THEORETICAL DETERMINATION OF SPECIFIC HEAT AND CRITICAL TEMPERATURE OF HIGH-T_C CUPRATE SUPERCONDUCTORS BASED ON INTRALAYER AND INTERLAYER INTERACTIONS

BY

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NOVEMBER, 2013

DECLARATION

DECLARATION BY THE STUDENT

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DEDICATION

To my lovely wife Vilary Chebet, daughters Patricia Chelangat and Elsie Chepchumba for their continuous moral support. I would not also forget my parents for their tireless effort to bring up in a scholarly manner.

ABSTRACT

The role of attractive interlayer and intralayer interactions in layered high-T_c Cuprate superconductors was investigated using a two-layer Hamiltonian. The Hamiltonian was formulated and diagonalized using Bogoliubov canonical transformations to get equations of the i^{th} state, E_i, specific heat, C_V in the superconducting state, and critical temperature, T_c. The heat capacity in the superconducting state was analyzed in the temperature domain 10 K $\leq$ T$\leq$ 100 K. The transition temperature obtained from the graph was 90.7K. This value is the same as that calculated from the derived equation of T_c for Yttrium Barium Copper Oxide which was considered in this study. The variation of transition temperature and on-site Coulomb repulsion *U* for fixed values of interlayer hopping, t, interlayer interaction, *W* was analyzed. The study reveals that an increase in interlayer hopping, t and interlayer *W* increases *U* which further enhances T_c. Hence interlayer and intralayer interactions play an important role in the enhancement of T_c in layered high-T_c Cuprates. There is agreement between the theoretical results, for instance, the values of C_V, T_c and C_s/C_n calculated in this thesis and the experimental results for the high-T_c superconductor Yttrium Barium Copper Oxide.

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LIST OF SYMBOLS AND ABBREVIATIONS

SYMBOL **MEANING**

a,b,c…………………………Cell Parameters

$a^{+}_{k\sigma}$ ……………………… Creation Operator

$a_{k\sigma}$ ……………………….Annihilation Operator

B ………………………… Magnetic flux

C_{el} …………………………. Electronic Specific Heat

C_V …………………………. .Heat Capacity

E …………………………… Total Energy

E_i …………………………… Energy of State i after diagonalization

E_f …………………………….Electric Field

E_f …………………………….Fermi Energy

ε_k …………………………….Energy of State k

H ……………………………Magnetic Flux

H_c …………………………. .Critical Field

H_{inter} ……………………….. Interlayer Hamiltonian

H_{intra} …………………….. …Intralayer Hamiltonian

J …………………………….Current density

k↑………………………….. Wave Vector Spin up

k↓………………………….. Wave Vector Spin down

k_B …………………………...Boltzmann constant

K_F ………………………. …Fermi wave Vector

m_k, m_{-k} ……………………..Number operator

T_c ……………………… Transition Temperature

u_k,v_k …………………….. Real numbers

σ ………………………...Conductivity

χ ………………………..Magnetic susceptibility

γ ……………………… .Sommerfeld Constant

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CHAPTER ONE

INTRODUCTION

1.1. Background

Superconductivity is the vanishing of the electrical resistance occurring in certain materials below a characteristic temperature called critical (transition) temperature, T_c. It was discovered by H. Kamerlingh in 1911 at Leiden, Holland. He found that when the temperature of pure frozen mercury was reduced below 4.2 K, its electrical resistance disappeared resulting in the flow of electrical current of the order 10^5 amperes. A number of pure metals alloys and doped semiconductors were found to have this property (Khanna, 2008).The electrical resistivity of a metallic conductor decreases gradually as the temperature is lowered. However, in ordinary conductors such as copper and silver, this decrease is limited by impurities and other defects. Even near absolute zero, a real sample of copper shows some resistance. Despite these imperfections, in a superconductor the resistance drops abruptly to zero when the material is cooled below its critical temperature. An electric current flowing in a loop of superconducting wire can persist indefinitely with no power source (Gallop, 1990).

In 1933, Meissner and Ochsenfeld (Meissner *et al.*, 1933) discovered that a metal cooled in the superconducting state in a moderate magnetic field expels the magnetic field from its interior. This phenomenon is called Meissner effect and this shows that such a superconducting material is diamagnetic. The relationship between the magnetic flux B and the magnetic field H is give by $B = H(1+4\pi\chi)$ where $\chi = M/H$ is magnetic susceptibility and *M* is magnetic intensity. When $\dot{B}$ =0 inside a superconductor for $T<T_c$, $\chi = -1/4\pi$, a condition for diamagnetism. The superconductivity exhibited by metals, alloys and doped semiconductors is called conventional superconductivity. The free electron model that gives a fairly good description of normal metals cannot be used to describe the properties of a superconductor (Meissner et.*al.*, 1933). It was not until 1957, when an acceptable microscopic theory for superconductivity based on the concept of pairing of electrons of opposite spins and momenta near the Fermi surface was given by Bardeen, Cooper and Schrieffer (BCS) (Bardeen *et al.*, 1957).

Superconductors are divided into two types depending on their characteristic behaviour in the presence of a magnetic field. Type I superconductors are comprised of pure metals, whereas type II superconductors are comprised primarily of alloys or intermetallic compounds. Both, however, have one common feature: below a critical temperature, T_c, their resistance vanishes. The critical temperature at which the resistance vanishes in a superconductor is reduced when a magnetic field is applied. The maximum magnetic field that can be applied to a superconductor at a particular temperature and still the material maintains superconductivity, is called the critical field, (H_{c1}.). This field varies enormously between type I and type II superconductors. The maximum critical field (H_{c1}) in any type I superconductor is about 2000 Gauss (0.2 Tesla), but in type II materials, superconductivity can persist to several hundred thousand Gauss (H_{c2}). At magnetic fields greater than H_{c1} in a type I superconductor and greater than H_{c2} in a type II superconductor, the material reverts to the normal state and regains its normal state resistance. A type I superconductor excludes the applied magnetic field from the center of the sample by establishing circulating currents on its surface that counteract the applied field. Type II superconductors; however, permit the field to penetrate through the sample in quantized amounts of flux. These quanta are comprised of circulating vortices of current and the flux contained in the vortices (Legget, 2006).

The effective interaction between a pair of electrons called Cooper pairs, results from the virtual exchange of a phonon between the two electrons constituting the pair. Such an interaction is called electron-phonon interaction. The strength of this electron-phonon interaction is maximum when the electrons are in states of equal and opposite momenta and of opposite spins and the energy difference $\Delta\varepsilon$ between the two electron states involved is less than the phonon energy $\hbar\omega$. It is found that the critical temperature for transition to the superconducting states depends on the isotopic mass. This lead to the understanding that the superconducting transition involved some kind of interaction with the crystal lattice. From Ohm's law, the current density J is given by,

$$J = \sigma E_f \qquad 2.1$$

Where E_f is the applied electric field. When the temperature $T<T_c$, the current density J becomes very large and the conductivity σ approaches infinity. Equation (2.1) then implies that the electric field $\vec{E}_f = 0$ inside a superconductor. For finite current flow, Maxwell's equation gives $\dot{B} = -c\left(\Delta \times \overrightarrow{E_f}\right) = 0$ which means $\dot{B}$ is a constant inside such a material. According to Meissner effect this constant could be zero. Since σ →0, a ring of a superconducting material could maintain persistent electrical currents for

years. The ratio of the resistance of the material in the superconducting state (R_s) to the resistance in the normal state (R_n) is of the order $\mathbf{R_s/R_n} < 10^{-15}$(Meissner et al., 1933).

For normal conductors, large electrical conductivity is accompanied by a large thermal conductivity. However, the thermal conductivity of a superconductor is less in the superconducting state when compared with the normal state, it approaches zero at very low temperatures. The transition temperature, T_c for the conventional superconductors is about 23.21 K (Kamerlingh 1911; Onnes, 1911).

The onset of superconductivity is accompanied by abrupt changes in various physical properties, which is the hallmark of phase transition. For example, the electronic heat capacity is proportional to the temperature in the normal regime. At the superconducting transition, it suffers a discontinuous jump and thereafter ceases to be linear. At low temperatures, it varies instead as $e^{-\alpha/T}$ for some constant α as shown in Figure 1.1 below (Junod, 1996).

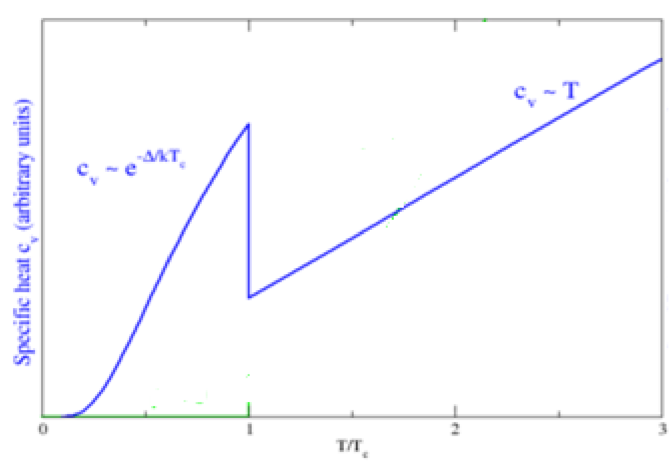

Figure 1.1: Variation of specific heat capacity, C_V with temperature.

