STRONG COUPLING MODEL FOR HIGH-\(T_C\) COPPER-OXIDE SUPERCONDUCTORS


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ABSTRACT

Model calculation have been carried out to obtain a modified effective two-dimensional dynamic interaction potential energy function in Copper-Oxide superconductors starting with modified Coulomb Potential Energy Function and Yukawa like Potential Energy Function. The calculations of Coulomb repulsive parameter, coupling strength, transition temperature, relaxation time, resistivity, specific heat, energy gap and thermal conductivity for LaSrCuO\(_4\) (Copper-Oxide superconductor consisting of one Cu-O layer per unit cell) are reported here. Our calculations show that the coupling between Cu-O conducting layers makes the effective two-dimensional dynamic interaction potential more attractive as well as less repulsive. The interaction potential energy function obtained by us is complex. Therefore, the complex nature of the present modified effective interaction potential energy function, responsible for resistivity has naturally been included.

KEYWORDS: High-\(T_C\) Superconductivity, Strong coupling theory, Electron-electron interaction

INTRODUCTION

Two-dimensional Layered Structure model has been proved successful [1-8] to understand the basic features of high-\(T_C\) Copper-Oxide superconductors (COS). However; the model suffers with mathematical inconsistency. The present model is an attempt to provide a prescription, which removes the inconsistency of the model, and also make it more viable for understanding the pairing mechanism in these superconductors. The salient features of the proposed prescription are:
1. The effective potential energy function obtained through the proposed model is complex ab-initio. Hence the resistivity of the material is included in a natural way.

2. The use of Yukawa like potential energy function provides a way to incorporate long-range correlation as desired by experimental observations [9-13].

3. It is capable of incorporating all possible exactions leading to pairing mechanism.

Theoretical results thus obtained have been successfully compared with experimental data.

FORMULISM

Case-I: Formulism based on Modified Coulomb Potential Energy Function

All the earlier investigations [14-17] based on layered structure model have taken three dimensional coulomb potential energy functions 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 \( r \to 0 \). 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 [18]. The modified coulomb potential energy function as proposed is also capable of incorporating long-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:

\[
V^o(r - r') = \frac{1}{2\pi^2 \epsilon_b^2} \frac{e^2 Si(Y | r - r' |)}{|r - r'|} 
\]

(1)

Where, \( Si(Y | r - r' |) \) 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 \( Si(x) = \sum_{m=0}^{\infty} \frac{(-1)^m x^{2m+1}}{(2m+1)!(2m+1)^2} \) and \( \epsilon \) is dielectric constant in vacuum \( \epsilon_b \) is static dielectric constant of background.

It is worth mentioning that the modified coulomb potential energy function as proposed in Eq. (1) is regular at the origin and leads to the usual coulomb potential energy function at large distances without introducing any additional parameter. The modified effective potential energy function can be obtained using Dyson diagrammatic technique. Taking two-dimensional Fourier transform, in the X-Y plane, and following the procedure [19] we get the modified bare potential energy function in two-dimensional plane as:

\[
V^o(q) = \frac{e^2}{\pi \epsilon_b^2} \int_0^\infty \frac{J_0(q \rho)}{\rho} Si(Yr) \rho d\rho 
\]

(2)

Here \( \rho = \sqrt{(X - X')^2 - (Y - Y')^2} \)

Now \( Si(Yr) \) can be written as...
\[ Si(Yr) = \frac{\pi}{2} - f(Yr)\cos(Yr) - g(Yr)\sin(Yr) \quad (3) \]

Where \[ f(Yr) = \int_{0}^{\infty} \frac{e^{-Yr t}}{t^2 + 1} dt \]

And \[ g(Yr) = \int_{0}^{\infty} \frac{t e^{-Yr t}}{t^2 + 1} dt \]

Using above expression of \( Si(Yr) \), \( V^o(q) \) can be written as

\[ V^o(q) = \frac{e^2}{\pi \varepsilon_b} \int_{0}^{\infty} \frac{J_1(q \rho)}{\rho} \left[ \frac{\pi}{2} - f(Yr)\cos(Yr) - g(Yr)\sin(Yr) \right] \rho d\rho \quad (4) \]

Or \[ V^o(q) = I_1 + I_2 + I_3 \quad (5) \]

Where \[ I_1 = \frac{e^2}{\pi \varepsilon_b} \int_{0}^{\infty} \frac{J_1(q \rho)}{\rho} \rho d\rho \quad (6) \]

\[ I_2 = -\frac{e^2}{\pi \varepsilon_b} \int_{0}^{\infty} \frac{J_1(q \rho)}{\rho} f(Yr)\cos(Yr) \rho d\rho \quad (7) \]

