value of the width of singularity ($D = \varepsilon_F$) contribute to the large value of this ratio. The coherence length decreases from 36 Å to 9 Å when the parameter $\Delta(0)/\varepsilon_F$ varies from 0.03 to 0.12. In conventional superconductors this ratio is very small ($\Delta(0)/\varepsilon_F \approx 10^{-4}$). The possibility of having a large value of $\Delta(0)/\varepsilon_F$ and short coherence length is related to the quasi-2D structure of the high- T_c superconductors [48, 49]. The large value of this parameter describes other properties such a scale of the critical region near T_c . In addition, we mention that the parameter $(\Delta(0)/\varepsilon_F)^2$ describes the shift in the dielectric function due to superconducting transition. This shift is negligibly small in conventional superconductors, but it is noticeable in high- T_c oxide superconductors [49].

To calculate this parameter, we start with the BCS expression giving the gap $\Delta(T)$ at temperature T

$$\Delta_k(T) = -\frac{1}{2} \sum_{k'} V_{k,k'} \frac{\Delta_k(T)}{\sqrt{\varepsilon_{k'}^2 + \Delta_k^2(T)}} \tanh\left(\frac{\sqrt{\varepsilon_{k'}^2 + \Delta_k^2(T)}}{2k_B T}\right). \quad (16)$$

At $T = 0$, the interaction is uniquely related to the phonon V_p which is constant in the range $2\hbar\omega_D$ centered about the Fermi level ε_F and the Eq. (16) is written as

$$1 = -\frac{1}{2} \sum_k \frac{V_p}{\sqrt{\varepsilon_k^2 + \Delta^2(0)}}. \quad (17)$$

After replacing the sum by integral, we have

$$\frac{2}{V_p} = \int_{\varepsilon_F - \hbar\omega_D}^{\varepsilon_F + \hbar\omega_D} \frac{n(\varepsilon) d\varepsilon}{\sqrt{(\varepsilon - \varepsilon_F)^2 + \Delta^2(0)}}. \quad (18)$$

Introducing Eq. (10) in Eq. (18), we obtain

$$\frac{1}{n_1 V_p} = \int_0^{\varepsilon_F + \hbar\omega_D} \frac{d\varepsilon}{\sqrt{(\varepsilon - \varepsilon_F)^2 + \Delta^2(0)}} \ln \frac{D}{\varepsilon - \varepsilon_F} + \frac{n_0}{n_1} \int_0^{\varepsilon_F + \hbar\omega_D} \frac{d\varepsilon}{\sqrt{(\varepsilon - \varepsilon_F)^2 + \Delta^2(0)}}. \quad (19)$$

Analytical calculation gives the following expression of the gap energy [29]

$$\Delta(0) = 2D \exp \left\{ \frac{n_0}{n_1} - \left[\frac{2}{n_1 V_p} + \left(\frac{n_0}{n_1} + \ln \frac{D}{\hbar \omega_D} \right)^2 - b \right]^{1/2} \right\} \quad (20)$$

where $b = \pi^2 / 6 = 1.6449$. When there is no singularity $n_1 = 0$ and $D = \hbar \omega_D$, we have the BCS formula: $\Delta(0) = 2\hbar \omega_D \exp(-1/n_0 V_p)$. When $n_0 = 0$ and $D = \varepsilon_F = k_B T_F$ where T_F is the Fermi temperature, we obtain the expression derived by Getino *et al*:

$$\Delta(0) = 2k_B T_F \exp \left(- \left[\left(2/n_1 V_p \right) + \left(\ln(T_F / \theta_D) \right)^2 - 1.64 \right]^{1/2} \right) \quad [14].$$

