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### **COMPARATIVE STUDY OF LAYERED STRUCTURE FORMULISMS FOR HIGH TEMPERATURE COPPER-OXIDE SUPERCONDUCTORS**

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### ABSTRACT

An effective two-dimensional dynamic interaction potential energy function has been developed to understand the pairing mechanism leading to high- $T_C$  superconductivity in copper-oxide superconductors. It has been carried out under perturbation approximation using Dyson diagrammatic formulism and the technique of Fourier transform by assuming layered structure of cooper-oxide superconductors as supported by X-ray diffraction and spectroscopic studies within the framework of BCS theory. Three different potentials namely Coulomb, Yukawa like and Modified have been employed. The effective two-dimensional dynamic interaction potential energy functions thus obtained are complex in nature ab-initio. The calculations of coupling strength, Coulomb repulsive parameter, transition temperature, relaxation time, resistivity, specific heat jump, energy gap and thermal conductivity are being carried out separately for each case taking LSCO as a sample. The calculated results calculations show that the coupling between Cu-O conducting layers makes the effective potential energy function more attractive and a less repulsive.

Keywords: Electron-electron interaction, High-T<sub>c</sub> Superconductivity, Strong coupling theory

### **INTRODUCTION**

The field of materials science got a new lease of life with the discovery of high- $T_c$  copper-oxide superconductors (COS) [1]. Banking on experimental observations that copper-oxide superconductors exhibit layered structure having Cu-O as conducting planes [2-11], a phenomenological layered structure model have been developed to understand pairing mechanism within the framework of BCS theory leading to high- $T_c$  superconductivity. The

basic ingredient of layered structure model is that a three-dimensional system is effectively reduced to two-dimensional one. Physically it amounts to the fact that these high- $T_c$ superconductors are constrained systems. From the dynamics point of view it is well known that the system under constrained motion with reduced degree of freedom has complex potential energy function. The imaginary part of the potential energy function accounts for the dissipation of energy or resistivity in the present case. During the course of earlier investigations [12-15] the layered structure model has been so developed that the calculated effective interaction potential energy function is real and to account for the resistivity, the potential energy function has been made complex employing somewhat artificial prescription. Our aim has been to rectify this weakness of the layered structure model. In the present investigation the modified formulism of layered structure model has been so developed that the effective interaction potential energy function is complex ab-initio. It is true that  $T_c$  is not describable within mean field theory because of phase fluctuations rather than amplitude fluctuations dominated systems. Nevertheless BCS theory has its relevance even in this context.

### MODEL

Experimental as well as theoretical studies of the inverse dielectric response function [4-5] suggest that copper-oxide superconductors possess a layered structure and their normal conducting state may be more like a doped semiconductor rather than a metal. Also, the crystallographic as well a spectroscopic studies [16-20] suggest a layered structure for COS. It has been further investigated that the change in the oxygen deficiency in copper-oxide superconductors develops free charge carriers in copper oxide conducting planes. We consider an array of two-dimensional layered electron gas model for La-Sr-Cu-O. It is assumed that the conduction of charge carriers is very pronounced in copper oxide plane (X-Y plane) and reasonably feeble perpendicular to the plane (Z-direction). Thus the charge carriers are strongly coupled with in the plane but weekly coupled with in the Z direction. The present model is based on following assumptions:

- 1. There is one Cu-O layer plane per unit cell.
- 2. Cu-O plane forms an infinite array of planes along Z-axis.
- 3. A non-conducting plane between Cu-O planes is considered as a uniform dielectric medium with a background dielectric response function taking as a constant  $\varepsilon_b$ .
- 4. The oxygen deficient Cu-O chain stabilizes the charge carriers in the conducting planes.

We shall carry out the study separately for all the three chosen potential energy functions.

### **Case-I: FORMULISM BASED ON COULOMB POTENTIAL ENERGY FUNCTION**

To obtain the effective two-dimensional dynamic interaction potential energy function we start with bare Coulomb potential energy function  $V^o |\vec{r} - \vec{r}'|$  for the pair of charge carriers existing in consecutive conducting planes given as:

$$V^{o} | \vec{r} - \vec{r}' | = \frac{1}{4\pi\varepsilon_{o}\varepsilon_{b}} \frac{e^{2}}{|\vec{r} - \vec{r}'|}$$
(1)

here  $\varepsilon_{\circ}$  is dielectric constant in vacuum  $\varepsilon_{b}$  is static dielectric constant of background.

Taking two-dimensional Fourier transform in the X-Y plane, and following the usual procedure [21] we get the bare potential energy function in two-dimensional plane as:

$$V^{o}(q,z,z') = \frac{e^{2}}{2 \in_{o} \in_{b} q} e^{-q(z-z')}$$
(2)

here  $\vec{q}$  is momentum transfer wave vector.

