TRANSITION TEMPERATURE OF SUPERCONDUCTING HYBRIDIZED CUPRATE SYSTEMS


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ABSTRACT
To study the properties of high-Tc superconducting Cuprates, it is assumed that the three- electron system contributes to the superconducting current. Two electrons constitute a pair called the Cooper pair which acts as a boson and the third electron which is a fermion surrounds the Cooper pair. Quantum Statistical mechanics of a mixture of bosons and fermions has been used to study the superconducting state.

Key Words: Hybridized Cuprate System, High-Tc Superconductivity, Coherence Length, Debye Frequency.

INTRODUCTION
Superconductivity is exhibited by elements, alloys and oxides with a range of compositions and structures. The copper oxide based materials and those of the conventional superconductors exhibit two classical characteristics of zero resistivity and the exclusion of magnetic field from its core. An increase in the electron-phonon coupling strength or the density of electronic states at the Fermi level is expected to raise the critical temperature values. When electrons move through the lattice, they tend to polarize the lattice as they interact with the ions. For lower mass lattice ions, a superconducting state may appear at a higher Tc.

High-Tc superconductivity was discovered (Ayodo et al., 2011) in 1986 using a Lanthanum-Barium-Copper Oxide (La-Ba-Cu-O) that gave a transition temperature (Tc) of 34K. (Wu et al., 1987) found that replacing Lanthanum with Yttrium raised Tc to 92K, a temperature higher than the boiling point of nitrogen, the most common refrigerant. There were more breakthroughs in 1993 when studies made on a Thallium-Mercury-Copper-Barium-Calcium-Oxygen ceramic by (Puri and Babbar, 2001) and a team of researchers yielded a transition temperature of 138K.

A theoretical model of high-Tc superconductivity based on the presence of charge stripes was presented by (Emery and Kivelson, 1994). However, the model was not applicable to cuprates since it has no charge spin separation. (Gaballe, 1993) proposed that H-Tc materials should be multi-component structures with more than two sites per unit cell, one of which is used to introduce charges. Composition should be near the metal-insulator Mott-transition. On the insulating side of Mott-transition, the localized states should have spin-1/2 ground state and anti-ferromagnetic ordering of the parent compound.

The optimal critical temperature, Tc, for cuprate superconductors and their doping curves was analyzed by (Oesterreicher, 2009). The phenomenon was explained in terms of bond-length ordering in the crystal denoting that all high–Tc superconducting materials organize themselves into patterns of local pairs of electrons or holes and electrons represented by doped radical bonds extending along correlated strings. The charge distribution along these strings of pairs of charges involves coupling of locally distorted bond-length order network through elastic interactions that influence transition temperature. However, the actual value of holes in the extended planar system was not known. Holes in most cuprates originate from the oxygen atoms pumped in the unit cell along the b-axis. Thus inter-atomic distance between oxygen and copper atoms must first be considered. This is because any amount of oxygen cannot be pumped into
the unit cell. Additionally, this theory does not take into consideration the temperature at which the atoms that generate the holes are introduced in the superconductor. This temperature is of great importance because it determines the whole concentration (Naqib, 2009).

The replacement of Oxygen with Chalcogenides was proposed by (Tsendin and Denisov, 2001) e.g. sulphur in YBaCuO, in large amount, will significantly increase critical temperature. In this model, attention is given to localized pairs of electrons and negative-U centres. Negative-U centres are centres of localized electrons that neighbor one another or simply the copper ion centres in the lattice with energy U. Transition of electrons from one centre to another in the process of forming Cooper pairs is guided by a matrix element. This study gives a slightly different approach in that it gives special consideration of the influence to the unpaired electrons on the Cooper pairs in the condensate to speculate on a possible conduction mechanism for High-Tc superconducting cuprates. Taking hint from this, we have proposed a three electron model in which a Cooper pair interacts with the third (unpaired) electron and have studied how this can lead to superconductivity.

The Three Electron Model

The quantum statistical mechanics postulates that elementary particles are either bosons or fermions. We have proposed a model where there is a bound pair of electrons in the condensed state and a third electron that interacts with the bound pair. The bound pair of electrons or the Cooper pair is considered to be a boson. This is because when two fermions with spins up and down form a pair, like the Cooper pair, for all practical purposes, the particle thus formed behaves like a boson, to be exact, it forms a composite probability function of bosons and that of fermions respectively. The distribution of electron pairs and the single electrons in the superconducting substrate, for example, is obtained from the free electron theory (Puri and Babbar, 2001) as;

\[
\frac{f_{BF}(E)}{\exp\left(\frac{E - \mu}{k_BT}\right) - 1} = \frac{2 \exp\left(\frac{E - \mu}{k_BT}\right)}{\exp\left(\frac{E - \mu}{k_BT}\right) + 1}
\]

Here, \(\mu\) is chemical potential for the mixture of bosons and fermions which according to our analysis is constant and equal to 2.5eV.