Equation (20) is applicable to low as well as high temperature superconductors. Numerical calculation shows that the gap energy $\Delta(0)$ increases when the effective mass increases. When the effective mass varies from $m^* = 2m_0$ to $m^* = 6m_0$, the gap energy increases from 4.763 meV to 17.874 meV for $\hbar \omega_D = 0.025$ eV, and from 9.546 meV to 39.80 meV for $\hbar \omega_D = 0.085$ eV. When the effective mass increases, the Fermi velocity V_F decreases while the gap energy increases. From this expression, we obtain for the parameter $\Delta(0) / D = \Delta(0) / \varepsilon_F$, the following expression

$$\frac{\Delta(0)}{D} = 2 \exp \left\{ \frac{n_0}{n_1} - \left[\frac{2}{n_1 V_p} + \left(\frac{n_0}{n_1} + \ln \frac{D}{\hbar \omega_D} \right)^2 - b \right]^{1/2} \right\} \quad (21)$$

In the weak coupling limit and the Debye energy $\hbar \omega_D$ is in the range 0.035 – 0.075 eV, the ratio $\Delta(0) / \varepsilon_F$ is in the range 0.01–0.30. In conventional superconductors, this ratio is very small ($\Delta(0) / \varepsilon_F \approx 10^{-4}$).

Introducing Eq. (21) in Eq. (15), we obtain the following expression of the coherence length

$$\xi_0 = \frac{a \sqrt{2}}{\pi^2 \theta^{n_0/n_1}} \exp \left[\frac{2}{n_1 V_p} + \left(\frac{n_0}{n_1} + \ln \frac{D}{\hbar \omega_D} \right)^2 - b \right]^{1/2} \quad (22)$$

The coherence length depends on the ratio n_0 / n_1 , on the phonon-interaction V_p , on the width of singularity D and on the Debye energy $\hbar \omega_D$. This expression shows that the ratio n_0 / n_1 contributes to the decrease in coherence length ξ_0 .

Figures (2) and (3) show that the coherence length ξ_0 decreases, when the effective mass m^* increases.

When m^* increases from $3m_0$ to $6m_0$ and V_p is in the range 0.10 – 0.14 eV, the coherence length ξ_0 decreases from 20 Å to 8 Å (Figure 3). When m^* varies from $3m_0$ to $6m_0$ and when the Debye energy is in the range 0.035 – 0.085 eV, the ratio ξ_0 / a decreases from 7 to 2 (Figure 3). In this case, the coherence length ξ_0 decreases from 28 Å to 8 Å.

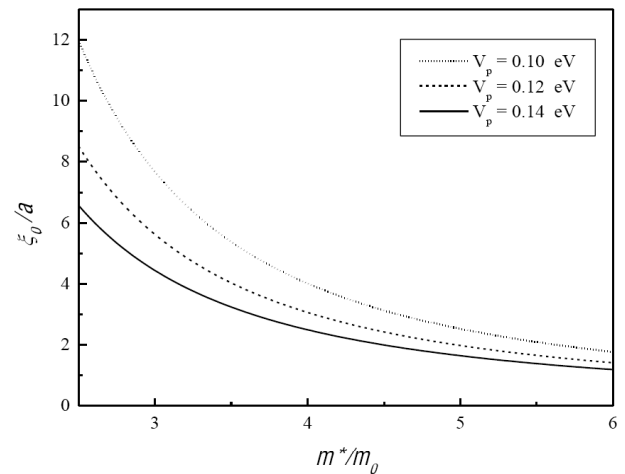


Figure 2: Variation of the coherence length ξ_0 with the effective mass m^* of carriers for different values of the phonon interaction V_p ($n_0 / n_1 = \pi / 4$ and $\hbar \omega_D = 0.065$ eV).

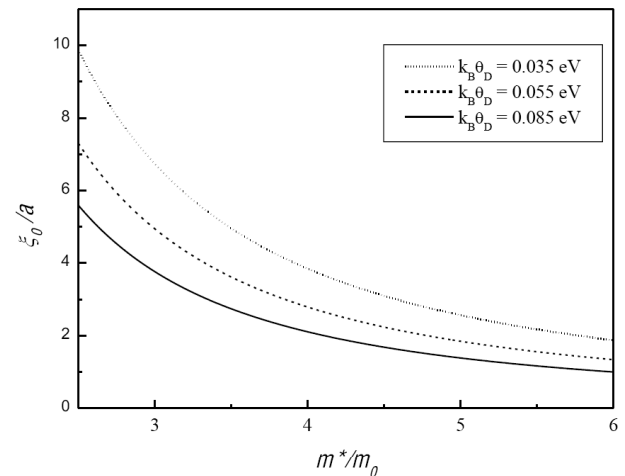


Figure 3: Variation of the coherence length ξ_0 with the effective mass of carriers m^* for different values of the Debye energy ($n_0 / n_1 = \pi / 4$ and $V_p = 0.14$ eV).