Now as the charge carriers are confined only in the two-dimensional conducting planes, z and z' can be represented by discrete variables nd and n'd respectively. Here n and n' are the numbers required to index the consecutive Oxygen deficient planes and d is the separation between them. From Eq. (2) it is evident that the bare two-dimensional potential energy function depends on (n-n') and not on n and n' separately. Hence it is mod of (n-n') i.e. |n-n'| appears in the expression of bare potential. Consequently Eq. (2) reduces to

$$V^{o}(q, |n-n'|) = \frac{e^{2}}{2 \in_{o} \in_{b} q} e^{-q|n-n'|d}$$
(3)

Assuming that the polarizability for a given conducting plane can be expressed as sum of the polarizabilities of all the possible charge carriers and all conducting planes to be identical, we obtain the effective potential energy function employing Dyson diagrammatic technique and using Discrete Fourier Transform (DFT) [22], as

$$V(q,\omega,k_z) = \frac{V^{\circ}(q,k_z)}{\varepsilon(q,\omega,k_z)}$$
(4)

where  $\mathcal{E}(q, \omega, k_z) = 1 - \prod (q, \omega) V^{\circ}(q, k_z) \prod (q, \omega) =$  Polarization function for the twodimensional conducting planes and

$$V^{\circ}(q,k_z) = \frac{e^2}{2\varepsilon_{\circ}\varepsilon_{b}q} \sum_{n-n'=-\infty}^{n-n'=\infty} V^{\circ}(q,|n-n'|)e^{ik_zd|n-n'}$$
(5)

This may be pointed out that earlier workers [12-15] have used mod of (n-n') only in the expression for  $V^{\circ}(q, |n-n'|)$  and not taking mod of (n-n') in the exponential occurring in Eq. (5). This arbitrary choice is mathematically inconsistent. As a matter of fact n and n' are the numbers used to index respective conducting layers and hence it is the mod of (n-n') viz. In-n'l contribute wherever it occurs in the formulism. Nevertheless for the sake of completeness and to bring out the clarity we have investigated the following possible options of (n-n') in Eq. (5). In table 1 the occurrence of (n-n') in term V<sup>o</sup> and in exponential term of Eq. (5) is designated as first and second positions, respectively.

Option	First position of n-	Second position of	$V^{\circ}(q,k_{\pi})$
	n′	n-n'	1 4 4 4 A
Ι	Mod	Mod	Finite output
II	Mod	Without mod	Finite output
III	Without mod	Mod	0
IV	Without mod	Without mod	0

Table 1: Summary of results with all possible options of (n-n') in Eq. (5)

From table 1 it is clear that the options III and IV gives null effective potential energy function leading to non-formation of cooper pairs and therefore, these options are of no use in present analysis of high- $T_c$  superconductivity. Further the option II in the table does bear finite value of effective potential energy function but this option is mathematically inconsistent, as we have already discussed. Thus the only possible and mathematically correct option is the first one, which is employed to develop the present model.

Following the usual technique [21], Eq. (5) yields

$$V^{\circ}(q,k_z) = \frac{e^2}{2\varepsilon_{\circ}\varepsilon_b q} \left[ \frac{1 + e^{-(q - ik_z d)}}{1 - e^{-(q - ik_z d)}} \right]$$
(6)

Form Eq.(4) and Eq.(6)we get

$$V(q,\boldsymbol{\omega},k_{z}) = \frac{\frac{e^{2}}{2\varepsilon_{\circ}\varepsilon qq} \left[\frac{1+e^{-qd}e^{ik_{z}d}}{1-e^{-qd}e^{ik_{z}d}}\right]}{1-\prod(q,\boldsymbol{\omega})\frac{e^{2}}{2\varepsilon_{\circ}\varepsilon_{b}q} \left[\frac{1+e^{-qd}e^{ik_{z}d}}{1-e^{-qd}e^{ik_{z}d}}\right]}$$
(7)

$$V(q, \omega, k_z) = \frac{\frac{e^2}{2\varepsilon_{\circ}\varepsilon qq} \left[ \frac{1 + e^{-qd} e^{ik_z d}}{1 - e^{-qd} e^{ik_z d}} \right]}{1 + P(q, \omega) \left[ \frac{1 + e^{-qd} e^{ik_z d}}{1 - e^{-qd} e^{ik_z d}} \right]}$$
(8)  
where  $P(q, \omega) = -\frac{e^2}{2\varepsilon_{\circ}\varepsilon_b q} \prod (q, \omega)$ 

A realistic calculation of  $P(q, \omega)$  requires a many-body treatment (marginal Fermi-liquid treatment) of a strongly correlated 2D system. However, here we use an RPA expression for  $P(q, \omega)$ , in order to see the coupling effects in a simple manner. We take  $P(q, \omega)$  [23] as

$$P(q,\omega) = \frac{qe^2k_F^2}{m^*\varepsilon_{\circ}\varepsilon_{b}\left[\frac{q^2V_F^2}{2} - \omega^2\right]}$$
(9)

where  $k_F$  and  $V_F$  are Fermi wave vector and Fermi velocity, respectively and m<sup>\*</sup> is effective mass of the charge carriers.