This exponential behavior is one of the pieces of evidence for the existence of the energy gap. The order of the phase transition was for a longtime a matter of debate. Experiments indicate that the transition is second order, meaning there is no latent heat. However in the presence of an external magnetic field, the material has finite latent heat, and hence transition is first order. The superconducting phase transition has lower entropy below the critical temperature than the normal phase.

Most of the physical properties of superconductors vary from material to material, such as the heat capacity, the critical temperature and critical magnetic field. On the other hand, there is a class of properties that are independent of the underlying material. For instance, all superconductors have exactly zero resistivity to low applied voltage when there is no magnetic field present or if the applied field does not exceed a critical value. The existence of these “universal” properties implies that superconductivity is a thermodynamic phase, and thus possesses certain distinguishing properties which are largely independent of microscopic details.

1.2. Statement of the problem

The study aims at establishing the role played by interlayer and intralayer interactions in high-T_c Cuprate superconductors. Studies have revealed that the interlayer and intralayer interactions play a significant role in enhancing transition temperature in layered cuprates. The discovery of high-T_c Cuprates superconductors and their properties which are quite different from the conventional BCS type superconductors has led to enormous theoretical research to look for the kind electron pairing mechanism that may exist in these superconductors (Kakani 2007; Anderson 1997). In the recent past several electron pairing mechanisms have been proposed which are different from the type of electron pairing mechanism used in BCS theory. Some of the electrons pairing mechanisms are known as resonance valence bond state, spin fluctuation, bipolarons, excitons, plasmons, fermion-boson and charge transfer electron pairing mechanism (Khanna, 2008).

A well known feature of the known high- T_c Cuprates is the presence of square planar CuO_2 layers which dominate most properties, (Dagatto 1994).

A common feature of the layered structure of all these high-T_c Cuprates is a two-dimensional copper- oxygen plane shown in figure 1.2, which is believed to be relevant to the conduction process in these systems. It is also believed that the superconductivity in these Cuprates seems to be controlled by the number of charge carriers (electrons or holes) in these layers through the oxidation states of the copper atoms (Dagatto,1994). More-over, the transition temperature increases with the number of CuO_2 layers in a unit cell upto three layers. The transition temperature T_c does not increase if the number of layers is more than three, thereafter it saturates. It was reported that the resistivity along a-directions and b-directions (ρ_{ab}) in copper oxide plane varies linearly with temperature whereas along c- direction (perpendicular to the plane) it varies as 1/T (Dinger, 1988).

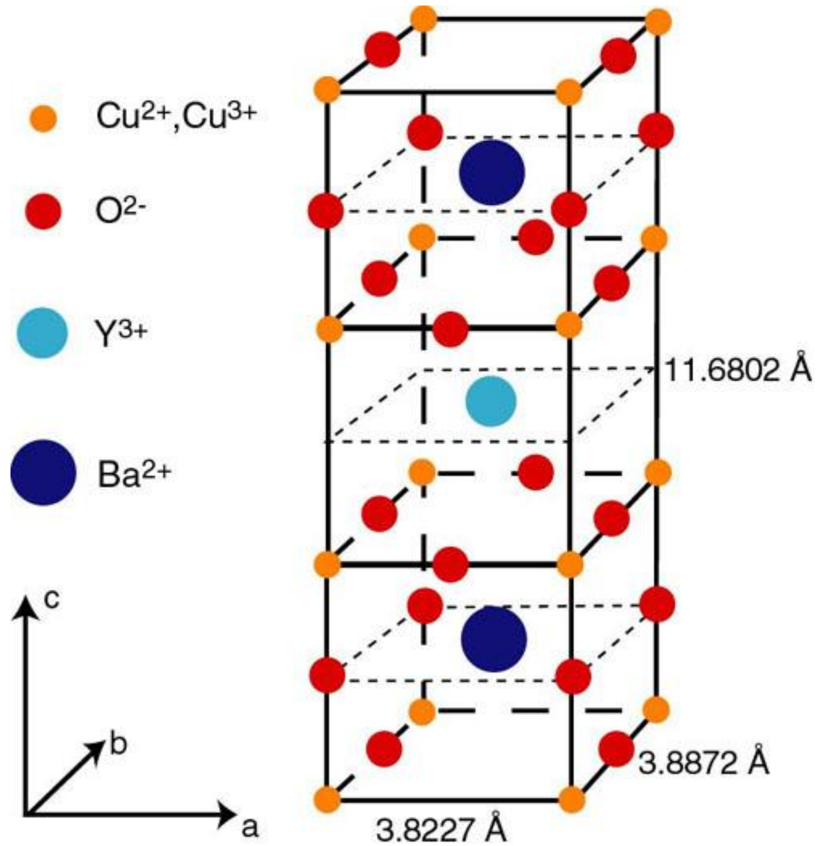

Figure 1.2: Unit cell of YBCO showing a, b, c axes and cell parameters(Dinger, 1988).

The influence of layered structure on the unusual properties of these Cuprates has been studied earlier also. It was proposed that interlayer and intralayer interactions play an important role in the increase of the superconducting transition temperature T_c, and in stabilizing superconducting order with respect to fluctuations (Khandka, 2006; Singh 2006). Hence the increase in T_c due to the increase in the number of layers in Cuprates clearly emphasizes that layered structure of the Cuprate compounds is crucial to high- T_c superconductors and plays an important role in establishing superconducting order.

To study the properties of multilayer Cuprates such as specific heat and transition temperature, we have to consider interlayer pairing along with intralayer pairing. The model Hamiltonian for such a system will have to be written and then diagonalized using Bogoliubov transformation to obtain the properties of such multilayer Cuprates.

1.3 Research objectives

1. To determine the specific heat capacity of high -T_c layered Cuprates based on intralayer and interlayer interactions.
2. To determine the critical temperature of high-T_c layered Cuprates based on intralayer and interlayer interactions.
3. To determine effect of intralayer and interlayer interactions on transition temperature of high-T_c layered Cuprates.

1.4 Justification of the Study

The question of how superconductivity can arise in high- temperature superconductors is one of the major unsolved problems of theoretical condense matter physics as of to-day. The exact mechanism that causes the electrons in these crystals to form pairs is not clear (Leggett, 2006). Despite intensive research and many promising leads, an acceptable explanation meant for all types of high-T_c superconductors has so far eluded scientists. One reason for this is that the materials in question are generally very complex, multi-layered crystals, for example, Bismuth Strontium Calcium Copper Oxide (BSCCO), making theoretical modeling difficult. Improving the quality and variety of samples also requires considerable research, both with the aim of improved characterization of the physical properties of existing compounds, and synthesizing new materials, often with the hope of increasing T_c. Technological research focuses on making high temperature superconductors (HTS) materials in sufficient quantities to make their use economically viable and optimizing their properties in relation to applications. The ultimate aim is to develop a superconducting material that can be used at room temperatures.

Technological applications benefit from both the higher critical temperature being above the boiling point of liquid nitrogen and also the higher critical magnetic field at which superconductivity is destroyed. In magnetic applications, the high critical magnetic field may be more valuable than the T_c itself.

1.5 Significance of the Study

The study will provide an insight into the role played by interlayer and intralayer interactions in the enhancement of superconducting transition temperature T_c in multilayer Cuprates. Other studies have revealed the factors which increase transition temperature in Cuprates. They include chemical compositions, cation substitutions, number of layers of CuO_2. The present research is directed towards the origin of high-temperature superconductivity and the charge carriers pairing mechanisms involved. One goal of all this research is room-temperature superconductivity (Mourachkine, 2004).

Superconductivity at room temperature would result in enormous savings for overhead power cables and equipment such as that used for Magnetic resonance imaging (MRI) scans. (www.news.leiden.edu/.../PhD candidate, 25/01/2012).

Superconducting magnets are used MRI, Nuclear magnetic resonance (NMR) machines, mass spectrometers and the beam-steering magnets used in particle accelerators. More recently, superconductors have been used to make digital circuits based on rapid single flux quantum technology and Radio frequency (RF) microwave filters for mobile phone base stations.

Some of the future promising applications of high-temperature superconductivity include high-performance smart grid, electric power transmission, transformers power storage devices, electric motors (e.g. for vehicle propulsion or maglev trains) magnetic levitation devices, fault current limiters, nanoscopic materials such as buckyballs, nanotubes, composite materials and superconducting magnetic refrigeration.

Some markets are arising where the relative efficiency, size and weight advantages of devices based on high-temperature superconductivity outweigh the additional costs involved. However, superconductivity is sensitive to moving magnetic fields so applications that use alternating current (e.g. transformers) will be more difficult to develop than those that rely upon direct current.