In Figure 4, we plot the ratio ξ_0 / a versus the phonon interaction V_p for different values of the Debye energy with effective mass $m^* = 2m_0$. This figure shows that the coherence length decreases with the

phonon-interaction V_p . When this interaction varies from 0.16 eV to 0.5 eV and when the Debye energy is in the range 0.035 – 0.085 eV, the ratio ξ_0/a decreases from 13.5 to 2. In this case, the coherence length ξ_0 decreases from 54 Å to 8 Å. We can see that the short coherence length in high- T_c oxide superconductors is mainly due to the large effective mass m^* . We can see also, even increase in V_p contributes to the decrease in ξ_0 .

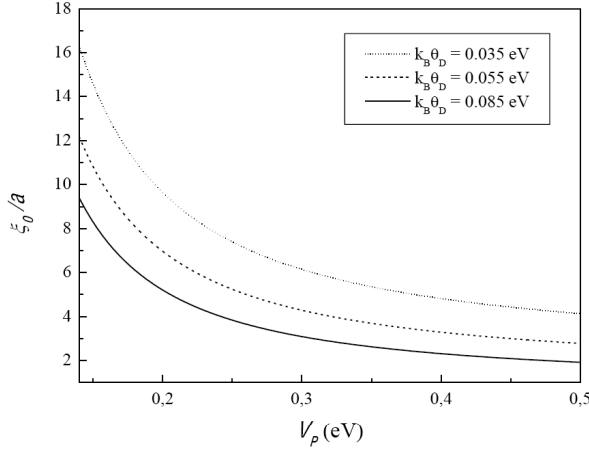


Figure 4: Variation of the coherence length ξ_0 with the phonon interaction V_p for different values of the Debye energy ($n_0/n_1 = \pi/4$ and $m^* = 2m_0$).

In Table 2, we calculate the coupling constant $\lambda_p = n_1 V_p$ and the gap energy $\Delta(0)$ from experimental results of the coherence length ξ_0 by using Eqs. (20) and (22). For yttrium compound $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, when the Debye energy $\hbar\omega_D$ is in the range 0.035 – 0.075 eV, we find the coupling constant λ_p between 0.09 and 0.17 and the gap energy $\Delta(0) = 33.80$ meV. The experimental results show that the maximum gap is between 23 meV and 40.5 meV [8, 50, 51]. For bismuth compounds, when the Debye energy is the range 0.055 – 0.075 eV, we find the constant coupling λ_p between 0.19 and 0.25 and $\Delta(0) = 38.77$ meV, $\Delta(0) = 35.99$ meV for Bi-2212 and Bi-2223, respectively. These results are in a good agreement with experimental results which show that the maximum gap is between 29 meV and 45 meV for Bi-2212 compound [9 - 11] and between 38 meV and 53 meV for Bi-2223 compound [9, 12].

In Table 3, we calculate the coupling constant λ_p and the coherence length ξ_0 from the experimental

results of the gap energy $\Delta(0)$. For lanthanum compound $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+x}$, when the Debye energy is in the range 0.045 – 0.075 eV, we find λ_p between 0.06 and 0.08 and the coherence $\xi_0 = 31$ Å. When the Debye energy $\hbar\omega_D$ is in the range 0.065 – 0.085 eV, we find the coupling constant λ_p between 0.214 and 0.245 and the coherence length $\xi_0 = 10$ Å for thallium compound $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+x}$. In this case, we find the coupling constant in the range 0.17 – 0.25 and the coherence lengths $\xi_0 = 14$ Å and $\xi_0 = 10.68$ Å for the mercury compound $\text{HgBa}_2\text{CuO}_{4+x}$ (Hg-1201, $T_c = 96 - 97$ K). These values of the coherence length correspond to the experimental values of the gap energy $\Delta(0) = 33$ meV [13] and $\Delta(0) = 44$ meV [8] respectively. For the mercury compound Hg-1212, we obtain the coupling constant in the range 0.24 – 0.28 and the coherence length $\xi_0 = 9.50$ Å corresponding to the experimental value of the gap energy $\Delta(0) = 55$ meV [13].

