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Research Article

TRANSITION TEMPERATURE OF SUPERCONDUCTING HYBRIDIZED CUPRATE SYSTEMS

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ABSTRACT
To study the properties of high-T_c 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-T_c 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 T_c.

High-T_C superconductivity was discovered (Ayodo *et al.*, 2011) in 1986 using a Lanthanum-Barium-Copper Oxide (La-Ba-Cu-O) that gave a transition temperature (T_c) of 34K.(Wu *et al.*, 1987) found that replacing Lanthanum with Yttrium raised T_C 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.

Atheoretical model of high-T_c 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-T_c 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, T_c, for cuprate superconductors and their dopping curves was analyzed by (Oesterreicher, 2009). The phenomenon was explained in terms of bond-length ordering in the crystal denoting that all high–T_c 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-T_c 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 boson hence we subject this system to the Bose-Einstein statistics (Marouchkine, 2004). The single electron is the polarization electron, which hops from one lattice site to another of similar symmetry. This electron is assumed to cause high frequency vibrations to the apical oxygen that contributes to electron-phonon coupling. The system of single electron will be governed by the Fermi-Dirac statistics (Oesterreicher, 2003). The distribution of electron pairs and the single electrons in the superconducting state will be guided by the probability function of bosons and fermions respectively. The distribution probability function of the mixture of fermions and bosons $f_{BF}(E)$, will be the sum of the probability function of bosons and that of fermions. This is because the interaction between the Cooper pair and the single electron is coulombic leading to,

$$f_{BF}(E) = \frac{2\exp\left(\frac{E-\mu}{k_B T}\right)}{\exp 2\left(\frac{E-\mu}{k_B T}\right) - 1} \qquad (1)$$

Here, μ 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;

$$N = \frac{v}{2\pi^2}\left[\frac{(2M)}{\hbar^2}\right]^{\frac{3}{2}} \int_0^{\infty} E^{\frac{1}{2}} f(E)\, dE \qquad (2)$$

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;

$$N = \frac{v}{2\pi^2}\left[\frac{(2M_e)}{3\hbar^2}\right]^{\frac{3}{2}} \int_0^{\infty} E^{\frac{1}{2}} f_{BF}(E)\, dE \qquad (3)$$

Using equation 1 in equation 3, fixing the upper limit to Fermi energy, E_F, integrating and simplifying gives;

$$N = \frac{v}{2\pi^2}\left[\frac{2M_e}{3\hbar^2}\right]^{\frac{3}{2}} k_B T \frac{E_F^{\frac{1}{2}}\left(-\mu^{\frac{1}{2}}\right) + \mu tanh^{-1}\left(\frac{E_F^{\frac{1}{2}}}{-\mu^{\frac{1}{2}}}\right)}{-\mu^{\frac{1}{2}}} \quad (4)$$

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

$$\frac{2}{V} = \int_{-k_B\theta_D}^{k_B\theta_D} N\frac{1}{E}\tanh\left(\frac{E}{2k_B T_c}\right) dE \quad (5)$$

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;

$$V_1 = \frac{M_q^2}{\hbar\omega_D} \quad (6)$$

where M_q is the matrix element of electron-phonon interaction and has the dimensions of energy and ω_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 ε_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;

$$V = \frac{rM_q^2 + 2\hbar\omega_D Ke^2}{\hbar\omega_D r} \quad (7)$$

On using equations (4) and (7) in equation (5) and using the approximations; sinhx≈x , tanhx≈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, ε,the value of T_c is found to be:

$$T_c = \frac{3\sqrt{3}v}{\pi^2}\epsilon\theta_D \frac{\left(\varepsilon M_q^2 + 2\hbar\omega_D Ke^2\right)}{2\hbar\omega_D\varepsilon}\left[\frac{M_e}{\hbar^2}\right]^{\frac{3}{2}}\left[E_F^{\frac{1}{2}} - \mu^{\frac{1}{2}}tanh^{-1}\left(\frac{E_F^{\frac{1}{2}}}{-\mu^{\frac{1}{2}}}\right)\right] \quad (8)$$

In this equation, θ_D is Debye temperature, T_c is critical temperature, E_F is Fermi energy of the superconductor and $\epsilon = k_B T$, 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(ω_D)	$\omega_D = 3.983\times10^{10}$Hz
Matrix element of electron-phonon interaction(M_q)	M_q = 0.5 eV
Coherence length for YBCO, ε	ε =15Å
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 lattice parameters. 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 = 135K has 3 copper oxide planes. However, the same cuprate with 2 copper oxide planes, Hg1212 has a lower T_c = 128K. (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 = 128K,while Tl2201 which has 1 copper oxide plane has a lower T_c = 95K. 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.