CHAPTER TWO

LITERATURE REVIEW

2.1 High – T_c Cuprates Superconductors

High- temperature superconductors (high- T_c) are materials that have a superconducting transition (T_c) above 30K (-243.2 ^{0}C).

"High-temperature" has three common definitions in the context of superconductivity:

1. Above the temperature of 30K that had historically been taken as the upper limit for BCS type superconductors or conventional superconductors. This is also above the 1973 record of 23K that had lasted until copper-oxide materials were discovered in 1986 with T_c in the range of 90K(Bednorz, 1986; Mueller, 1986).
2. Having a transition temperature that is a larger fraction of the Fermi temperature than for conventional superconductors such as elemental mercury or lead. This definition encompasses a wider variety of unconventional superconductors and is used in the context of theoretical models.
3. Greater than the boiling point of liquid nitrogen (77K or -196^{0}C). This is significant for technological applications of superconductivity because liquid nitrogen is a relatively inexpensive and easily handled coolant.

There are several families of Cuprate superconductors and they can be categorized by the elements they contain and the number of adjacent copper-oxide layers in each superconducting block. For example, Yttrium Barium Copper Oxide (YBCO) and Bismuth Strontium Calcium Copper Oxide (BSCCO) can alternatively be referred to as

Y123 and Bi2201/Bi2212/Bi2223 depending on the number of layers in each superconducting block (*n*). The superconducting transition temperature has been found to peak at an optimal number of layers in each superconducting block, typically *n*=3.

In 1986 Bednorz and Muller discovered superconductivity in a lanthanum- based Cuprate which had a transition temperature of 35K (Bednorz *et al.*, 1995).It was later found by Chu and Wu (1988) that replacing the Lanthanum with yttrium making YBCO raised the critical temperature to 92K which was important because liquid nitrogen could then be used as a refrigerant since its boiling point is 77K at atmospheric pressure (Chu *et al.*, 1988). Until Fe-based superconductors were discovered in 2008 (Bednorz, 1986; Muller 1986; Xiao- Li, 2008), the term high-temperature superconductor was used interchangeably with Cuprate superconductor for compounds such as Bismuth Strontium Calcium Copper Oxide (BSCCO) and Yttrium Barium Copper Oxide (YBCO).All known high-T_c superconductors are type-II superconductors. In contrast to type- I superconductors which expel all magnetic fields due to Meissner effect , type-II superconductors allow magnetic fields to penetrate their interior in quantized units of flux creating `holes` or `tubes` of normal metallic regions in the superconducting bulk. Consequently, high- T_c superconductors can sustain much higher magnetic fields (Khanna *et al.*, 2008).

The discovery of possible high –T_c superconductivity in Lanthanum – Barium – Copper-Oxide (La- Ba –Cu-O, T_c=30K) system (Bednorz et al., 1986) was important and decisive breakthrough in the high- T_c superconductivity research. The great success with La-Ba-Cu-O and La-Sr-Cu-O compounds, led to the discovery of multilayered compounds whose transition temperatures were more than 90K. By March 2007, the world record for high T_c superconductivity was held by a ceramic superconductor consisting of Thallium, Mercury; Copper, Barium, Calcium, Strontium and Oxygen (T_c =138 K). Many other Cuprates superconductors have been discovered, and some of them with their values of T_c are given in table 1.1

Table 1.1: Some of the Superconducting Oxides (Khanna, 2008).

Formulae	**Highest T_c(K)**
$YBa_2Cu_3O_{7-s}$	92
$Bi_2Sr_2CaCu_2O_8$	90
$Bi_2Sr_2CaCu_2O_{10}$	122
$Tl_2Ba_2CaCu_2O_8$	110
$Tl_2Ba_2Ca_2Cu_3O_{10}$	127
$TlBa_2CaCu_2O_7$	90
$HgBa_2Ca_2Cu_3O_8$	135
$HgBa_2Ca_2Cu_3O_x$	133
$Bi_2Sr_2Ca_2Cu_3O_{10}$(BSCCO)	110
$YBa_2Cu_3O_7$(YBCO)	90

2.2. Characteristics of High-Temperature Superconductors

There are three main characteristics of high-T_c superconducting copper oxides.

i) Strong correlations on copper

ii) Anisotropy

iii) Large electron-phonon coupling

2.2.1 Strong correlations on copper

In superconducting copper oxides, the valence state of copper is Cu^{2+}. The copper ion has one hole with spin $S={}^{1}/_{2}$ in the 3-D shell and this hole is localized since the energy barrier prevents the transfer of the hole to the neighboring oxygen site. The magnetic moments associated with spin ½ of Cu^{2+} are coupled by supper – exchange interaction to a given anti-ferromagnetic ground state with Neel temperature $T_n \geq$ 300K. When the oxygen content is increased, additional holes mainly of oxygen P_a character are transferred into O (2P) states in CuO_2 planes. These holes form a band of states within energy gap for the Cu charge excitation. When the number of holes increases further, they tend to align adjacent spins in a parallel configuration that leads to a Mott insulator-metal transition and the materials become a superconductor.

Thus, the only motion possible is the alternating spin $\alpha = [½,-{}^{1}/_{2}]$, where the energy band splits into two narrow Hubbard bands separated by 2U, where U is the Coulomb on site energy, the lower band being fully occupied by anti-ferromagnetically aligned electrons and the upper band being empty.

Anderson argued that the strong correlations in the CuO_2 planes are best described by a single-band Hubbard model with on-site repulsion. Strong Coulomb repulsion and hole correlation play a crucial role in the 2-dimensional CuO_2 sub-lattice. It is essential here in the CuO_2 planes that the charge carriers are confined to (Anderson, 1997).

2.2.2 Anisotropy

Due to the layered structure (quasi-two-dimensional nature of structure), high-T_c superconductors exhibit a strongly anisotropic superconducting behavior which favours superconducting currents flowing in CuO_4 planes. This implies that the coupling between adjacent conducting layers is in the form of a tunneling process.

2.2.3 Large Electron-Phonon Coupling

Superconductivity is due to an effective attraction between conduction electrons. Since two electrons experience a repulsive Coulomb force, there must be an additional attractive force between two electrons when they are placed in a metallic environment. In conventional superconductors, this force is known to arise from the interaction with the ionic system. For T_c to be large, the Electron-Phonon Coupling constant should also be large. Doglov observations showed an evidence for strong electron-Phonon Coupling. Also the self consistent band structure calculation gave large values of the coupling constant (Khanna, 2008).

2.3 Theories of High Temperature Superconductivity (HTS)

Two decades of experimental and theoretical research, with over 100,000 published papers on the subject (Mark, 2001) have discovered many common features in the properties of high-temperature superconductors (Leggett, 2006) but as of 2009, there was no widely accepted theory to explain their properties. Cuprate superconductors differ in many important ways from conventional superconductors, such as elemental mercury or lead, which are adequately explained by the BCS theory. There also has been much debate as to high-temperature superconductivity coexisting with magnetic ordering in YBCO (Sanna *et al*., 2004), iron-based superconductors, several Cuprates and other exotic superconductors, and the search continues for other families of materials. High Temperature Superconductors are Type- II superconductors, which allow magnetic fields to penetrate their interior in quantized units of flux, meaning that much higher magnetic fields are required to suppress superconductivity. The layered structure also gives a directional dependence to the magnetic field response.

A number of theories have been proposed as possible explanation for high-T_c superconductivity. Most of these theories require that there should be an attractive interaction between the charge carriers resulting in the formation of pairs which act as bosons, and can undergo Bose-Einstein condensation. The proposed theories fall into the following three main categories:

(i) Interaction through phonons (lattice vibrations)

(ii) Interaction through charges (charge fluctuations)

(iii) Interaction through unpaired spins (spin fluctuations)

2.3.1 Bipolaron theory

Polaron is defined as a Fermionic quasiparticle composed of a charge and its accompanying polarization field. A slow moving electron in a dielectric crystal, interacting with lattice ions through long range forces will permanently be surrounded by a region of lattice polarization and deformation caused by the moving electron. Moving through the crystal, the electron carries the lattice distortion with it, thus one speaks of a cloud of phonons accompanying the electron. Polarons have spin, though two closely-spaced Polarons called bipolaron are spinless. The assembly of these bound pairs can undergo superconducting transition at temperatures below the Bose-Einstein condensation temperature T_c.

2.3.2 Exciton Theory

Excitons are bound states of electron-hole pair created by electrostatic interaction between an electron in the excited state and a hole in the ground state. Oxides superconductors have a layered structure and thus a multiband nature of electron spectrum. It is therefore highly probable to have excitons. Since, here the energy responsible for coupling is of the order of electron energies, much higher T_c can be obtained. Some of the Exciton models are:

i. Plasma excitations which have a quasi-two-dimensional electronic Spectrum which gives rise to the appearance of weakly damped Acoustic plasmons (Ruvalds, 1987).

ii. Collective electron excitation connected to copper – oxygen charge transfer (Varma, 1987)

2.3.3 Spin Bag Theory

Schrieffer (1992) proposed a model in which boson excitations are responsible for superconducting pairing in copper oxide high-T_c compounds. When a mobile hole passes through the CuO_2lattice, it creates a region of local depression in which copper spins are aligned anti-ferromagnetically. When another hole passes through this region, it gets attracted to this region of lower potential energy resulting in the appearance of a magnetic polaron that moves with a deformed cloud. High- T_c and wave pairing are conditioned by a strongly anisotropic region due to anti-ferromagnetic spin fluctuations.

