Anisotropy of the gap energy in high T_C Copper Oxides

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Within the frame work of BCS phonon-mediated pairing with a logarithmic (2D) Van Hove Singularity in the density of states, we study the anisotropy of superconductors gap taking into account the anisotropy of attractive coupling and the coulomb repulsion .The results show that gap is more disperse and can explain some observed experimental data.

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I. INTRODUCTION

The discovery of High -Temperature superconductivity in Copper oxides presents a serious challenge to the conventional BCS model. Experimental evidence of a very small isotope effect [1] and the absence of saturation in normal state resistivity [2], observed in $YBa_2Cu_3O_{7-X}$, as well as other Cu oxides indicate that the electron-phonon coupling is very weak so that its contribution to T_C is much smaller. Since the origin of cuprate superconductivity is found in the CuO_2 planes, which are weakly coupled together along the perpendicular axis, their electronic structure will be quasi-two dimensional (2D). This necessarily leads at least to one Van-Hove Singularity **(**VHS) coinciding with a saddle point in the ε (k) surface. These saddle points being present in all 2D-band structure. To resolve this contradiction between High T_C and weak coupling V.H.S in density of state N (ε) near the Fermi energy was proposed as a T_C enhancement mechanism within the fram work of the phonon -mediated pairing [3-4]. Many experiments of angle resolve photoemission spectroscopy (ARPES) have confirmed the existence of saddle points (V.H.S) at the Fermi level in different Copper oxides compounds by different groups [5-7]. The origin of a 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 the model of 2 D electrons with the presence of V.H.S in the band structure has already explained certain number of experimental facts; i .e. high T_C, Anomalous isotope effect [4,8], very small values of the coherence length [9] and the properties of the gap energy $\Delta(T)$ [10,11]. It is clear that models are not able to explain the strong gap anisotropy and the ratio $\eta = 2\Delta(T=0)/ K_B T_C$ which is much larger than the usual BCS value (3.52) .A large value, as it was experimentally observed could be explained by a large anisotropy of attractive coupling constant $V_{kk'}$, adding the repulsion part of the electron-electron interaction. This last repulsion is known to be essential to explain other properties of such systems, as for instance the existence of antiferromagnetic phase [12].

The purpose of this paper is to study the anisotropy of the superconductors gap within a VHS scenario taking into account the anisotropy of attractive coupling and the coulomb repulsion.

II. ANISOTROPY BCS GAP EQUATION IN VHS SCENARIO

The simplest band structure that we can take for square CuO_2 lattice of two dimensions is:

$$\varepsilon(k) = -2t(\cos(k_X a) + \cos(k_X a)) + 4t'\cos(k_X a)\cos(k_X a) \quad (1)$$

Where t and t' are the transfers integrals between nearest neighbour and the second nearest neighbour respectively, k_X and k_Y the components of the wave vector. This gives a square Fermi surface and the V.H.S corresponding in this approximation to half filling. Also this leads to the logarithmic density of state near a saddle point that we take as [9]**:**

$$N(\varepsilon) = \begin{cases} n_0 + n_1 \log \dfrac{D}{|\varepsilon - \varepsilon_S|} & \text{for } \varepsilon \in]-D, D[\\ n_0 & \text{for } \varepsilon \in]-w/2, -D[\cup]D, w/2[\end{cases} \quad (2)$$

Where D is the width of the V.H.S $D = 16t\sqrt{1-r^2}$ with $r = t'/t$ and $n_1 = N/\pi^2 D$ where N is the total number of carrier charge, $n_1$and n_0 are related by the following relation: $(n_0 / n_1 = 2(\pi^2 - 1))$ D/W. Where W is the band width.
The BCS equation giving the gap is:

$$\Delta_k = -\frac{1}{N}\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} \tanh\left(\frac{E_{k'}}{2K_B T}\right) \quad (3)$$

Where $E_k^2 = \varepsilon_k^2 + \Delta_k^2$

at $T = 0^\circ K$ this equation is written as:

$$\Delta_k = -\frac{1}{2}\sum_{k'}\frac{V_{kk'}}{N}\frac{\Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}} \quad (4)$$

We take the electron -electron attractive potential $V_{kk'}$ between two electrons states of wave vector k and k′, as:

$$V_{kk'} = \begin{cases} W_{kk'} + U & \text{if } |\varepsilon_k| \text{ and } |\varepsilon_{k'}| < \eta\omega \\ U & \text{otherwise} \end{cases} \quad (5)$$

Where U is the coulomb repulsion between electrons.