When the coupling constant is in the range 0.06 – 0.30 and the Debye energy in the range 0.025 – 0.085 eV, we obtain simultaneously the experimental values of the gap energy $\Delta(0)$ and the coherence length ξ_0 . In the following section, we take into account the Coulomb repulsion V_C and study its effect on the coherence length.

5. EFFECT OF THE COULOMB REPULSION

The Coulomb repulsion V_C plays a fundamental role in superconductivity. This interaction has a strong effect on the gap energy $\Delta(0)$ but does not suppress the superconductivity. The Coulomb interaction reduces the gap energy $\Delta(0)$ which leads to the increase in coherence length ξ_0 . The expression of the gap energy deduced from Force-Bok formula through the relation $2\Delta(0) = Rk_B T_c$, is given by [52]

$$\Delta(0) = R \frac{D}{2} \exp \left[\frac{n_0}{n_1} + 0.819 - \sqrt{F} \right] \quad (23)$$

where

$$F = \left[\left(\frac{2}{n_1 V_p - n_1 V_C^*} \right) + \left(\frac{n_0 + 0.819}{n_1} \right)^2 + \left(\ln \frac{D}{\hbar\omega_D} \right)^2 - 2 \times 0.99 - 2 \frac{n_0}{n_1} \ln \frac{2.28 \hbar\omega_D}{D} \right]^{\frac{1}{2}} \quad (24)$$

and

Table 2: Theoretical Values of the Coupling Constant $\lambda_p = n_1 V_p$ and the Gap Energy $\Delta(0)$ Obtained from Experimental Values of the Coherences Length ξ_0 of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ and TI-2223 ($D = 0.5 \text{ eV}$, $n_0/n_1 = 4$) and of Bismuth Compounds ($D = 0.3225 \text{ eV}$, $n_0/n_1 = \pi$).

| Compounds | ξ_{exp} (Å) | $\lambda_p = n_1 V_p$ Eq. 22 | $\hbar\omega_D$ (eV) | Δ_{the} (meV) Eq. 20 | Δ_{exp} (meV) |
|---|------------------------|----------------------------------|-------------------------|---------------------------------------|-----------------------------|
| $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ $T_c = 89 \text{ (K)}$ | 16 Refs. 1 and 2 | 0.16886 0.11315 0.093393 | 0.035 0.055 0.075 | 33.80 | 23 – 40 Refs. 8 and 48 |
| TI-2223 $T_c = 125 \text{ K}$ | 13.6 Ref. 3 | 0.211111 0.130811 0.10495 | 0.035 0.055 0.075 | 39.789 | |
| Bi-2223 $T_c = 110 \text{ K}$ | 9.7 Ref. 4 | 0.232613 0.212352 0.198258 | 0.055 0.065 0.075 | 35.99 | 43 ± 5 Ref. 10 |
| Bi-2212 $T_c = 92 \text{ K}$ | 9 ± 1 Ref. 4 | 0.248468 0.225345 0.209709 | 0.055 0.065 0.075 | 38.77 | 36 ± 2 Ref. 9 |

$$V_C^* = \frac{V_c}{1 + \mu \left[\frac{1}{2} \left(\ln \frac{D}{\hbar\omega_D} \right)^2 + \frac{n_0}{n_1} \ln \frac{D}{\hbar\omega_D} \right]} \quad (25)$$

where $\mu = n_1 V_C$. With $R_{\text{BCS}} = 3.53$, we can write the expression of the gap energy as the form

$$\Delta(0) = 2 D \exp \left\{ \frac{n_0}{n_1} - \left[\frac{2}{n_1 V_p - n_1 V_C^*} + \left(\frac{n_0}{n_1} + \ln \frac{D}{\hbar\omega_D} \right)^2 - c \right]^{\frac{1}{2}} \right\} \quad (26)$$

where $c = 1.32$. We remark that this expression is obtained by replacing $\lambda_p = n_1 V_p$ by $\lambda_p - \mu^* = n_1 V_p - n_1 V_C^*$ in our expression (Eq. 20).