2.3.4 Friedel's theory of Van-Hove anomaly

Friedel proposed that superconductivity is due to electron-phonon coupling of delocalized carriers. Since the carriers are confined to the CuO_2 planes, high – T_c super-conductors exhibit quasi two dimensional Fermi surface. The band structure for holes leads to electronic density of states at or very near the Fermi surface which has Van Hove singularity.

2.3.5 Resonating Valence Bond (RVB) State Theory.

A Quantum spin liquid or singlet liquid state is called a Resonating Valence Bond state. Anderson (1987) found that the whole wealth of experimental results on the so-called high–T_c superconducting compounds could not fit in honest way to conventional BCS theory.

The departures were in two fronts; the first one is that high-T_c superconductivity is not due to phonon-induced pairing of electrons. The second and perhaps the most important one is that in these superconductors, superconductivity arises not from Cooper pair condensation but the condensation of new quasi-particles of positive charge which are now called holons. Anderson refers to ceramic superconductors as, strange insulators, strange metal and strange superconductors. Superconducting transition temperature T_c is generally large, of the order of 92K and above. There are indicators of unstable superconductivity even at room temperatures. The superconductor-normal metal tunneling is anomalous since there is a strong ultrasonic attenuation and velocity of sound anomaly. The infrared absorption is very different as compared to the BCS compounds. Wide discrepancies are there in the gap measurements obtained from different experiments such as tunneling infrared absorption.

The remarkable fact is the vicinity of the insulating phase to the superconducting phase in that at very low temperature the system directly goes from an insulator to a superconductor.It was the inelastic neutron scattering in La_2CuO_{u-y} that had shown a clear indication for the presence of a quantum spin (RVB state) liquid. Anderson generalized Pauling's theory of resonant valence bond to make it relevant to high-T_c oxide compounds. In this model, valence electrons are bounded singlet anti-ferromagnetic pairs (Magnetic singlet pairs) which become mobile as in a liquid in the presence of mobile holes.

Superconductivity is assumed to be due to:

i. Condensation of holons with $\langle b_i^+, b_j \rangle \neq 0$ pairing is by interlayer tunneling of Holons.

ii. Tunneling of pairs of electrons between the layers under the condensation of spinon pairing amplitude $\Delta_{ij} \neq 0$.

Although much progress has been made in understanding the mechanisms that may ultimately lead to the development of a comprehensive theory for the high-T_c

superconductivity, the nature of the pairing mechanism that may finally describe the properties of such systems is still unknown.

2.3.6 Ginzburg-Landau Theory.

Ginzburg-Landau theory, named after Vitaly Lazarevich Ginzburg and Lev Landau, is a mathematical theory used to describe superconductivity. In its initial form, it was postulated as a phenomenological model which could describe type-I superconductors without examining their microscopic properties. Later a version of Ginzburg- Landau theory was derived from the Bardeen-Cooper-Schrieffer microscopic theory by Lev Gorkov, thus showing that it also appears in some limit of microscopic theory and giving microscopic interpretation of all its parameters (Dasgupta, 2011). Based on Landau's previously established theory of second-order phase transitions, Ginzburg and Landau (Ginzburg *et al*., 2004) argued that the free energy, F, of a superconductor near the superconducting transition can be expressed in terms of a complex order parameter field, ψ, which is non-zero below a phase transition into a superconducting state and is related to the density of the superconducting component. In Ginzburg- Landau theory the electrons that contribute to superconductivity were proposed to form a superfliud (Ginzburg, 2004). Ginzburg and Landau observed the existence of two types of superconductors depending on the energy of the interface between the normal and superconducting states. The most important finding from Ginzburg-Landau theory was made by Alexei Abrikosov in 1957. He used Ginzburg-Landau theory to explain experiments on superconducting alloys and thin films. He found that in a type-II superconductor in a high magnetic field, the field penetrates in the form of hexagonal lattice of quantized tubes of flux (Abrikosov, 2003).

2.4 Heat capacity of Cuprates and Transition temperature.

In Cuprates such as $YBa_2Cu_3O_{7-\delta}$, the mechanism of binding holes as carriers into Cooper pairs with high-T_c is still discussed with high intensity. For the high –T_c superconductors, there is a very interesting large group activity, for pairing model involving substances with phonon, polarons, bipolarons, exciton, charge density fluctuation (Ruvalds,1996) spin density fluctuation, magnons and resonating- bond state (Kirtley,2000;Tsuei,2000). Nevertheless, the B.C.S theory and the Cooper pairing concept remains the cornerstone of almost all-current theories of superconductivity. Of course, one should take into account the effects of the co existence of charge density fluctuations and the antiferromagnetic spin fluctuations in describing the pairing force in Cuprates (Varshney *et al*., 2003).

Among various Cuprates hole doped $YBa_2Cu_3O_{7-\delta}$ ($T_c \approx$ 90K) systems are widely analyzed experimentally since good crystals with a very sharp superconducting transition at T_c can be prepared. One of the interesting aspects of this structure is that δ can be varied over a wide range while the orthorhombic structure and superconductivity are maintained. For approximately $0 < \delta < 0.5$, the system is orthorhombic, while for $\delta \approx 1.0$, it is tetragonal. The orthorhombic phase of $YBa_2Cu_3O_{7-\delta}$ is composed of two- dimensional CuO_2 layers as well as one-dimensional (ID) CuO chains. Quite generally the superconductivity occurs primarily in the planes and that the existing chains are less crucial.

Traditional proofs of revealing thermal properties, particularly, heat capacity, were used extensively on under, optimized and overdoped samples. Salient features of the reported specific heat measurements include a linear term ($\gamma'T$) at very low temperatures, an upturn in C (T) of superconducting version in the vicinity of T_c and a bump in the normal state region near to room temperature (Junod, 1996). It is noteworthy that the specific heat anomaly in the vicinity of T_c both in pure and chemically substituted samples of $YBa_2Cu_3O_{7-\delta}$ is weak in comparison to conventional low T_c superconductors. On the theoretical side the observation of this anomalous behavior has therefore been of considerable interest. It seems essential to point out that these anomalies represent a deviation from the BCS prediction. It is useful to understand first the possible difficulties in explaining the observed anomalous behavior. As far as a linear term in the low temperature domain, it is unclear that $\gamma'T$ is associated with non-superconducting phase or is an intrinsic property due to vanishing of energy gap over a portion of Fermi-surface. Secondly, in the vicinity of T_c, the lattice contribution to specific heat is dominating, so separation of Fermionic term from the bosonic (Phononic) effect is not straight forward without an accurate model for phononic specific heat with many unknown input parameters. Apart from these, there is a good probability of having other phase transitions, either electronic or lattice near to the room temperature region. In an attempt to reveal the reported upturn in the vicinity of transition temperature, it is worth noting that measured specific heat differs from usual lattice contribution. It is known that the high-T_c superconductors, in particular $YBa_2Cu_3O_{7-\delta}$ have very complicated electronic structures (Anderson, 1997).

Above T_c, the electronic specific heat is linear. $C_{el}=\gamma T$ where γ is the Sommerfeld constant. Below T_c the electronic specific heat is determined by the microscopic mechanism of high-

T_c superconductors. The specific heat measurements show a discontinuity in C (T) of superconducting version in the vicinity of transition temperature (Dorbolo *et al.*, 1998).

For high-T_c Cuprates the evaluation of electronic specific heat is not quite straight forward as measured data include contributions from both the electrons and phonons. In passing, we may add that the separation of the lattice specific from the total specific heat is indeed constrained by considerable fluctuation effects influencing the temperature dependence of specific heat close to T_c. In the vicinity of T_c, the specific heat is dominated by lattice contribution. Despite limitations and use of free parameters for the estimation of lattice and electronic specific heat, the present theoretical model of the heat capacity of high- T_c $YBa2Cu3O7_{-\delta}$ superconductor reveals the anomalous behaviour reported experimentally.

The election scattering rate at low temperature is inversely proportional to Fermi energy ($\varepsilon_f \approx 0.1eV - 0.3eV$) and the value of ε_f is low in doped Cuprates as compared to conventional metals which implies that Coulomb interactions may dominate over other excitations (lattice and spin wave) in the temperature domain of interest(Ferreira *et al.*, 1988).