The electron-electron interaction via phonons $W_{kk'}$ is written as:

$$W_{kk'} = \begin{cases} V\left[1 + a(k_x - k'_x)^2 + b(k_y - k'_y)^2\right] \\ \text{for} \quad |\varepsilon_k| \text{ and } |\varepsilon_{k'}| \ \pi \ \eta\omega \\ 0 \quad \text{otherwise} \end{cases} \quad (6)$$

where ω is the cut off energy of phonon, V is not dispersed interaction, a and b are the constants. We can noted that the same form of $W_{kk'}$ is used before by Béal.Monod et al [13-14], and in the limit a = b = 0 we rediscover the BCS model. Taking in to account the expression of ε (k) in equation (1) by choosing the ε_F as the origin of energy axis, only the electrons near the Fermi level formed a Cooper pairs in our model, and a = b = -1 which corresponds to « d » symmetry, the equation (6) is written as :

$$W_{kk'} = -V\left[1 + (\varepsilon + \varepsilon')A\right] = W(\varepsilon, \varepsilon') \quad (7)$$

Where A is a constant (independent on the k and k′):

$$A = \frac{2}{(k_F a)^2}\frac{1}{t}\frac{1}{\cos k_x^F a} \ ;$$

$\cos k_x^F a$ is obtained in the some manner in the reference [15](k_x^F is the Fermi wave vector in x direction). The equation (3) is transformed to:

$$\Delta_k = -\frac{1}{2}\int_{-\frac{w}{2}}^{\frac{w}{2}} \left(W_{kk'}(\varepsilon, \varepsilon') + U\right)\frac{\Delta(\varepsilon')}{\sqrt{\varepsilon'^2 + \Delta^2(\varepsilon')}} N(\varepsilon')d\varepsilon' \quad (8)$$

To solve this self-consistant equation we propose the following form of the gap:

$$\Delta(\varepsilon) = \Delta_0(1 + \varepsilon.B) \quad (9)$$

Where Δ_0 is the gap at Fermi level and B is a constant which are obtained numerically.

In ordre to calculate the ratio $\eta = 2\Delta(T = 0)/k_B T_c$ we need the expression T_c for the disperse $V_{kk'}$ (where T_c is the transition temperature between normal state and superconductivity state), the T_c expression is obtained by the following condition $(\Delta(T = T_c) = 0)$:

$$1 = -\frac{1}{N}\sum_{k'} V_{kk'}\frac{1}{2\varepsilon(k')}\tanh\frac{\varepsilon(k')}{2K_B T_c} \quad (10)$$

Taking into account the equation (2), (4) and equation (10) T_C is obtained by solving the following relation:

$$a_2(\log 2K_B T_c)^2 - b_2(\log 2K_B T_c) - c_2 = 0 \quad (11)$$

Where:

$$a_2 = Aq\varepsilon + (q - 1)$$

$$b_2 = 2(q - 1)(c_1 + 1) + 2\log D((q - 1) + Aq\varepsilon) + 2Aq\varepsilon(c_1 + 1)$$

$$c_2 = 2c_1\log\frac{W}{2\eta\omega} + \left(\log\frac{D}{\eta\omega}\right)^2 - 2c_1(\log\eta\omega)a_2 - a_2\left(2\log D\log\eta\omega - \log^2\eta\omega\right) - 2(c_1 + 1)a_2 + \frac{q}{\lambda}$$

With:

$$c_1 = \frac{n_0}{n_1}; \lambda = \frac{Vn_1}{2}$$

Where λ is the coupling constant.

III. RESULTS AND DISCUSSION

In recent works Hocquet et al [16] have studied anisotropy of gap parameter in cuprate oxides superconductors. They have set a model to hamiltonien including both the Hubbard intra-atomic repulsion U and effective coupling constant $V_{kk'}$ between electrons, with in the logarithmic Van Hove singularity in the electronic density of states .J. Bouvier et al [11] have taken a classical electron-electron potential $V_{kk'}$ between two electron states of waves vector k and k′ via electron-phonon coupling, by assuming that $|\varepsilon_{kk'}| \le \eta\omega$, the term $\frac{(\eta\omega)^2}{\varepsilon_{kk'}^2 - (\eta\omega)^2}$ is taken as -1.They have written Δ_k in a Fourier expression

$(\Delta = \Delta_0 + \Delta_1 \cos\phi)$. The result shows no dispersion of the gap and the ratio $\eta = 2\Delta(T=0)/k_B T_c$ has a fixed value 3.7. Recently S. Prakash [17] has studied the anisotropy of gap parameter in cuprate superconductors. He found that Δ_k consists of a constant part and an oxillatory part which varies as $\sin^2 k_x a$. But all these models are no able to explain the different values observed in various experiments.

In this work we are interested to YBCuO system .The numerical calculation neede Some physical parameter such k_F = 0.5 $10^8 cm^{-1}$ [18], $\eta\omega/t$ = 0.2 [16]. To evaluated values of the ration we need T_C (equation11) and $\Delta(Tc = 0)$ from equation (8). The solution obtained for Δ(ε) presents a maximum value. In the first step we have been interested to ratio r_o corresponding to this maximum value (r_0= 2 Δ_{max} / $K_B T_c$).

In figure 1 we have plotted the variation of r_0 as function of (q=V/U) for different λ .