And \[ I_3 = -\frac{e^2}{\pi \varepsilon_b} \int_{0}^{\infty} \frac{J_1(q \rho)}{\rho} g(Yr)\sin(Yr) \rho d\rho \quad (8) \]

After carrying out the integral Eq. (6) yields

\[ I_1 = \frac{e^2}{2 \varepsilon_o \varepsilon_b} e^{-q(z-z')}(9) \]

It is found [19] that layering effect is significant for small values of \( qd \) only. We shall therefore, confine our discussion and analysis in the limit of small \( qd \). In this limit (small \( qd \)) \( I_2 \) and \( I_3 \) get simplified and are given as

\[ I_2 = -\frac{e^2}{2 \varepsilon_o \varepsilon_b Y} - \frac{5}{24} \frac{e^2 q^2}{\varepsilon_o \varepsilon_b Y^3} - \frac{e^2 q^2 (z-z')^2}{8 \varepsilon_o \varepsilon_b Y} \quad (10) \]

And \[ I_3 = -\frac{e^2}{2 \varepsilon_o \varepsilon_b Y} + \frac{1}{24} \frac{e^2 q^2}{\varepsilon_o \varepsilon_b Y^3} - \frac{e^2 q^2 (z-z')^2}{8 \varepsilon_o \varepsilon_b Y} \quad (11) \]

Now using Eq.(9), Eq.(10) and Eq.(11) the two-dimensional modified bare Coulomb potential energy function Eq.(5) reduces to

\[ V^o(q, z, z') = \frac{e^2}{2 \varepsilon_o \varepsilon_b} e^{-q(z-z')} - \frac{e^2}{\pi \varepsilon_b Y} - \frac{e^2 q^2}{6 \varepsilon_o \varepsilon_b Y^3} - \frac{e^2 q^2 (z-z')^2}{4 \varepsilon_o \varepsilon_b Y} \quad (12) \]

As the charge carriers are confined only in the two-dimensional conducting planes, \( z \) and \( z' \) can be represented by discrete variables \( n \) and \( n' \) 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. (12) it is evident that the modified 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. \( \ln-n' \) appears in the expression of modified bare potential. Consequently Eq. (12) reduces to

\[
V^o(q,n,n') = \frac{e^2}{2\varepsilon e} \frac{1}{q} e^{-\frac{q}{\varepsilon e} n' d} - \frac{e^2}{\pi\varepsilon e Y} \frac{e^2 q^2}{6\pi\varepsilon e Y^3} - \frac{e^2 q^2}{4\pi\varepsilon e Y} (13)
\]

Assuming that polarizability for a given conducting plane can be expressed as sum of the polarizability of all the possible charge carriers and all conducting planes to be identical, we obtain the modified effective potential energy function employing Dyson diagrammatic technique and using Discrete Fourier Transform (DFT) [20], as

\[
V(q,\omega,k_z) = \frac{V^o(q,k_z)}{\epsilon(q,\omega,k_z)} (14)
\]

Where \( \epsilon(q,\omega,k_z) = 1 - \prod_{n} (q,\omega) \)

\[
\prod_{n} (q,\omega) = \text{Polarization function for the two-dimensional conducting plane}
\]

\[
V^o(q,k_z) = \frac{e^2}{2\varepsilon e} \sum_{n-n'} (q|n-n'|) e^{ik_z (n-n')} (15)
\]

It is worth to emphasize that the earlier workers [14-17] have obtained the effective potential energy function using mod of \( (n-n') \) only in the expression for \( V^o(q,|n-n'|) \) and not taking mod of \( (n-n') \) in the exponential occurring in Eq. (15). 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. \( \ln-n' \) contributes wherever it occurs in the formalism. Following the technique [19], and taking mod of \( (n-n') \) wherever it occurs in formulism, Eq. (15) yields

\[
V^o(q,k_z) = \frac{e^2}{2\varepsilon e} \left[ \frac{1+e^{(q-k)d}}{1-e^{-(q-k)d}} \right] - \frac{e^2}{\pi\varepsilon e Y} \frac{e^2 q^2}{6\pi\varepsilon e Y^3} \left[ \frac{1+e^{(k-d)}}{1-e^{-(k-d)}} \right] - \frac{e^2 q^2 d^2}{2\pi\varepsilon e Y} e^{ikz} \left( \frac{1+e^{(k-d)}}{1-e^{-(k-d)}} \right) (16)
\]