CHAPTER THREE

THEORY AND DERIVATIONS

3.1 Formulation of the Problem

The model Hamiltonian for a multilayer system of Cuprates can be written as,

$$H = H_{intra} + H_{inter} \qquad 3.1$$

Where H_{intra} refers to the Intralayer pairing part of the Hamiltonian, and H_{inter} refers to the interlayer pairing part of the Hamiltonian. We can write,

$$H_{intra} = \sum_{r,k,\sigma} \varepsilon_k a^{+}_{r,k,\sigma} a_{r,k,\sigma} + U \sum_{r,k,k'\sigma} a^{+}_{r,k+q\uparrow} a^{+}_{r,k'-q\downarrow} a_{r,k'\downarrow} a_{r,k\uparrow} \qquad 3.2$$

$$H_{inter} = (-t) \sum_{r,s,k,\sigma} a^{+}_{r,k,\sigma} a_{s,k,\sigma} + W \sum_{r,s,k,k',\sigma,\sigma' q} a^{+}_{r,k+q,\sigma} a^{+}_{s,k'-q,\sigma'} a_{s,k',\sigma} a_{r,k,\sigma} \qquad 3.3$$

Here r = 1 (2) and s = 2 (1) are the layer indices for a two layer system such that when the layer r is denoted by 1, the layer s is denoted by 2 and vice versa (i.e. when r = 2, then s = 1)

$a^{+}_{k\sigma}$ is the creation operator, and $a_{k\sigma}$ is the annihilation operator of charge carriers in CuO_2 plane with the wave vector 'k' and spin 'σ'. The first term in equation (3.2) represents the energy of free charge carriers within the CuO_2 plane, and the second term indicates attractive intralayer interaction between the charge carriers; U is a measure of such interactions (on-site repulsion).

The first term in Equation(3.3) represents the direct hopping of charge carriers between the layers, t is the interlayer hopping and the second term represents attractive interlayer interaction 'W' and it contains the contributions from exciton or Plasmons mediated interaction and direct Coulomb interaction between charge carriers of different layers. Here W is negative (attractive nature) and for the repulsive case U > 0, the hopping integral t is taken to be positive (Zhang *et.al*., 1992).

To study the physical properties, we have to diagonalize using Bogoliubov transformation the Hamiltonian in Equation (3.1) using (3.2) and (3.3)

$$H_{\text{int}ra} = \sum_{r,k,\sigma} \varepsilon_k a^+_{r,k,\sigma} a_{r,k,\sigma} + U \sum_{r,k,k'\sigma} a^+_{r,k+q\downarrow} a^+_{r,k'-q\downarrow} a_{r,k'\downarrow} a_{r,k\uparrow}$$

Using Bogoliubov transformation

$$\left.\begin{aligned} \mathrm{b}_{\mathrm{k}} &= u_k a_k - v_k a^+_{-k} \\ b_{-k} &= u_k a_{-k} + v_k a^+_k \end{aligned}\right\} \qquad 3.4$$

Their complex conjugates are

$$\left.\begin{aligned} b^+_k &= u_k a^+_k - v_k a_{-k} \\ b^+_{-k} &= u_k a^+_{-k} + v_k a_k \end{aligned}\right\} \qquad 3.5$$

The inverse transformation of equations (3.4) and (3.5) are

$$\left.\begin{aligned} a_k &= u_k b_k + v_k b_{-k}^{+} \\ a_{-k} &= u_k b_{-k} - v_k b_k^{+} \\ a_k^{+} &= u_k b_k^{\;+} + v_k b_{-k} \\ a_{-k}^{+} &= u_k b_{-k}^{+} - v_k b_k \end{aligned}\right\} \qquad 3.6$$

Substituting 3.6 into the first term of the Hamiltonian in Equation (3.2), that is the energy of free charge carriers, say H_1, we have:

$$H_1 = \sum_{r,k,\sigma} \varepsilon_k a_{r,k,\sigma}^{+} a_{r,k,\sigma}$$

$$= \sum_k \varepsilon_k \left(u_k b_k^{\;+} + v_k b_{-k}\right)\left(u_k b_k + v_k b_{-k}^{\;+}\right)$$

$$= \sum_k \varepsilon_k \left(u_k^{\;2} b_k^{\;+} b_k + u_k v_k b_k^{\;+} b_{-k}^{\;+} + u_k v_k b_{-k} b_k + v_k^{\;2} b_{-k} b_{-k}^{\;+}\right)$$

$$= \sum_k \varepsilon_k \left(u_k^{\;2} b_k^{\;+} b_k + v_k^{\;2} b_{-k} b_{-k}^{\;+}\right) + \sum_k \varepsilon_k \left(u_k v_k b_k^{\;+} b_{-k}^{\;+} + u_k v_k b_{-k} b_k\right) \qquad 3.7$$

A new pair of number operators is defined as

$$\left.\begin{aligned} & b_k^{\;+} b_k = m_k,\; b_{-k}^{\;+} b_{-k} = m_{-k},\; b_{k'}^{\;+} b_{k'} = m_{k'} \\ & b_k b_k^{\;+} = m_k + 1,\; b_{-k} b_{-k}^{\;+} = m_{-k} + 1,\; b_{-k'}^{\;+} b_{-k'} = m_{-k'} \end{aligned}\right\} \qquad 3.8$$

Using the number operators in Equation (3.8), H_1 becomes

$$H_1 = \sum_k \varepsilon_k \left[\left(u_k{}^2 m_k + v^2 m_{-k} + v_k{}^2\right) + u_k v_k \left(b_k{}^+ b_{-k}{}^+ + b_{-k} b_k\right)\right]$$

$$= \sum_k \varepsilon_k \left[v_k{}^2 + \left(u_k{}^2 m_k + v_k{}^2 m_{-k}\right) + u_k v_k \left(b_k{}^+ b_{-k}{}^+ + b_{-k} b_k\right)\right]$$

$$= \sum_k \varepsilon_k v_k{}^2 + \sum_k \varepsilon_k \left(u_k{}^2 m_k + v_k{}^2 m_{-k}\right) + \sum_k \varepsilon_k u_k v_k \left(b_k{}^+ b_{-k}{}^+ + b_{-k} b_k\right) \qquad 3.9$$

H_1 contains three terms, the first term is a constant, the second term contains the number Operators m_k, m_{-k} and the third term is the off-diagonal term containing the products $b_k{}^+ b_{-k}{}^+$ and $b_{-k} b_k$

Dealing with the second term of the Hamiltonian in Equation (3.2), say H_2

$$H_2 = U \sum_{r,k,k'\sigma} a^+_{r,k+q\uparrow} a^+_{r,k'-q\updownarrow} a_{r,k'\downarrow} a_{r,k\uparrow}$$

$$= U \sum_k \left(u_k b_k{}^+ + v_k b_{-k}\right)\left(u_k b_{-k}{}^+ - v_k b_k\right)\left(u_k b_{-k} - v_k b_k{}^+\right)\left(u_k b_k + v_k b_{-k}{}^+\right)$$

The product of the last two terms of H_2 is;

$$H_3 = U \sum_k \left(u_k{}^2 b_{-k} b_k + u_k v_k b_{-k} b_{-k}{}^+ - u_k v_k b_k{}^+ b_k - v_k{}^2 b_k{}^+ b_{-k}{}^+\right) \qquad 3.10$$

Operating with $\left(u_k b_{-k}{}^+ - v_k b_k\right)$ on Equation (3.10) from the left, we have,

$$H_4 = U\sum_k \Big(u_k{}^3 b_{-k}{}^+ b_{-k} b_k + u_k{}^2 v_k b_{-k}{}^+ b_{-k} b_{-k}{}^+ - u_k{}^2 v_k b_{-k}{}^+ b_k{}^+ b_k$$

$$- u_k v_k{}^2 b_{-k}{}^+ b_k{}^+ b_{-k}{}^+ + u_k{}^2 v_k b_k b_{-k} b_k - u_k v_k{}^2 b_k b_{-k} b_{-k}{}^+$$

$$+ u_k v_k{}^2 b_k b_k{}^+ b_k + v_k{}^3 b_k b_k{}^+ b_{-k}{}^+ \Big) \qquad 3.11$$