### **Analysis of Coulomb Potential Energy Function**

### 1. Cut-off Frequency and Attractive and Repulsive Frequency Ranges

The cut-off frequency, which gives the upper cut-off limit for attractive potential energy function, is obtained as follows:

The average dynamic permittivity  $\varepsilon(q, \omega)$  is computed as

$$\boldsymbol{\varepsilon}(q,\omega) = \frac{d}{2\pi} \int_{-\pi/d}^{+\pi/d} \boldsymbol{\varepsilon}(q,\omega) k_z dk_z$$
(10)  
where  $\boldsymbol{\varepsilon}(q,\omega,k_z) = 1 + P(q,\omega) \left[ \frac{1 + e^{-qd} e^{ik_z}}{1 - e^{-qd} e^{ik_z}} \right]$ 

Thus on integrating, Eq. (10) yields

$$\varepsilon(q,\omega) = 1 + P(q,\omega) + i \frac{2P(q,\omega)}{\pi} \ln\left(\frac{A+1}{A-1}\right)$$
(11)  
where  $A = e^{qd}$ 

The zeros of Real  $\varepsilon(q, \omega)$  i.e. Re  $\varepsilon(q, \omega)$  give the cut-off frequency  $\omega_c$ . Hence we have

$$\Rightarrow 1 + P(q, \omega_c) = 0 \tag{12}$$

On solving Eq. (12) and using Eq. (9) we get

$$\boldsymbol{\omega}_{c} = \sqrt{\frac{q^{2}V_{F}^{2}}{2} + \frac{qe^{2}k_{F}^{2}}{m^{*}\boldsymbol{\varepsilon}_{o}\boldsymbol{\varepsilon}_{b}}}$$
(13)

The frequency range in which interaction potential energy function is attractive can be obtained as follows.

Using Eq. (13) and Eq. (9) (RPA polarization)  $\operatorname{Re} \varepsilon(q, \omega)$  becomes

$$\operatorname{Re}\varepsilon(q,\omega) = \frac{\omega_c^2 - \omega^2}{\frac{q^2 V_F^2}{2} - \omega^2}$$
(14)

and the range in which interaction potential energy function is attractive, is defined as  $\operatorname{Re} \varepsilon(q, \omega) < 0$ 

Thus there are two possibilities to fulfill this condition:

$$\frac{q^2 V_F^2}{2} < \omega^2 < \omega_c^2$$
(15)  
and  $\frac{q^2 V_F^2}{2} > \omega^2 > \omega_c^2$ 
(16)

$$\sqrt{\frac{q^2 V_F^2}{2}} \le \omega \le \sqrt{\frac{q^2 V_F^2}{2} + \frac{q e^2 k_F^2}{m^* \varepsilon_{\circ} \varepsilon_b}}$$
(17)

For the values of  $\omega$ , lying beyond the inequality in Eq. (17), V(q,  $\omega$ ) is repulsive.

### 2. Analysis and Comparison of Effective and Bare Potential Energy Functions

Effective two-dimensional dynamic potential energy function obtained in Eq. (8) is complex ab-initio. Therefore, in the present formulism the complex nature of potential energy function, responsible for the resistivity of the material has been included in natural way. This gets rid of all ad-hoc prescriptions as are being used in earlier investigations [12-15] to make the effective potential energy function complex in nature. We have investigated the behavior of bare and effective potential energy functions as given by Eq. (6) and Eq. (8) respectively with respect to qd for a given  $\cos\theta$  (where  $\theta = K_z d$ ) and  $\omega$ . For the sake of completeness a comparison of present results has been done with that of earlier investigators [12-15] as well.