The expression of the coherence length is written as

$$\xi_0 = \frac{a\sqrt{2}}{\pi^2 e^{n_0/n_1}} \exp \left[\frac{2}{\lambda_p - \mu^*} + \left(\frac{n_0}{n_1} + \ln \frac{D}{\hbar\omega_D} \right)^2 - b \right]^{\frac{1}{2}} \quad (27)$$

where $\mu^* = n_1 V_C^*$. We have made some numerical calculation using Eqs. (26) and (27) with $D = 0.3225$

eV, $\hbar\omega_D = 0.065 \text{ eV}$ and $n_1/n_0 = \pi/4$.

Figure (5) shows that, the gap energy $\Delta(0)$ decreases with the parameter μ . For example, when the parameter μ varies from 0.08 to 0.3, the gap energy $\Delta(0)$ decreases from 36.25 meV to 12.61 meV for $\lambda_p = 0.28$, and from 44.59 meV to 21.79 meV for

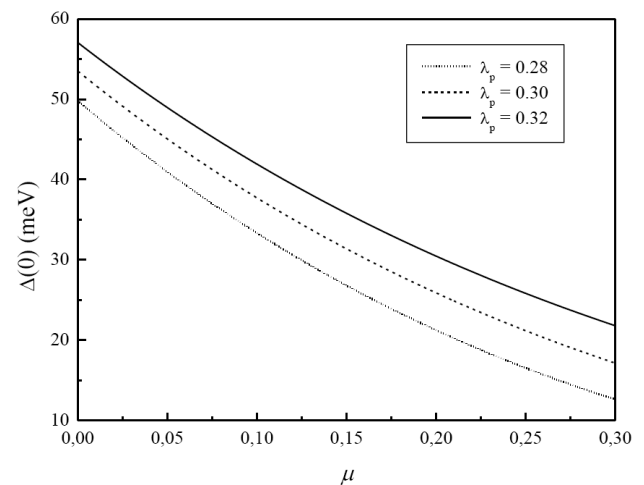


Figure 5: Variation of the gap energy $\Delta(0)$ with the parameter $\mu = n_1 V_p$ for different values of the coupling constant λ_p ($D = 0.3225 \text{ eV}$, $n_0/n_1 = \pi/4$ and $\hbar\omega_D = 0.065 \text{ eV}$).

Table 3: Theoretical Values of the Coupling Constant $\lambda_p = n_1 V_p$ and the Coherence Length ξ_0 Obtained from Experimental Values of the Gap Energy of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ($D = 0.5$ eV, $n_0/n_1 = 4$, $n_0/n_1 = 4$), for Thallium Compound TI-2201 and Mercury Compounds Hg-1201, Hg-1212 ($D = 0.3225$ eV, $n_0/n_1 = 4$).

| Compounds | ξ_0 (Å) Eq. 22 | $\lambda_p = n_1 V_p$ Eq. 20 | $\hbar\omega_D$ (eV) | $\Delta_{\text{exp}}(0)$ (meV) |
|---|-------------------------|---------------------------------|-------------------------|--------------------------------|
| $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ $T_c = 38 - 39$ K | 31.11 31.05 31.00 | 0.0835 0.0669 0.0606 | 0.045 0.065 0.085 | 17.5 Ref. 6 |
| $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+x}$ (TI-2201) $T_c = 92.5$ K | 11.10 10.91 10.76 | 0.2456 0.2273 0.2138 | 0.065 0.075 0.085 | 43 Ref. 9 |
| $\text{HgBa}_2\text{CuO}_{4+x}$ (Hg-1201) $T_c = 96 - 97$ K | 14.18 13.95 13.76 | 0.1988 0.1865 0.1775 | 0.065 0.075 0.085 | 33 Ref. 11 |
| $\text{HgBa}_2\text{CuO}_{4+x}$ (Hg-1201) $T_c = 96 - 97$ K | 10.88 10.68 10.52 | 0.2504 0.2315 0.2177 | 0.065 0.075 0.085 | 44±4 Ref. 9 |
| $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+x}$ (Hg-1212) $T_c = 123$ K | 9.67 9.51 9.36 | 0.2814 0.2573 0.2405 | 0.065 0.075 0.085 | 50 Ref. 11 |