Operating with $\left(u_k b_k{}^+ + v_k b_{-k}\right)$, on Equation (3.11) from the left, finally we have,

$$H_5 = U\sum_k \Big(u_k{}^4 b_k{}^+ b_{-k}{}^+ b_{-k} b_k + u_k{}^3 v_k b_k{}^+ b_{-k}{}^+ b_{-k} b_{-k}{}^+$$

$$- u_k{}^3 v_k b_k{}^+ b_{-k}{}^+ b_k{}^+ b_k - u_k{}^2 v_k{}^2 b_k{}^+ b_{-k}{}^+ b_k{}^+ b_{-k}{}^+$$

$$- u_k{}^3 v_k b_k{}^+ b_k b_{-k} b_k - u_k{}^2 v_k{}^2 b_k{}^+ b_k b_{-k} b_{-k}{}^+$$

$$+ u_k{}^2 v_k{}^2 b_k{}^+ b_k b_k{}^+ b_k + u_k v_k{}^3 b_k{}^+ b_k b_k{}^+ b_{-k}{}^+$$

$$+ u_k{}^3 v_k b_{-k} b_{-k}{}^+ b_{-k} b_k + u_k{}^2 v_k{}^2 b_{-k} b_{-k}{}^+ b_{-k} b_{-k}{}^+$$

$$- u_k{}^2 v_k{}^2 b_{-k} b_{-k}{}^+ b_k{}^+ b_k - u_k v_k{}^3 b_{-k} b_{-k}{}^+ b_k{}^+ b_{-k}{}^+$$

$$- u_k{}^2 v_k{}^2 b_{-k} b_{-k}{}^+ b_k{}^+ b_k - u_k v_k{}^3 b_{-k} b_{-k}{}^+ b_k{}^+ b_{-k}{}^+$$

$$+ u_k v_k{}^3 b_{-k} b_k b_k{}^+ b_k + v_k{}^4 b_{-k} b_k b_k{}^+ b_{-k}{}^+ \qquad 3.12$$

Equation (3.12) can be re-written such that the first term contains four operators, the second term is the off-diagonal term containing the product $b_k{}^+ b_{-k}{}^+$ and $b_{-k} b_k$ and the third term contains the number operators m_k and m_{-k}. Also using the number operators given in Equation (3.8) H_5 becomes,

$$H_5 = U\sum_k \Big[\Big\{\Big(u_k^{\,4} b_k^{\,+} b_{-k} b_{-k} b_k + v_k^{\,4} b_{-k} b_k b_k^{\,+} b_{-k}^{\,+} - u_k^{\,2} v_k^{\,2} b_k^{\,+} b_{-k}^{\,+} b_k^{\,+} b_{-k}^{\,+}$$

$$- u_k^{\,2} v_k^{\,2} b_{-k} b_k b_{-k} b_k \Big\} + \Big\{\Big(u_k^{\,3} v_k \left(m_{-k} + 1\right) b_k^{\,+} b_{-k}^{\,+}$$

$$- u_k^{\,3} v_k m_k b_k^{\,+} b_{-k}^{\,+} + u_k v_k^{\,3} m_k b_k^{\,+} b_{-k}^{\,+}$$

$$- u_k v_k^{\,3} \left(m_{-k} + 1\right) b_k^{\,+} b_{-k}^{\,+} + u_k^{\,3} v_k \left(m_{-k} + 1\right) b_{-k} b_k$$

$$- u_k^{\,3} v_k m_k b_{-k} b_k + u_k v_k^{\,3} m_k b_{-k} b_k - u_k v_k^{\,3} \left(m_{-k} + 1\right) b_{-k} b_k \Big\}$$

$$+ \Big\{\Big(u_k^{\,2} v_k^{\,2} m_k m_k + u_k^{\,2} v_k^{\,2} \left(m_{-k} + 1\right)\left(m_{-k} + 1\right)$$

$$- u_k^{\,2} v_k^{\,2} m_k \left(m_{-k} + 1\right) - u_k^{\,2} v_k^{\,2} m_k \left(m_{-k} + 1\right)\Big\}\Big]$$

Factoring out the operators $b_k^{\,+} b_{-k}^{\,+}, b_{-k} b_k$ in the second term and the common term $u_k^{\,2} v_k^{\,2}$ in the third term, H_5 becomes,

$$H_5 = U\sum_k \Big(u_k^{\,4} b_k^{\,+} b_{-k}^{\,+} b_{-k} b_k + v_k^{\,4} b_{-k} b_k b_k^{\,+} b_{-k}^{\,+} - u_k^{\,2} v_k^{\,2} b_k^{\,+} b_{-k}^{\,+} b_k^{\,+} b_{-k}^{\,+}$$

$$- u_k^{\,2} v_k^{\,2} b_{-k} b_k b_{-k} b_k \Big) + U\sum_k \Big[\Big\{u_k^{\,3} v_k \left(m_{-k} + 1\right) - u_k^{\,3} v_k m_k$$

$$+ u_k v_k^{\,3} m_k - u_k v_k^{\,3} \left(m_{-k} + 1\right)\Big\} b_k^{\,+} b_{-k}^{\,+} + b_{-k} b_k \Big]$$

$$+ U\sum_k u_k^{\,2} v_k^{\,2} \left[m_k m_k + \left(m_{-k} + 1\right)\left(m_{-k} + 1\right) - 2 m_k \left(m_{-k} + 1\right)\right]$$

Since m_k and m_{-k} are real numbers, then $m_k = m_{-k}$, H_5 reduces to,

$$H_5 = U\sum_k \left(u_k{}^4 b_k{}^+ b_{-k}{}^+ b_{-k} b_k + v_k{}^4 b_{-k} b_k b_k{}^+ b_{-k}{}^+ - u_k{}^2 v_k{}^2 b_k{}^+ b_{-k}{}^+ b_k{}^+ b_k{}^+\right.$$

$$\left. - u_k{}^2 v_k{}^2 b_{-k} b_k b_{-k} b_k \right) + U\sum_k \left[\left\{u_k{}^3 v_k (m_{-k} + 1) - u_k{}^3 v_k m_k\right.\right.$$

$$\left.\left. + u_k v_k{}^3 m_k - u_k v_k{}^3 (m_{-k} + 1)\right\} b_k{}^+ b_{-k}{}^+ + b_{-k} b_k \right]$$

$$U\sum_k u_k{}^2 v_k{}^2 \left[m_k{}^2 + m^2{}_{-k} + 2m_{-k} + 1 - 2m_k m_{-k} - 2m_k\right]$$

Or

$$H_5 = U\sum_k \left(u_k{}^4 b_k{}^+ b_{-k}{}^+ b_{-k} b_k + v_k{}^4 b_{-k} b_k b_k{}^+ b_{-k}{}^+ - u_k{}^2 v_k{}^2 b_k{}^+ b_{-k}{}^+ b_k{}^+ b_{-k}{}^+\right.$$

$$\left. - u_k{}^2 v_k{}^2 b_{-k} b_k b_{-k} b_k \right) + U\sum_k \left[\left\{u_k{}^3 v_k (m_{-k} + 1) - u_k{}^3 v_k m_k\right.\right.$$

$$\left.\left. + u_k v_k{}^3 m_k - u_k v_k{}^3 (m_{-k} + 1) \right\} b_k{}^+ b_{-k}{}^+ + b_{-k} b_k \right]$$

$$+ U\sum_k u_k{}^2 v_k{}^2 \left[2m_k{}^2 + 2m_k + 1 - 2m_k{}^2 - 2m_k\right]$$

Or

$$H_5 = U\sum_k \left(u_k{}^4 b_k{}^+ b_{-k}{}^+ b_{-k} b_k + v_k{}^4 b_{-k} b_k b_k{}^+ b_{-k}{}^+ - u_k{}^2 v_k{}^2 b_k{}^+ b_{-k}{}^+ b_k{}^+ b_{-k}{}^+\right.$$

$$\left. - u_k{}^2 v_k{}^2 b_{-k} b_k b_{-k} b_k \right) + U\sum_k \left[\left\{u_k{}^3 v_k (m_{-k} + 1) - u_k{}^3 v_k m_k\right.\right.$$

$$+u_k v_k^{\ 3} m_k - u_k v_k^{\ 3}(m_{-k}+1)\}b_k^{\ +} b_{-k}^{\ +} + b_{-k} b_k\Big] + U\sum_k u_k^{\ 2} v_k^{\ 2} \qquad 3.13$$

H_5 contains three terms, the first term contains four operators, the second term is off-diagonal term and the third term is a constant.

The off-diagonal term in H_1 (Equation 3.9) say H_6, is,

$$H_6 = \sum_k \varepsilon_k u_k v_k \left(b_k^{\ +} b_{-k}^{\ +} + b_{-k} b_k\right)$$

The off-diagonal terms in H_5 (Equation 3.13) say H_7, are,

$$H_7 = U\sum_k \Big[\{u_k^{\ 3} v_k (m_{-k}+1) - u_k^{\ 3} v_k m_k + u_k v_k^{\ 3}(m_{-k}+1)\}b_k^{\ +} b_{-k}^{\ +} + b_{-k} b_k\Big]$$

To diagonalize the Hamiltonian, equating the sum of the off-diagonal terms in H_6 and H_7 equal to zero and by neglecting the terms with four operators, we get:

$$\sum_k \varepsilon_k \Big[u_k v_k \left(b_k^{\ +} b_{-k}^{\ +} + b_{-k} b_k\right)\Big] + U\sum_k \Big[\{u_k^{\ 3} v_k (m_{-k}+1) - u_k^{\ 3} v_k m_k$$

$$+ u_k v^3{}_k m_k - u_k v^3{}_k (m_{-k}+1)\}b^+{}_k b^+{}_{-k} + b_{-k} b_k\Big] = 0$$