The bare and effective potential energy functions obtained by earlier workers [12-15] following arbitrary prescription as mentioned above (option II of Table 1), are:

$$V^{\circ}(q,k_{z}) = \frac{e^{2}S(q,K_{z})}{2\varepsilon_{\circ}\varepsilon_{b}q}$$
(18)  
Where  $S(q,k_{z}) = \frac{Sinh(qd)}{Cosh(qd) - Cos(K_{z}d)}$ 

$$V(q,\omega,k_z) = \frac{e^2}{2\varepsilon_{\circ}\varepsilon_b q} \frac{S(q,K_zd)}{1 + P(q,\omega)S(q,K_zd)}$$
(19)

On the basis of the calculations following inferences can be drawn:

★ The behavior of effective potential energy function with respect to qd has been investigated. The value of  $\omega$  is chosen within the range for which the dielectric response function leads to the formation of cooper pairs. The real of effective potential energy function of the present model exactly same as the total effective potential energy function obtained by earlier workers [12-15] (here termed as Old V). The total effective potential

energy function of the present model is linear sum of its real and imaginary parts. Hence it is much more attractive as compare to Old V. Therefore, it is envisaged that if a sample is so prepared that charge carriers in conducting planes are guided such that they practically suffer elastic collisions in the forward direction (q is small and  $\cos\theta \approx 1$ ), the sample has enhanced probability of exhibiting high transition temperature.

★ The behavior of bare potential energy function with qd is being investigated for  $\cos\theta=0.9$  and  $\omega=10^{13}$  Hz. The results are consistent with the behavior of effective potential energy function as discussed above.

## Case-II: FORMULISM BASED ON YUKAWA LIKE POTENTIAL ENERGY FUNCTION

Similar formulation is being done starting with short-range Yukawa like potential energy function  $V^o |\vec{r} - \vec{r}'|$  for the pair of charge carriers existing in consecutive conducting planes to incorporate the all possible excitons as exchange particle and it is given as:

$$V^{o} \mid \vec{r} - \vec{r}' \models \frac{1}{4\pi\varepsilon_{o}\varepsilon_{b}} \frac{e^{2}e^{-\mu|\vec{r} - \vec{r}'|}}{\mid \vec{r} - \vec{r}'\mid}$$
(20)

Talking two- dimensional Fourier transform and following the procedure [21] we get the potential energy function in two- dimensional plane as:

$$V^{o}(Q, z, z') = \frac{e^{2}}{2 \in_{o} \in_{b} Q} e^{-Qbn-n^{\gamma}}$$
(21)

Where  $Q = \sqrt{\mu^2 + q^2}$  and  $\mu = m_{\text{exch}}c/\hbar$ 

Following the technique as we have opted in Case-I, the bare and effective potential energy functions thus obtained are given here respectively in Eq. (22) and Eq. (23)

$$V^{\circ}(Q,k_z) = \frac{e^2}{2\varepsilon_{\circ}\varepsilon_b Q} \left[ \frac{1 + e^{-(Q - ik_z d)}}{1 - e^{-(Q - ik_z d)}} \right]$$
(22)

$$V(Q, \omega, k_z) = \frac{\frac{e^2}{2\varepsilon_s \varepsilon q Q} \left[ \frac{1 + e^{-Qd} e^{ik_z d}}{1 - e^{-Qd} e^{ik_z d}} \right]}{1 + P(Q, \omega) \left[ \frac{1 + e^{-Qd} e^{ik_z d}}{1 - e^{-Qd} e^{ik_z d}} \right]}$$
(23)

## Case-III: FORMULISM BASED ON MODIFIED COULOMB POTENTIAL ENERGY FUNCTION

All the earlier investigations [12-15] based on layered structure model have taken three dimensional Coulomb potential energy function for the pair of charge carriers belonging to the consecutive conducting planes as the starting point. Its well known that the Coulomb

potential energy function has ultra violet singularity viz. the potential energy function becomes infinite in the limit when  $r \rightarrow 0$ . The problem is perplexing and leads to number of unphysical situations like infinite self energy, infinite self momentum, pre-accelerated phenomenon, run away solutions and like that. In order to circumvent these difficulties and to provide physically acceptable solutions a modified Coulomb potential energy function has been proposed by Gupta [24]. This modified Coulomb potential energy function is also capable of incorporating short-range co-relations between the pair of electrons forming Cooper pairs. To obtain the modified effective two-dimensional dynamic interaction potential energy function we start with modified bare Coulomb potential energy function for the pair of charge carriers existing in consecutive conducting planes, given as:

$$V^{\circ} \mid \vec{r} - \vec{r}' \models \frac{1}{2\pi^{2}\varepsilon_{\circ}\varepsilon_{b}} \frac{e^{2}Si(Y \mid \vec{r} - \vec{r}' \mid)}{\mid \vec{r} - \vec{r}' \mid}$$
(24)

where,  $Si(Y | \vec{r} - \vec{r'}|)$  is an exponential function and has following limiting behavior:

In the limit when x is large  $Si(x) = \pi/2$  and in the limit when x is small Si(x) can be represented as infinite series given as  $Si(x) = \sum_{m=0}^{m=\infty} \frac{(-1)^m (x)^{2m+1}}{(2m+1)(2m+1)!}$ 

It is worth mentioning that the modified Coulomb potential energy function as proposed in Eq. (28) is regular at the origin and leads to the usual Coulomb potential energy function at large distances without introducing any additional parameter. The modified bare and effective potential energy functions thus obtained are respectively given here in Eq.(29) and Eq.(30)

$$V^{\circ}(q,k_{z}) = \frac{e^{2}}{2\varepsilon_{\circ}\varepsilon_{b}q} \left[\frac{1+e^{-(q-ik_{z}d)}}{1-e^{-(q-ik_{z}d)}}\right] - \left[\frac{e^{2}}{\pi\varepsilon_{\circ}\varepsilon_{b}Y} + \frac{e^{2}q^{2}}{6\pi\varepsilon_{\circ}\varepsilon_{b}Y^{3}}\right] \left[\frac{1+e^{ik_{z}d}}{1-e^{ik_{z}d}}\right] - \left[\frac{e^{2}q^{2}d^{2}}{2\pi\varepsilon_{\circ}\varepsilon_{b}Y}e^{ik_{z}d}\left(\frac{\left(1+e^{ik_{z}d}\right)}{\left(1-e^{ik_{z}d}\right)^{3}}\right)\right]$$
(25)

$$V(q,\omega,k_{z}) = \frac{\frac{e^{2}}{2\varepsilon_{o}\varepsilon_{b}q} \left[ \left( \frac{1+e^{-(q-ik_{z}d)}}{1-e^{-(q-ik_{z}d)}} \right) - \left[ \frac{2q}{\pi Y} + \frac{q^{3}}{3\pi Y^{3}} \right] \left[ \frac{1+e^{ik_{z}d}}{1-e^{ik_{z}d}} \right] - \left[ \frac{q^{3}d^{2}}{2\pi Y} e^{ik_{z}d} \left( \frac{\left(1+e^{ik_{z}d}\right)}{\left(1-e^{ik_{z}d}\right)^{3}} \right) \right] \right]}{1+P(q,\omega) \left[ \left( \frac{1+e^{-(q-ik_{z}d)}}{1-e^{-(q-ik_{z}d)}} \right) - \left[ \frac{2q}{\pi Y} + \frac{q^{3}}{3\pi Y^{3}} \right] \left[ \frac{1+e^{ik_{z}d}}{1-e^{ik_{z}d}} \right] - \left[ \frac{q^{3}d^{2}}{2\pi Y} e^{ik_{z}d} \left( \frac{\left(1+e^{ik_{z}d}\right)}{\left(1-e^{ik_{z}d}\right)^{3}} \right) \right] \right]} \right]}$$

$$(26)$$

### **RESULTS AND DISCUSSIONS**

# Coupling Strength ( $\lambda$ ), Coulomb Repilsive Parameter ( $\mu^*$ ) and Transition Temperature ( $T_c$ )

Employing the present formulism, we have calculated  $\lambda$ ,  $\mu^*$  and  $T_c$  for La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> cuprate superconductor, which consists of one Cu-O layer per unit cell, using [25] following formulae

$$\lambda = 2 \int_{0}^{\omega_{c}} \frac{\alpha^{2}(\omega)F(\omega)}{\omega} d\omega$$
(27)

where  $\alpha^2(\omega)F(\omega)$  is the Eliasberg function and  $F(\omega)$  is the boson density of states.  $\alpha^2(\omega)F(\omega)$  can be given by [26]

$$\alpha^{2}(\omega)F(\omega) = N_{\circ} << \operatorname{Im}V(q, \omega, k_{z}) >>$$
(28)

where  $\langle \operatorname{Im} V(q, \omega, k_z) \rangle$  is the average of the imaginary part of  $V(q, \omega, k_z)$  over q and  $k_z$ . The averaging over  $k_z$  is done over whole range i.e.;  $-\pi/d \leq k_z \leq \pi/d$ , while averaging over q is done in the range  $0 \leq q \leq q_c$ .

$$\mu^* = \frac{\mu}{\left[1 + \mu \ln(E_F / \omega_c)\right]}$$
(29)

where  $\mu$  is the averaged Coulomb repulsion and  $E_F$  is the Fermi energy at absolute zero.  $\mu$  can be defined as :

$$\mu = \frac{N_{o}}{q_{c}^{2}} \int_{-1}^{+1q_{c}} V(q,0,k_{z}) q dq d(\cos(k_{z}d))$$
(30)

where  $q_c$  is the upper cut-off value of q,  $N_o$  is the density of states at Fermi surface.