When a boson and a fermion interact the resulting system will be a fermion, thus the total number of electrons in our system is obtained from the free electron theory (Puri and Babbar, 2001) as;

\[
N = \frac{v}{2\pi^2} \left(\frac{2M}{\hbar^2}\right)^{3/2} \int_0^{\infty} E^{3/2} f(E) dE
\]

where \(v\) is volume of the unit cell of the superconducting substrate, \(M\) is the mass of the electrons and \(E\) is the energy of the system, \(f(E)\) is the probability function, which in our case, will be \(f_{BF}(E)\). We take the mass, \(M_e\) of the electrons as the reduced mass of the Cooper pair and that of the single electron. Thus;

\[
N = \frac{v}{2\pi^2} \left(\frac{2M_e}{3\hbar^2}\right)^{3/2} \int_0^{\infty} E^{3/2} f_{BF}(E) dE
\]
Using equation 1 in equation 3, fixing the upper limit to Fermi energy, $E_F$, integrating and simplifying gives:

$$N = \frac{\nu}{2\pi^2} \frac{2M_q^2}{3\hbar^2} \frac{1}{k_B T} \left[ \frac{1}{E_F} \left( -\mu^2 \right) + \mu \tanh^{-1} \left( \frac{1}{E_F} \frac{1}{-\mu^2} \right) \right]$$

(4)

The standard Berdeen-Cooper-Schriffer (BCS) formalism (Menon et al., 2001) applied to delocalized quasi-particles with a well defined density of states gives:

$$\frac{2}{\nu} = \int_{-k_B \theta_D}^{k_B \theta_D} N \frac{1}{E} \tanh \left( \frac{E}{2k_B T_c} \right) dE$$

(5)

where $T_c$ is the transition temperature, $V$ is the coupling potential of Cooper pairs and $N$ is the total number of electrons.

In our calculations, $V$ becomes the effective interaction potential of the Cooper pairs with the unpaired electrons.

Coupling potential of the Cooper pairs (Khanna, 2008) is given by:

$$V_1 = \frac{M_q^2}{\hbar \omega_D}$$

(6)

where $M_q$ is the matrix element of electron-phonon interaction and has the dimensions of energy and $\omega_D$ is Debye frequency. The interaction potential for Cooper pairs and the unpaired electrons is considered as Coulombic and is given by; $V_2 = \frac{2ke^2}{r}$, where $r$ is the mean distance between the Cooper pair and the single electron and $K = \frac{1}{4\pi \varepsilon_0 \varepsilon_r}$, in which case $\varepsilon_r$ is relative permittivity of the superconductor and it is equal to 500 for cuprates. The total coupling potential, $V$, between Cooper pairs and the unpaired electrons becomes; $V = V_1 + V_2$ which gives;

$$V = \frac{rM_q^2 + 2\hbar \omega_D Ke^2}{\hbar \omega_D r}$$

(7)

On using equations (4) and (7) in equation (5) and using the approximations; $\sinh x \approx x$, $\tanh x \approx x$ for small values of $x$, and the mean distance, $r$, between the Cooper pair and the unpaired electron to be equal to coherence length, $\varepsilon$, the value of $T_c$ is found to be:

$$T_c = \frac{3\sqrt{3} \nu}{\pi^2} \frac{\theta_D}{2} \frac{\left( eM_q^2 + 2\hbar \omega_D Ke^2 \right)}{2\hbar \omega_D \varepsilon} \left[ \frac{M_q^2}{\hbar^2} \right]^{\frac{3}{2}} \left[ \frac{1}{E_F^2} - \mu^2 \tanh^{-1} \left( \frac{1}{E_F} \frac{1}{-\mu^2} \right) \right]$$

(8)

In this equation, $\theta_D$ is Debye temperature, $T_c$ is critical temperature, $E_F$ is Fermi energy of the superconductor and $\varepsilon = k_B T$, where $T$ is the temperature of the system. The equation gives the critical temperature of high-$T_c$ superconducting cuprates. Equation (8) is referred to as the Three Electron- $T_c$ equation.