This implies that**,**

$$\sum_k \varepsilon_k u_k v_k + U\sum_k \Big[u_k^{\ 3} v_k (m_{-k}+1) - u_k^{\ 3} v_k m_k + u_k v_k^{\ 3} m_k - u_k v_k^{\ 3}(m_{-k}+1)\Big] = 0 \qquad 3.14$$

Or

$$b_k^{\ +} b_{-k}^{\ +} + b_{-k} b_k = 0$$

Since m_k are real numbers, $m_k = m_{-k}$, Equation (3.14) reduces to;

$$\sum_k \varepsilon_k u_k v_k + U\sum_k \left[u_k^3 v_k m_{-k} + u_k^3 v_k - u_k^3 v_k m_k + u_k v_k^3 m_k - u_k v_k^3 m_{-k} - u_k v_k^3\right] = 0$$

$$\sum_k \varepsilon_k u_k v_k + U\sum_k \left(u_k^3 v_k - u_k v_k^3\right) = 0$$

$$\sum_k \left[\varepsilon_k u_k v_k + U\left(u_k^3 v_k - u_k v_k^3\right)\right] = 0 \qquad 3.15$$

Obtaining the constant term from Equation (3.9) and (3.13), we get,

$$\sum_k \varepsilon_k v_k^2 + U\sum_k u_k^2 v_k^2 \qquad 3.16$$

Similarly for H_{inter}

$$H_{inter} = (-t)\sum_{r,s,k,\sigma} a^+_{r,k,\sigma} a_{s,k,\sigma} + W \sum_{r,s,k,k',\sigma,\sigma' q} a^+_{r,k+q,\sigma} a^+_{s,k'-q,\sigma} a_{s,k',\sigma'} a_{r,k,\sigma} \qquad 3.17$$

Using Equation (3.6), the first term of the Hamiltonian, say H_8 in Equation (3.17) becomes,

$$H_8 = (-t)\sum_{r,s,k,\sigma} a^+_{r,k,\sigma} a_{s,k,\sigma}$$

$$= -t\sum_k \left(u_k b_k^+ + v_k b_{-k}\right)\left(u_k b_k + v_k b_{-k}^+\right)$$

$$= -t\sum_k \left(u_k^2 b_k^+ b_k + u_k v_k b_k^+ b_{-k}^+ + u_k v_k b_{-k} b_k + v_k^2 b_{-k} b_{-k}^+\right)$$

$$= -t\sum_k \left(u_k^2 b_k^+ b_k + v_k^2 b_{-k} b_{-k}^+\right) - t\sum_k \left(u_k v_k b_k^+ b_{-k}^+ + u_k v_k b_{-k} b_k\right)$$

Using the number operators given in Equation (3.8), H_8 becomes,

$$H_8 = -t\sum_k \left[\left(u_k{}^2 m_k + v_k{}^2 m_{-k} + v_k{}^2\right) + u_k v_k \left(b_k{}^+ b_{-k}{}^+ + b_{-k} b_k\right)\right]$$

$$= -t\sum_k \left[v_k{}^2 + \left(u_k{}^2 m_k + v_k{}^2 m_{-k}\right) + u_k v_k \left(b_k{}^+ b_{-k}{}^+ + b_{-k} b_k\right)\right]$$

$$= -t\sum_k v_k{}^2 - t\sum_k \left(u_k{}^2 m_k + v_k{}^2 m_{-k}\right) - t\sum_k u_k v_k \left(b_k{}^+ b_{-k}{}^+ + b_{-k} b_k\right) \qquad 3.18$$

Dealing with the second part of the Hamiltonian in Equation (3.17), say H_9, we have,

$$H_9 = W \sum_{r,s,k,k',\sigma,\sigma' q} a^+_{r,k+q,\sigma} a^+_{s,k'-q,\sigma'} a_{s,k'\sigma'} a_{r,k,\sigma}$$

$$H_9 = W\sum_k \left(u_k b_k{}^+ + v_k b_{-k}\right)\left(u_k b_{-k}{}^+ + v_k b_k\right)\left(u_k b_{-k} - v_k b_k{}^+\right)\left(u_k b_k + v_k b_{-k}{}^+\right)$$

The product of the last two terms is,

$$H_{10} = W\sum_k \left(u_k{}^2 b_{-k} b_k + u_k v_k b_{-k} b_{-k}{}^+ - u_k v_k b_k{}^+ b_k - v_k{}^2 b_k{}^+ b_{-k}{}^+\right) \qquad 3.19$$

Operating with $\left(u_k b_{-k}{}^+ - v_k b_k\right)$ on Equation (3.19) on the left, we have,

$$H_{11} = W\sum_k \Big(u_k{}^3 b_{-k}{}^+ b_{-k} b_k + u_k{}^2 v_k b_{-k}{}^+ b_{-k} b_{-k}{}^+ - u_k{}^2 v_k b_{-k}{}^+ b_k{}^+ b_k$$

$$- u_k v_k{}^2 b_{-k}{}^+ b_k{}^+ b_{-k}{}^+ + u_k{}^2 v_k b_k b_{-k} b_k - u_k v_k{}^2 b_k b_{-k} b_{-k}{}^+$$

$$+ u_k v_k{}^2 b_k b_k{}^+ b_k + v_k{}^3 b_k b_k{}^+ b_{-k}{}^+ \qquad 3.20$$

Operating with $\left(u_k b_k^{+} + v_k b_{-k}\right)$ on Equation (3.20) from the left, finally we have,

$$
\begin{aligned}
H_{12} = W\sum_k \Big(& u_k^{4} b_k^{+} b_{-k}^{+} b_{-k} b_k + u_k^{3} v_k b_k^{+} b_{-k}^{+} b_{-k} b_{-k}^{+} \\
& - u_k^{2} v_k^{2} b_k^{+} b_{-k}^{+} b_k^{+} b_{-k}^{+} + u_k^{3} v_k b_k^{+} b_{-k}^{+} b_k^{+} b_k \\
& - u_k^{3} v_k b_k^{+} b_k b_{-k} b_k - u_k^{2} v_k^{2} b_k^{+} b_k b_{-k} b_{-k}^{+} \\
& + u_k^{2} v_k^{2} b_k^{+} b_k b_k^{+} b_k + u_k v_k^{3} b_k^{+} b_k b_k^{+} b_{-k}^{+} \\
& + u_k^{3} v_k b_{-k} b_{-k}^{+} b_{-k} b_k + u_k^{2} v_k^{2} b_{-k} b_{-k}^{+} b_{-k} b_{-k}^{+} \\
& - u_k^{2} v_k^{2} b_{-k} b_{-k}^{+} b_k^{+} b_k - u_k v_k^{3} b_{-k} b_{-k}^{+} b_k^{+} b_{-k}^{+} \\
& - u_k^{2} v_k^{2} b_{-k} b_k b_{-k} b_k - u_k v_k^{3} b_{-k} b_k b_{-k} b_{-k}^{+} \\
& + u_k v_k^{3} b_{-k} b_k b_k^{+} b_k + v_k^{4} b_{-k} b_k b_k^{+} b_{-k}^{+} \qquad 3.21
\end{aligned}
$$

Using the number operators of Equation (3.8), H_{12} becomes,

$$
\begin{aligned}
H_{12} = W\sum_k \Big[\Big\{ & u_k^{4} b_k^{+} b_{-k} b_{-k} b_k + v_k^{4} b_{-k} b_k b_k^{+} b_{-k}^{+} - u_k^{2} v_k^{2} b_k^{+} b_{-k}^{+} b_k^{+} b_{-k}^{+} \\
& - u_k^{2} v_k^{2} b_{-k} b_k b_{-k} b_k \Big\} + \Big\{ u_k^{3} v_k \left(m_{-k} + 1\right) b_k^{+} b_{-k}^{+} \\
& - u_k^{3} v_k m_k b_k^{+} b_{-k}^{+} + u_k v_k^{3} m_k b_k^{+} b_{-k}^{+} \\
& - u_k v_k^{3} \left(m_{-k} + 1\right) b_k^{+} b_{-k}^{+} + u_k^{3} v_k \left(m_{-k} + 1\right) b_{-k} b_k \\
& - u_k^{3} v_k m_k b_{-k} b_k + u_k v_k^{3} m_k b_{-k} b_k - u_k v_k^{3} \left(m_{-k} + 1\right) b_{-k} b_k \Big\}
\end{aligned}
$$

$$+\left\{u_k^{\,2}v_k^{\,2}m_k m_k + u_k^{\,2}v_k^{\,2}(m_{-k}+1)(m_{-k}+1)\right.$$
$$\left.-u_k^{\,2}v_k^{\,2}m_k(m_{-k}+1) - u_k^{\,2}v_k^{\,2}(m_{-k}+1)\right\}\Big] \qquad 3.22$$