and 
$$T_c = 0.7\omega_c \exp\left[\frac{-(1+\lambda)}{\lambda - \mu^*}\right]$$
 (31)

For case-I we have calculated coupling strength ( $\lambda$ ) and Coulomb repulsive parameter ( $\mu^*$ ) with the help of Eq. (8) considering small-angle scattering of charge carriers at the Fermi surface.  $\omega_c$  is obtained from Eq. (13). With the help of Eq. (27), (29) and (31), we have computed T<sub>c</sub> for La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> at x=0.15. For computation we used m<sup>\*</sup>=4m<sub>e</sub>, k<sub>F</sub>=0.2833 Å<sup>-1</sup>, d=13.25Å, q<sub>c</sub>=0.0239 Å<sup>-1</sup> and  $\varepsilon_b$ =22 [25]. We obtained  $\lambda$ = 1.54 and  $\mu^*$ =0.02 and T<sub>c</sub>=39.6 K. We thus find that our calculated values of  $\lambda$ ,  $\mu^*$  and T<sub>c</sub> are in good agreement with the experimentally observed value [27-28].

For case-II we have calculated coupling strength ( $\lambda$ ) and Coulomb repulsive parameter ( $\mu^*$ ). The obtained values are  $\lambda$ = 1.59 and  $\mu^*$ =0.03 and T<sub>c</sub>=39.7 K. We thus find that our calculated values of  $\lambda$ ,  $\mu^*$  and T<sub>c</sub> are in good agreement with the experimentally observed value [27-28]. For case-III we have obtained  $\lambda$ =1.66 and  $\mu^*$ =0.05 and T<sub>c</sub>=39.9 K. Which are in good agreement with the experimentally observed value [27-28].

The computed values of  $\lambda$ ,  $\mu^*$  and  $T_c$  fairly agrees with the experimentally measured values. The important intrinsic parameters which characterize  $La_{2-x}Sr_xCuO_4$  and related COS are effective mass of charge carriers, two-dimensional carrier density and background dielectric constant. In order to see how the variation in these parameters affects the  $T_c$ , we have computed the  $T_c$  as a function of  $m^*$  and  $\varepsilon_b$ . It should be noted here that larger value of  $\varepsilon_b$  in our model calculation gives rise to smaller value of plasmon energy. Again, smaller plasmon energy results in smaller  $T_c$  value in our calculation. Therefore, the behavior of  $T_c$ 

with  $\varepsilon_b$ , is what one expect from our model calculation. Further we have also ploted  $T_c$  as a function of m<sup>\*</sup>. We notice that similar to variation of  $T_c$  with  $\varepsilon_b$ ,  $T_c$  decreases on increasing m<sup>\*</sup>. Larger value of m<sup>\*</sup> yields smaller value of plasma frequency which could be used in pair formation. Further, it is implied that a smaller boson frequency results in a smaller value of  $T_c$ . We thus find that our calculated results are consistent with the generally expected behavior of  $T_c$  with m<sup>\*</sup>. We also notice that  $T_c$  first decreases rapidly and then slowly on increasing m<sup>\*</sup>.

### **Relaxation Time and Resistivity**

Following classical Drude relation, we have

$$\rho = \frac{m^2}{ne^2\tau} \tag{32}$$

where  $m^*$  is the effective mass of the charge carrier, the n and  $\tau$  are the carriers density per unit volume and the relaxation time for scattering of charge carriers from phonon like bosons respectively. In other words  $\tau$  is mean time to absorb or emit a phonon like boson. The n can be related to  $n_s$  via the relation  $n_s = nv$ , where v is the number of Cu-O planes per unit length. The inverse of relaxation time ( $\tau$ ) at temperature (T) higher than Debye temperature, for the scattering of charge carriers in a two- dimensional (2D) conduction Cu-O plane (a-b plane) is given as [29]

$$\frac{1}{\tau} = \frac{V_F}{\Lambda} = n_i \langle \sigma \rangle V_F \tag{33}$$

where  $\Lambda$  is mean free path and is given by

Let  $\sigma(\theta)$  be the cross section per unit solid angle for scattering of conduction electron by an impurity atom. The electrical resistivity is concerned the change on scattering of the projection of the wave vector along the axis of the current flow. Thus the effective average cross section for resistivity is

$$\langle \sigma \rangle = 2\pi \int_{-\pi}^{+\pi} d\theta \sin \theta \sigma(\theta) (1 - \cos \theta)$$
 (34)

and

$$\sigma(\theta) = \left(\frac{m}{4\pi^2\hbar}\right)^2 |V(q)|^2$$
(35)

Where V(q) is effective potential energy function.

where the last factor on the right hand side weights the average according to the change of  $k_z$ . The associated relaxation frequency is given by Eq. (39).