Form Eq. (14) and Eq. (16) we get

\[
V(q,\omega,k_z) = \frac{e^2}{2\varepsilon e} \left[ \frac{1+e^{(q-k)d}}{1-e^{-(q-k)d}} \right] - \frac{e^2}{\pi\varepsilon e Y} \frac{e^2 q^2}{6\pi\varepsilon e Y^3} \left[ \frac{1+e^{(k-d)}}{1-e^{-(k-d)}} \right] - \frac{e^2 q^2 d^2}{2\pi\varepsilon e Y} e^{ikz} \left( \frac{1+e^{(k-d)}}{1-e^{-(k-d)}} \right) (17)
\]
\[ V(q, \omega, k_z) = \frac{e^2}{2\varepsilon \varepsilon_0 q} \left( 1 + e^{-i(kz - d)} \right) - \frac{2q}{\pi^2} + \frac{q^3}{3\pi^3} \left[ 1 + e^{-i(kz - d)} \right] - \frac{q^3 d^2}{2\pi^3} \left( \frac{1 + e^{-i(kz - d)}}{1 - e^{-i(kz - d)}} \right) \]

\[ 1 + P(q, \omega) \left( 1 + e^{-i(qz - d)} \right) - \frac{2q}{\pi^2} + \frac{q^3}{3\pi^3} \left[ 1 + e^{-i(qz - d)} \right] - \frac{q^3 d^2}{2\pi^3} \left( \frac{1 + e^{-i(qz - d)}}{1 - e^{-i(qz - d)}} \right) \]

Where \( P(q, \omega) = -\frac{e^2}{2\varepsilon \varepsilon_0 q} \prod_{\omega} (q, \omega) \)

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 \( P(q, \omega) \) [21], in order to see the coupling effects in a simple manner. We take \( P(q, \omega) \) as

\[ P(q, \omega) = \frac{q \varepsilon^2 k_F^2}{m^* \varepsilon \varepsilon_0 \left( \frac{q^2 V_F^2}{2} - \omega^2 \right)} \]

Where \( k_F \) and \( V_F \) are Fermi wave vector and Fermi velocity, respectively and \( m^* \) is effective mass.

**Case-II: Formulism based on Yukawa like Potential Energy Function**

To obtain the effective two-dimensional dynamic potential energy function we start with short-range Yukawa like potential energy function, \( V^\omega | \vec{r} - \vec{r}' | \), for the pair of charge carriers existing in consecutive conducting planes to incorporate all possible exactions as exchange particle. It is given as:

\[ V^\omega | \vec{r} - \vec{r}' | = \frac{1}{4\pi\varepsilon \varepsilon_0 | \vec{r} - \vec{r}' |} e^{\left( \frac{q^2 \varepsilon^2 k_F^2}{m^* \varepsilon \varepsilon_0 \left( \frac{q^2 V_F^2}{2} - \omega^2 \right)} \right)} \]

Here \( \varepsilon_0 \) is dielectric constant in vacuum \( \varepsilon_0 \) is static dielectric constant of background and \( \mu \) is inverse Compton wavelength of exchange particle, given as \( \mu = m_{exch} c / \hbar \)

Following the similar prescription as adopted in case-I the bare and effective potential energy functions thus obtained are given here respectively:

\[ V^\omega(Q, k_z) = \frac{e^2}{2\varepsilon \varepsilon_0 Q} \left( 1 + e^{-iQz - d} \right) \]

\[ V(Q, \omega, k_z) = \frac{e^2}{2\varepsilon \varepsilon_0 Q} \left( 1 + e^{-iQz - d} \right) \]

Here \( Q = \sqrt{\mu^2 + q^2} \) and \( q \) is momentum transfer wave vector.
RESULT AND DISCUSSION

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 thus obtained, is as follows:

\[ \omega_c = \sqrt{\frac{q^2V_F^2}{2} + \frac{q^2k_F^2}{m^*\varepsilon_b}} \]  
\[ (23) \]

The frequency range in which modified effective interaction potential energy function is attractive can be given as:

\[ \sqrt{\frac{q^2V_F^2}{2}} \leq \omega \leq \sqrt{\frac{q^2V_F^2}{2} + \frac{q^2k_F^2}{m^*\varepsilon_b}} \]  
\[ (24) \]

For the values of \( \omega \), lying beyond the inequality in Eq. (24), \( V(q, \omega) \) is repulsive.