The result shows that r_0 decreases as q increases and find the BCS limit for larger q (when the coulomb

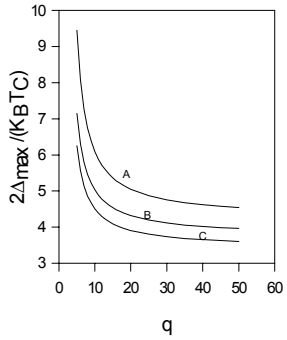

FIG. 1 : 2□(0) max / ($K_B T_C$) as a function of q a for differents values of □ : □ = 0.05 (curve A)
□ = 0.1 (curve B) and □ = 0.15 (curve C) for r = 0.

repulsion is very weak). For a fixed q, r_0 also decreases as λ increases. The copper oxides superconductors are characterised by a strong coulomb repulsion U (q =V/U), the values of q are weak(2≤ q ≤20) and a weak coupling λ ≤ 0.15.

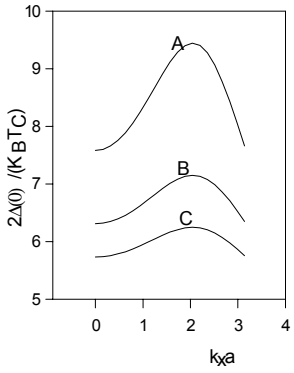

FIG. 2 : 2□(0) max / ($K_B T_C$) as a function of k_x a for different values of □ : □ = 0.05 (curve A)
□ = 0.1 (curve B) and □ = 0.15 (curve C) for q = 5.

In figure 2 we plot the dispersion of $\eta = 2\Delta(T=0)/k_B T_c$ as function of $k_x a$ for different values of λ = 0.05 (Curve A), λ =0.1 (Curve B) and λ = 0.15 (Curve C) in the case where r =0.

The result shows that the dispersion of η is more pronounced for weak coupling and their values are far from the BCS one. In the case λ =0.05 the ratio varies between 7.5 and 9.5 .The variation on $k_x a$ is in argument with the result obtained by [18].

In order to approach the experiment observation for the gap dispersion we have included the effect of the second nearest-neighbour in our model.

In figure 3 we show the variation of $\eta = 2\Delta(T=0)/k_B T_c$ as function of different values of λ taking the effect of nearest-neighbour r =0.15. The ratio η is more disperse in this case. For λ=0.05, it varied between 3.5 and 9.1. Such dispersion is reduced as the coupling constant λ increases in the region $\pi/4 \le k_x a \le 3\pi/4$, but η becomes slowly otherwise and the effect of λ is inversed. Here we show that dispersion depends on many physical parameters such ηω (cut off energy of phonon), λ (coupling constant λ= (Vn_1)/2) , D (singularity width) and on the ratio q = V/U.

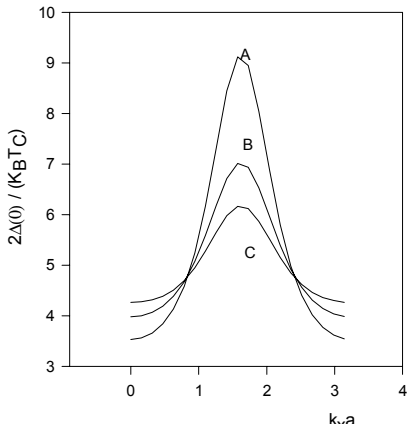

FIG. 3 : □ = 2□(0) max / ($K_B T_C$) as a function of k_x a for differents values of □ : □ = 0.05 (curve A)
□ = 0.1 (curve B) and □ = 0.15 (curve C) for q = 5 and r = 0.15.

The effect of the nearest-neighbour on the gap dispersion is plotted in figure4. The increasing of r gives a more disperse gap. In the case of λ =0.05, q(V/U) = 5 and r =0.15, the gap ratio varied between 3.5 and 9. This result is in agreement with different observed experimental values which themselves depend on the quality, the nature of contact points and the method used to measure the gap.

Contrary to the previous works Hocquet et al [16], Bouvier et al [11] and S.Prakach et al [17] who have

studied the dispersion of Δ in Copper oxides and where ther results can not explain the experiment results, our approach due to the dispersion of $V_{kk'}$ can predicte a more dispersion of the ratio η.

In conclusion the dispersion of the gap ratio $2\Delta(T=0)/k_B T_c$ can be explained by the dispersive interaction between the charge carrier $V_{kk'}$ on the one hand and to the effect of the nearest-neighbour in the electronic structure on the other hand.

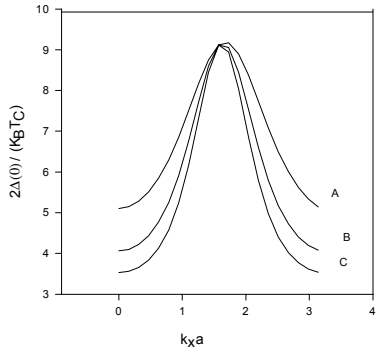

FIG. 4 : □ = 2□(0) max / ($K_B T_C$) as a function of k_x a for differents values of r : r = 0.15 (curve A) r = 0.1 (curve B) and r = 0.15 (curve C) for q = 5 and □ = 0.15.

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