The calculated relaxation time and resistivity for La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> at x=0.15 comes out to be  $\tau = 3.9 \times 10^{-14} Sec$ ,  $\rho = 0.7317 \mu\Omega meter$  for case-I,  $\tau = 3.4 \times 10^{-14} Sec$ ,  $\rho = 0.839 \mu\Omega meter$  for case-II and  $\tau = 3.2 \times 10^{-14} Sec$ ,  $\rho = 0.8918 \mu\Omega meter$  for case-III. For computation we used m<sup>\*</sup>=4m<sub>e</sub>, k<sub>F</sub>=0.2833 Å<sup>-1</sup>, d=13.25Å, q<sub>c</sub>=0.0239 Å<sup>-1</sup>,  $\varepsilon_{b}=22$  [25] and carrier

concentration  $n_s = 1.277 \times 10^{18} m^{-2}$ . The above calculated values are in good agreement with experimental results. Further we notice that resistivity explicitly depends upon intrinsic parameters such as  $\varepsilon_b$ , m<sup>\*</sup> and n<sub>s</sub> of COS. Computed results are in good agreement with the results obtained in earlier investigations [32-34].

#### **Specific Heat Jump at Transition Temperature**

The relation between specific heat difference,  $\Delta C(T)$ , of superconducting and normal state,  $\Delta F(T)$ , at any temperature T may be obtained from the solution of Eliashberg equations. Eliashberg equations are a set of two coupled equations for the pairing potential and the renormalized Matsubara Frequencies [35-36]. In addition to knowledge of the solutions of the Eliashberg equations an expression for the free- energy difference between normal and superconducting state  $\Delta F(T)$  is required which is given by Daams et al [35] and Rainer et al [36]. The relation  $\Delta C$  and  $\Delta F(T)$  may therefore be obtained as [37-38],

$$\Delta C(T_c) = T \frac{d^2 \Delta F(T)}{dT^2}$$
(36)

The free energy,  $\Delta F(T)$ , depends on the single spin electronic density of states at Fermi surface N<sub>o</sub>, the electron-boson spectral density  $\alpha^2(\omega)F(\omega)$  and the Coulomb pseudo potential  $\mu^*$ . The normalized specific heat jump (R) at T=Tc can these be given by an empirical relation [39-40]

$$R \equiv T_c \frac{\left\lfloor \frac{d\Delta C(T)}{dT} \right\rfloor_{T_c}}{\Delta C(T_c)}$$
(37)

By defining two arbitrary parameters the empirical relation for R can be simplified to [38]

$$R = 2.634 \left[ 1 + 38 \left( \frac{T_c}{\omega_{\ln}} \right)^2 \ln \left( \frac{\omega_{\ln}}{3.2T_c} \right) \right]$$
(38)

where  $\omega_{ln}$  is an appropriate average boson frequency related to Eliashberg function  $\alpha^2(\omega)F(\omega)$ and first introduced by Allen and Dynes [41]. The  $\omega_{ln}$  is defined as

$$\omega_{\rm ln} \equiv \exp\left[\frac{2}{\lambda}\int_{0}^{\infty}\frac{\alpha^{2}(\omega)F(\omega)}{\omega}d\omega\right]$$
(39)

We have obtained  $\omega_{ln}$  using our calculated value of  $\lambda$  and  $\alpha^2(\omega)F(\omega)$ . Our computed  $\lambda$  and  $\alpha^2(\omega)F(\omega)$  are given by Eq. (27) and Eq.(28) respectively. For computation we have used same experimental data as used before. The normalized specific heat (R) at T=T<sub>c</sub> is then obtained using our calculated value of  $\omega_{ln}$  along with the evaluated value of T<sub>c</sub> from our model calculation. Our calculated value of R for La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> comes out to be 2.64, 2.64 and 2.65 respectively for case-I, case-II and case-III respectively, which is consistent with the experimental results [42].

### **Energy Gap**

The gap equation at finite temperature  $(\beta = 1/k_B T)$  is

$$\frac{1}{N_{\circ}V} = \int_{0}^{\hbar\omega_{D}} \frac{d\varepsilon}{\left(\varepsilon^{2} + \Delta^{2}\right)^{1/2}} \tanh\left[\frac{1}{2}\beta\left(\varepsilon^{2} + \Delta^{2}\right)^{1/2}\right]$$
(40)

Near T<sub>c</sub> the energy gap may be expressed as

$$\Delta(T) = 3.2k_B T_c \left[ 1 - \frac{T}{T_c} \right]^{1/2}$$
(41)

Geilikman and his colleagues [43] obtained the Energy gap equation at T=0K with the use of Eliashberg equation and the following expression were obtained

$$2\Delta(0)/k_{B}T_{c} = 3.52 \left[ 1 + \alpha \left(\frac{T_{c}}{\widetilde{\omega}}\right)^{2} \ln \left(\frac{\widetilde{\omega}}{T_{c}}\right) \right]$$
(42)

where  $\alpha = 5.3$  and  $\tilde{\omega}$  is a characteristic phonon frequency.