$\lambda_p = 0.32$. On the other hand, the ratio ξ_0/a increases with the parameter μ . When this parameter μ varies from 0.08 to 0.3, the ratio ξ_0/a increases from 2.55 to 7.33 for $\lambda_p = 0.28$, and from 2 to 4.24 for $\lambda_p = 0.32$. In this case, the coherence length ξ_0 increases from 8 Å to 29.32 Å (Figure 6).

If we choose $n_1 = 0.1$ states/eV, the Coulomb repulsion V_C is in the range 0.8 – 3 eV. The gap energy increases with the phonon-interaction V_p and decreases with the Coulomb repulsion V_C while the coherence length decreases with V_p and increases with V_C . With these values of the phonon-interaction V_p and electron-electron interaction V_C , we obtain simultaneously the experimental values of the gap energy and the coherence length.

6. CONCLUSION

In this approach, we have presented a formula of the density of states. The more realistic model contains

a logarithmic term $(1/2D)\ln(D/\varepsilon)$ plus a constant one n_0 . This form of the density of states has been also obtained from tight-binding model [37]. From this form of the density of states, we have calculated the Fermi velocity v_F and the gap energy $\Delta(0)$. With the expressions of v_F and $\Delta(0)$, we have deduced a formula of the coherence length ξ_0 by using the BCS theory. In this formula, the coherence length decreases with the phonon-interaction V_p and the effective mass of carriers m^* . Within the BCS theory, the singular logarithmic density of states can explain simultaneously the large gap energy and the short coherence length. In order to have the experimental values of the gap energy $\Delta(0)$ and the coherence length ξ_0 , the constant coupling λ_p is in the range 0.06 – 0.30 and the effective mass tends to be large ($2m_0 - 6m_0$). Our numerical calculation shows that the Fermi velocity v_F is in the range $(1 - 2) \cdot 10^7 \text{cm.s}^{-1}$. The electron-phonon interaction V_p plays a fundamental role in high- T_c superconductors as well as the classical superconductors. In the weak coupling, our theoretical values of the coherence length are in a good

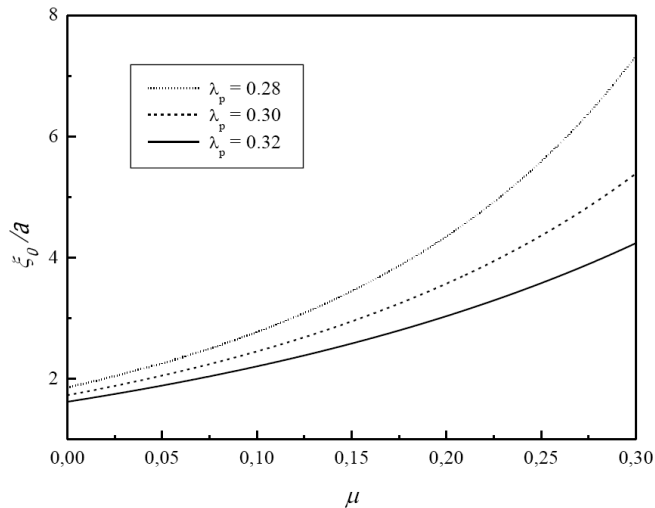


Figure 6: Variation of the coherence length ξ_0 with the parameter $\mu = n_1 V_p$ for different values of the coupling constant λ_p ($D = 0.3225$ eV, $n_0/n_1 = \pi/4$ and $\hbar\omega_D = 0.065$ eV).

agreement with experimental results, a much better agreement could have obtained by fitting the model parameters.

We mention that the superconducting gap ratio both in d-wave pairing and in strong coupling, is still smaller than experimental results, but it is interesting to develop this work in d-wave pair function and in strong coupling and compare with our results.

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