RESULTS AND DISCUSSION

Variation of $T_c$ with various physical quantities is given by equation (8). Values of the different parameters used to get $T_c$ are given below:
Debye frequency for metals($\omega_D$) $\omega_D = 3.983 \times 10^{10}$ Hz

Matrix element of electron-phonon interaction($M_q$) $M_q = 0.5$ eV

Coherence length for YBCO, $\varepsilon$ $\varepsilon = 15$ Å

Chemical potential for the mixture of fermions and bosons $\mu = 2.5$ eV

The Critical temperature appears as an extensive property of the system as it varies linearly with volume of the unit cell (Figure 1). Essentially, the volume of the unit cell of a cuprate can be increased by increasing the number of copper oxide layers per unit cell is influenced by the increased lattice parameter. This work, therefore indicates that increasing the number of copper oxide layers can raise the value of $T_c$. This agrees with experimental results (Marouchkine, 2004). Mercury cuprate Hg1223 which has the highest $T_c = 135$K has 3 copper oxide planes. However, the same cuprate with 2 copper oxide planes, Hg1212 has a lower $T_c = 128$K. (Cooper et al., 1990) also obtained a linear variation of $T_c$ with unit cell volume of Molybdenum-Boron superconductor. $T_c$ increased linearly with $v$ up to $T_c$=10K. Beyond this point, $T_c$ remained constant for all values of $v$. In the family of thallium cuprates, Tl 1224 with 3 copper oxide planes has $T_c = 128$K, while Tl2201 which has 1 copper oxide plane has a lower $T_c = 95$K. In Yttrium cuprates, YBCO, $T_c$ increases with increase in oxygen content pumped along the b-axis (Tsendin and Denisov, 2001). This is because the holes that enhance superconductivity in this compound are contributed by the oxygen atoms. Thus to increase $T_c$ in YBCO, the volume of the unit cell should be increased.

It is a known fact that external pressure affects $T_c$ through changing unit cell volume. However, it should be noted that external pressure and temperature are related via general thermodynamic relations. Since external pressure changes the volume of the unit cell, it means $T_c$ can vary with unit cell volume and this is the result we got in our manuscript.

![Figure 1: Variation of critical temperature, $T_c$ with unit cell volume, $v$.](image-url)
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Figure 2 shows hyperbolic variation of critical temperature with Debye frequency. \( T_c \) increases with decrease in Debye frequency and as \( \omega_D \) approaches \( 0.8 \times 10^{13} \) Hz, \( T_c \) becomes constant. Debye frequency that gives the highest rise in \( T_c \) is in the range 0 to \( 2 \times 10^{13} \) Hz. Room temperature \( T_c \approx 300 \text{K} \) can only be achieved if Debye frequency is \( 1.4 \times 10^{13} \) Hz. The variation of critical temperature with Debye frequency is a new idea to the area of High \( T_c \) superconductivity in that many researchers were limited to the variation of critical temperature with Debye temperature. (Jain and Kachhava, 1980) expressed critical temperature in terms of phonon frequency. We have obtained the value of \( T_c \) in terms of Debye frequency. Considering the natural frequency of vibration of the superconducting charge carriers near the Fermi surface as equal to Debye frequency then our model suggests that his frequency must be low in order to facilitate superconductivity because the energy of the superconducting charges must be as low as possible. Low frequency implies low energy. This then explains why most of the superconducting electrons have been found to be concentrated close to the Fermi level of the superconductor (Menon et al., 2001). Fermi level is the highest filled energy level at 0K.

![Figure 2: Graph of critical temperature, \( T_c \) Vs Debye frequency, \( \omega_D \).](image)

![Figure 3: Variation of Critical Temperature, \( T_c \) with Coherence length, \( \varepsilon \).](image)
Critical temperature is high for small values of coherence length and low for large values of coherence length (Figure 3). The high values of critical temperature are obtained when coherence length or the mean distance between the Cooper pair and the unpaired electron is reduced below 3Å. High transition temperature \( (T_c \approx 300K) \) can be achieved if the coherence length is 2Å and the energy of the system \( \varepsilon = \frac{k_B T_c}{2} = 0.2583eV \). Experimental results of \( T_c \) and \( \varepsilon \) along the a-b plane of the unit cell for various groups of cuprates (Oesterreicher, 2003) show that NCCO, which has the highest coherence length of 58Å has the lowest \( T_c \) of 24K while Hg1223 cuprate which has the smallest coherence length of 13Å has the highest \( T_c \) of 135K. Our calculations seem to agree with these experimental observations.

**Conclusion**

In this work, we have formulated a theory of High-\( T_c \) superconductivity based on a three electron model of what we now refer to as a hybridized cuprate system. It is clear that an unpaired electron, 2Å away from the Cooper pair will interact with the Cooper pair in such a way as to raise the critical temperature of the system to the much desired \( T_c = 300K \) (Room temperature \( T_c \)). Bulk superconductivity is possible since the results show linear variation of \( T_c \) with the volume of the superconducting substrate. However, the process of fabricating increased volume or multilayered superconductors may not be easy. Careful construction of the superconductor in such a way that the Debye frequency be lower than \( 2 \times 10^{13} \)Hz will also enable us to achieve \( T_c = 300K \).

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**REFERENCES**