2. To test the validity of our model we have calculated the following properties

We have computed following for \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) at \( x=0.15 \) in both the cases which are well in agreement with theoretical and experimental results [22-25]. For computation we used \( m^* = 4m_e \), \( k_F = 0.2833 \text{ Å}^{-1} \), \( d = 13.25 \text{Å} \), \( q_c = 0.0239 \text{ Å}^{-1} \) and \( \varepsilon_b = 22 \) and carrier concentration \( n_s = 1.277 \times 10^{18} \text{ m}^{-2} \)

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Physical Quantity</th>
<th>Case-I</th>
<th>Case-II</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Coupling Strength</td>
<td>1.66</td>
<td>1.54</td>
</tr>
<tr>
<td>2</td>
<td>Coulomb repulsive parameter</td>
<td>0.05</td>
<td>0.02</td>
</tr>
<tr>
<td>3</td>
<td>Transition temperature</td>
<td>39.9 K</td>
<td>39.6 K</td>
</tr>
<tr>
<td>4</td>
<td>Relaxation time</td>
<td>( 3.2 \times 10^{-14} \text{ Sec} )</td>
<td>( 3.9 \times 10^{-14} \text{ Sec} )</td>
</tr>
<tr>
<td>5</td>
<td>Resistivity</td>
<td>( \rho = 0.8918 \mu\Omega \text{meter} )</td>
<td>( 0.7317 \mu\Omega \text{meter} )</td>
</tr>
<tr>
<td>6</td>
<td>Specific heat</td>
<td>2.65</td>
<td>2.65</td>
</tr>
<tr>
<td>7</td>
<td>Energy gap</td>
<td>( 2.72 \times 10^{-21} \text{ Joule} )</td>
<td>( 1.921 \times 10^{-21} \text{ Joule} )</td>
</tr>
<tr>
<td>8</td>
<td>Thermal conductivity</td>
<td>0.0393 Watt-m/K</td>
<td>0.038 Watt-m/K</td>
</tr>
</tbody>
</table>

CONCLUSIONS

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

1. The formalism required to develop model calculations for layered structure systems has 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 results in constrained system. The occurrence of complex nature of an effective
potential energy function is a direct consequence of the constrained system. Earlier investigators have used an ad-hoc prescription in an artificial way, in order to incorporate the imaginary part of potential energy function. Therefore, it can be concluded that our formalism provides mathematically correct and physically logical layered structure model.

2. An attempt has been made to develop a formalism, which incorporates all possible excitons as exchange particles may be responsible for the formation of Cooper pairs. In this formalism the only free parameter is mass of exchange particle, which can be obtained by the band theory of solids. Nevertheless the present investigations indicate that very light particles \( m_{\text{exch}} \approx 10^{-34-35} \text{Kg} \) are being exchanged responsible for the formation of Cooper pair. Further the results are highly sensitive if the mass of exchange particle is greater than \( 10^{-34} \text{Kg} \) (say \( 10^{-32} \) to \( 10^{-33} \text{Kg} \)) and less sensitive if the mass of exchange particle is larger than \( 10^{-34} \text{Kg} \). This suggests that effectively zero mass particles are exchanged for the formation of Cooper pairs.

3. An attempt has also been made to use a bare potential energy function, which is free from singularities ab-initio. Following Prof. Gupta a modified Coulomb potential energy function has been employed.

4. The effective two-dimensional dynamic interaction potential energy function thus developed is attractive in the region of plasma frequency mode. It is therefore indicated that plasmons are providing the main contribution for the formation of Cooper pairs in copper-oxide superconductors.

5. The values of coupling strengths \( \lambda \) deduced by us are found to be greater than 1 this favors the occurrence of the strong coupling theory. Also, the Coulomb repulsive parameter \( \mu^* \) obtained by us is exceedingly small \(( \approx 0.03 \) which indicates that repulsion between the electrons of a Cooper pair is very small. It also leads to strong coupling theory.

6. 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 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-\( T_c \) superconductors prefers scattering in forward direction \(( \cos \theta \approx 1 \) ). This provides a criterion to look for the materials, which may exhibit superconducting property, viz the materials which have the tendency for suffering scattering in forward direction, as the potential candidates for seeking transition in superconducting state.

7. From our calculations it is evident that almost identical results are obtained for the physical parameters analyzed during the course of present investigation for both the cases. Thus the investigated properties of the systems like LSCO do not explore the region where the three chosen potential energy functions have distinct behavior. At very short distances modified Coulomb potential energy function has characteristically different behavior as compared to Yukawa like potential energy functions. Nevertheless the use of modified Coulomb potential energy function makes the theory mathematically consistent and free from singularity, which has played important role in classical electrodynamics, right from its inception. Investigation of microscopic
phenomenon like nuclear tunneling may provide a distinction between both potential energy functions chosen by us.

In conclusion, though our calculations are model dependent, yet the consistent agreement of our calculations with available experimental data seems to indicate that the layered structure model based on reduced dimensionality describe some gross features of high-\(T_c\) superconductors, quantitatively.

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REFERENCES