With the help of Eq.(42) energy gap parameter  $(2\Delta(0))$  is calculated for all three cases separately using same experimental data as used before for LSCO sample. The calculated values are  $1.921 \times 10^{-21}$  Joule ,  $1.92 \times 10^{-21}$  Joule and  $2.72 \times 10^{-21}$  Joule for case-I, case-II and case-III respectively. Results are in good agreement with experimental data [44]. For the sake of completeness variation of energy gap with qd is also studied. It is observed that the energy gap remains constant for large values of qd, for small values of qd the energy gap increases and practically infinite for zero qd.

#### **Thermal Conductivity**

We know that in a real superconductor the mean free path for collision between one quasi-particle and another  $(l_e)$  is always much greater than that for collisions between quasi-particles and lattice defects (l), so that hydrodynamic flow of the normal fluid is not possible. We shall only consider only the case where thermal conduction is electronic and where it is limited by collisions with static effects and not phonons. A successful theory for this case was developed by Bardeen Rickayzen, and Tewordt (BRT) [45]; it was based straightforwardly on a solution of the Boltzmann equation for the excitation gas, and it yielded the following result for the thermal conductivity:

$$K = \frac{k_F^2 l}{3\pi^2 \hbar T} \int_{\Delta}^{\infty} E \sqrt{E^2 - \Delta^2} \, \tau dE \, \frac{\partial f}{\partial E}$$
(43)

where l is the mean free path of the quasi-particles (equal to that for electrons in the normal state) and  $f(E) = [\exp(\beta E) + 1]^{-1}$  is the Fermi distribution for the quasi-particles at temperature T.

We have computed Thermal conductivity (K) for  $La_{2-x}Sr_xCuO_4$  at x=0.15 with the help of Eq.(43) for all the three cases. For present computation we have considered same experimental data as used before. Calculated value of thermal conductivity (K) is 0.038, 0.0387 and 0.0393 Watt meter/K for case-I, case-II and case-III respectively. From computation we observe that thermal conductivity increases with rising temperature. However, this may be pointed out here that thermal conductivity is less pronounced in LSCO because transition temperature for LSCOs are around 40 K and for low temperature (around up to 65 K) thermal conductivity is not much pronounced. On the other hand thermal conductivity is highly pronounced at higher temperature. The present results are in good agreement with the experimental data [46-50].

### CONCLUSION

On the basis of our investigation on copper-oxide superconductors, following conclusions are being drawn.

- 1. The formulism required to develop model calculations for layered structure systems have been made mathematically consistent and physically logical ab-initio. As a matter of fact the reduction of three-dimensional system to an effective two-dimensional system gives reduced degree of freedom. The occurrence of complex nature of an effective potential energy function is a direct consequence of the reduction of degree of freedom. Earlier investigations have used an ad-hoc prescription in an artificial way in order to incorporate reduced degree of freedom. Therefore, it can be concluded that our formulism provides mathematically correct and physically logical layered structure model.
- 2. An attempt has also been made to use a potential energy function, which free from singularities ab-initio. Following Gupta [24] a modified Coulomb potential energy function has been employed. For the sake of completeness we have extended model calculation on the basis of present formulism for 123 (having two conducting layer per unit cell) systems and 223 (having three conducting per unit cell) systems are in progress and shall be reported through our future communications.
- 3. Following the prescription as given by Y M Gupta [21] we have confined our investigations in the region of small momentum transfer with reference to scattering between free electrons inside the materials. This facilitates us to choose with the well-supported experimental evidence that the only electrons are the charge carriers in dielectric response function. In conventional explanation for the reason of transition temperature in superconductors two types of charge carriers are required in dielectric response function so to cover the whole region of momentum transfer. However, there is no clear-cut experimental support in favor of the charge carriers other than electrons. From the analysis it is concluded that high-T<sub>c</sub> superconductors prefers scattering in forward direction ( $Cos\theta \approx 1$ ). This provides a criteria to look for the materials which may exhibit superconducting property viz the materials which have the tendency for suffering scattering in forward direction, are the stronger candidates for seeking transition in superconducting state.

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