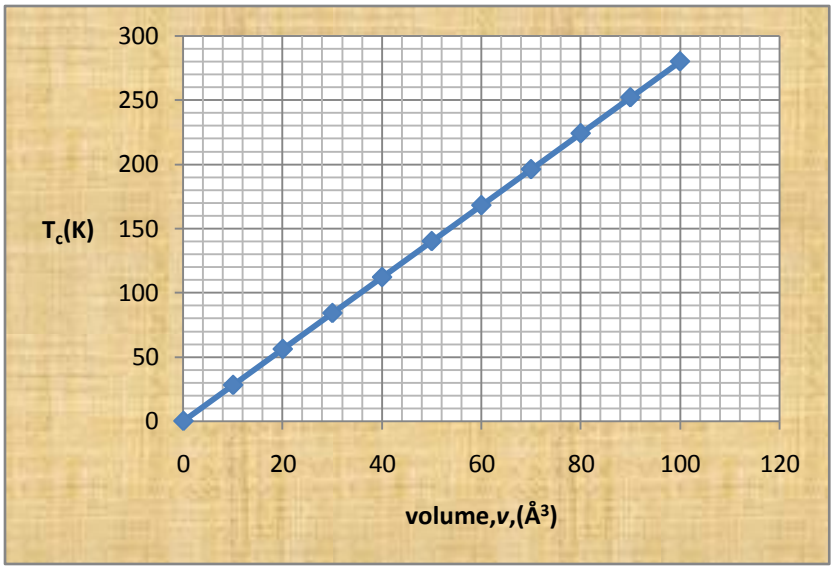

Figure 1: Variation of critical temperature,T_c with unit cell volume, *v*.

Figure 2 shows hyperbolic variation of critical temperature with Debye frequency. T_c increases with decrease in Debye frequency and as ω_D approaches 0.8×10^{13} Hz,T_c becomes constant. Debye frequency that gives the highest rise in T_c is in the range 0 to 2×10^{13} Hz. Room temperature $T_c \approx 300$K can only be achieved if Debye frequency is 1.4×10^{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.

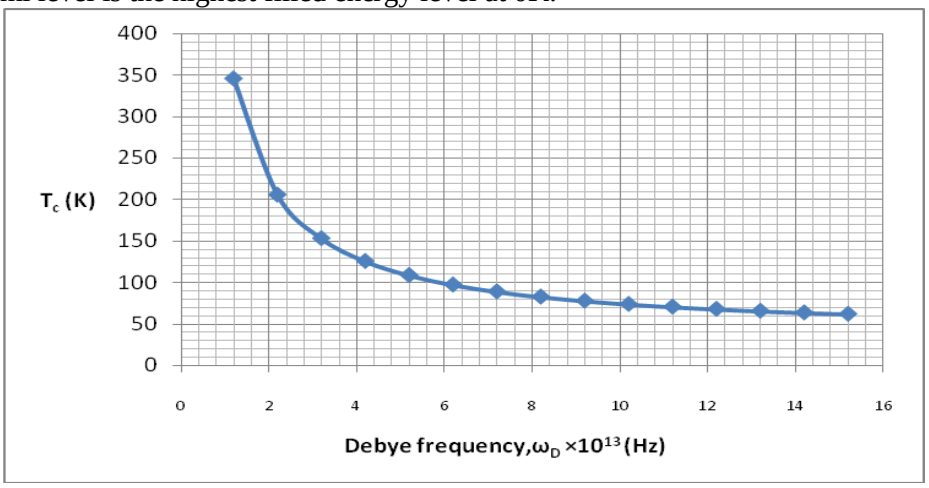

Figure 2: Graph of critical temperature, T_c Vs Debye frequency, ω_D.

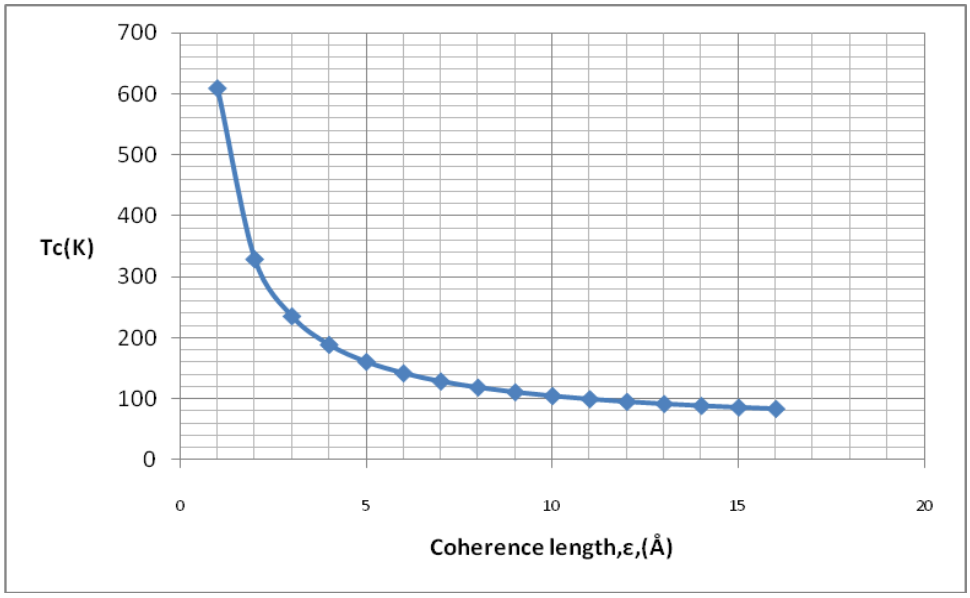

Figure 3: Variation of Critical Temperature, T_c with Coherence length,ε.

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 $\in = k_B T_c = 0.2583eV$ · Experimental results of T_c and ε 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 away that the Debye frequency be lower than 2×10^{13}Hz will also enable us to achieve T_c=300K.

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