Factoring out the operators $b_k^{\,+}b_{-k}^{\,+}, b_{-k}b_k$ in the second term and the common term $u_k^{\,2}v_k^{\,2}$ in the third term of Equation (3.22), H_{12} becomes,

$$H_{12} = W\sum_k \Big(u_k^{\,4}b_k^{\,+}b_{-k}^{\,+}b_{-k}b_k + v_k^{\,4}b_{-k}b_k b_k^{\,+}b_{-k}^{\,+} - u_k^{\,2}v_k^{\,2}b_k^{\,+}b_{-k}^{\,+}b_k^{\,+}b_{-k}^{\,+}$$
$$-u_k^{\,2}v_k^{\,2}b_{-k}b_k b_{-k}b_k\Big) + W\sum_k \Big[\Big\{u_k^{\,3}v_k(m_{-k}+1) - u_k^{\,3}v_k m_k$$
$$+u_k v_k^{\,3}m_k - u_k v_k^{\,3}(m_{-k}+1)\Big\}b_k^{\,+}b_{-k}^{\,+} + b_{-k}b_k\Big]$$
$$+W\sum_K u_k^{\,2}v_k^{\,2}\big[m_k m_k + (m_{-k}+1)(m_{-k}+1) - 2m_k(m_{-k}+1)\big]$$

Or

$$H_{12} = W\sum_k \Big(u_k^{\,4}b_k^{\,+}b_{-k}^{\,+}b_{-k}b_k + v_k^{\,4}b_{-k}b_k b_k^{\,+}b_{-k}^{\,+} - u_k^{\,2}v_k^{\,2}b_k^{\,+}b_{-k}^{\,+}b_k^{\,+}b_{-k}^{\,+}$$
$$-u_k^{\,2}v_k^{\,2}b_{-k}b_k b_{-k}b_k\Big) + W\sum_k \Big[\Big\{u_k^{\,3}v_k(m_{-k}+1) - u_k^{\,3}v_k m_k$$
$$+u_k v_k^{\,3}m_k - u_k v_k^{\,3}(m_{-k}+1)\Big\}b_k^{\,+}b_{-k}^{\,+} + b_{-k}b_k\Big]$$
$$+W\sum_k u_k^{\,2}v_k^{\,2}\big[2m_k^{\,2} + 2m_k + 1 - 2m_k^{\,2} - 2m_k\big]$$

Or

$$H_{12} = W\sum_k \Big(u_k^{\,4} b_k^{\,+} b_{-k}^{\,+} b_{-k} b_k + v_k^{\,4} b_{-k} b_k b_k^{\,+} b_{-k}^{\,+} - u_k^{\,2} v_k^{\,2} b_k^{\,+} b_{-k}^{\,+} b_k^{\,+} b_{-k}^{\,+}$$
$$- u_k^{\,2} v_k^{\,2} b_{-k} b_k b_{-k} b_k \Big) + W\sum_k \Big[\Big\{u_k^{\,3} v_k \left(m_{-k}+1\right) - u_k^{\,3} v_k m_k$$
$$+ u_k v_k^{\,3} m_k - u_k v_k^{\,3}\left(m_{-k}+1\right)\Big\}\Big(b_k^{\,+} b_{-k}^{\,+} + b_{-k} b_k\Big]$$
$$+ W\sum_k u_k^{\,2} v_k^{\,2} \qquad 3.23$$

The off-diagonal term in Equation (3.18) is,

$$-t\sum_k u_k v_k \left(b_k^{\,+} b_{-k}^{\,+} + b_{-k} b_k\right) \qquad 3.24$$

The off-diagonal terms in Equation (3.23) are,

$$W\sum_k \Big[\Big\{u_k^{\,3} v_k \left(m_{-k}+1\right) - u_k^{\,3} v_k m_k$$
$$+ u_k v_k^{\,3} m_k - u_k v_k^{\,3}\left(m_{-k}+1\right)\Big\}\Big(b_k^{\,+} b_{-k}^{\,+} + b_{-k} b_k\Big] \qquad 3.25$$

To diagonalize the Hamiltonian, equate the sum of terms in Equation (3.24) and (3.25) to zero, let the terms with m_k and m_{-k} in H_8 to vanish and neglecting the terms containing four operators of H_{12} we get,

$$-t\sum_k u_k v_k \left(b_k^{\,+} b_{-k}^{\,+} + b_{-k} b_k\right) + W\sum_k \Big[\Big\{u_k^{\,3} v_k \left(m_{-k}+1\right) - u_k^{\,3} v_k m_k$$
$$+ u_k v_k^{\,3} m_k - u_k v_k^{\,3}\left(m_{-k}+1\right)\Big\}\Big(b_k^{\,+} b_{-k}^{\,+} + b_{-k} b_k\Big] = 0$$

Or

$$-t\left[\sum_k u_k v_k + W\sum_k \left\{u_k{}^3 v_k\left(m_{-k}+1\right) - u_k{}^3 v_k m_k + u_k v_k{}^3 m_k - u_k v_k{}^3\left(m_{-k}+1\right)\right\}\right] b_k{}^+ b_{-k}{}^+ + b_{-k} b_k = 0$$

This implies,

$$-t\sum_k u_k v_k + W\sum_k \left\{u_k{}^3 v_k\left(m_{-k}+1\right) - u_k{}^3 v_k m_k + u_k v_k{}^3 m_k - u_k v_k{}^3\left(m_{-k}+1\right)\right\} = 0$$

$$-t\sum_k u_k v_k + W\sum_k \left\{u_k{}^3 v_k m_{-k} + u_k{}^3 v_k - u_k{}^3 v_k m_k + u_k v_k{}^3 m_k - u_k v_k{}^3 m_{-k} - u_k v_k{}^3\right\} = 0 \quad 3.26$$

Since $m_k = m_{-k}$, Equation (3.26) reduces to,

$$-t\sum_k u_k v_k + W\sum_k \left(u_k{}^3 - u_k v_k{}^3\right) = 0 \quad 3.27$$

From Equation (3.18) and (3.23), the sum of constant terms for H_{inter} is

$$-t\sum_k v_k{}^2 + W\sum_k u_k{}^2 v_k{}^2 \quad 3.28$$

From $H = H_{intra} + H_{inter}$

The sum of off- diagonal terms from Equations (3.15) and (3.27) becomes

$$\sum_k \left[\varepsilon_k u_k v_k + U\left(u_k^{\ 3} v_k - u_k v_k^{\ 3}\right)\right] - \sum_k \left[t u_k v_k + W\left(u_k^{\ 3} v_k - u_k v_k^{\ 3}\right)\right] = 0$$

Or

$$\sum_k \left[(\varepsilon_k - t) u_k v_k + (U + W)\left(u_k^{\ 3} v_k - u_k v_k^{\ 3}\right)\right] = 0$$

The sum of constant terms from Equation (3.16) and (3.28) becomes:

$$\sum_k \varepsilon_k v_k^{\ 2} + U \sum_k u_k^{\ 2} v_k^{\ 2} - t \sum_k v_k^{\ 2} + W \sum_k u_k^{\ 2} v_k^{\ 2} = H_{diagonal}$$

$$\sum_k (\varepsilon_k - t) v_k^{\ 2} + (U + W) \sum_k u_k^{\ 2} v_k^{\ 2} = H_{diagonal} = E_i \qquad 3.29$$

For electrons (Fermions)

$u_k^{\ 2} + v_k^{\ 2} = 1$, (Plakida, 1995), this implies that when,

$u_k = 0$, Then $v_k = 0$ and

$u_k = 1, v_k = 0$

These combinations are not acceptable since they do not give any physically important results. Thus $u_k = v_k = \frac{1}{\sqrt{2}}$ will be the only useful values.

From equation (3.29) the energy of the state i, E_i , is given by,

$$E_i = \left[(\varepsilon_k - t) v_k^{\ 2} + u_k^{\ 2} v_k^{\ 2} (U + W)\right] \qquad 3.30$$

Substituting the values of u_k and v_k, Equation (3.30) becomes,

$$E_i = \frac{1}{2}(\varepsilon_k - t) + \frac{1}{4}(U + W) \qquad 3.31$$

The temperature dependence of the energy E_i will be introduced through the thermal activation factor e^{-E_i/k_BT}. The system energy E_i will be multiplied by e^{-E_i/k_BT} such that the energy of the system becomes $E = E_i e^{-E_i/k_BT}$.

Equation (3.31) changes to,

$E = \left[\frac{1}{2}(\varepsilon_k - t) + \frac{1}{4}(U + W)\right] e^{-E_i/k_BT}$ Where k_B is the Boltzmann Constant

Where $\varepsilon_k = \varepsilon_f$

Hence,

$$E = \left[\frac{1}{2}\left(\frac{\hbar^2 k_F{}^2}{2m} - t\right) + \frac{1}{4}(U + W)\right] e^{-E_i/k_BT} \qquad 3.32$$

$$E = E_i e^{-E_i/k_BT} \qquad 3.33$$

Where $E_i = \frac{1}{2}\left(\frac{\hbar^2 k_F{}^2}{2m} - t\right) + \frac{1}{4}(U + W)$

The energy expression in Equation (3.34) will be used to calculate the heat capacity and transition temperature T_c of Cuprates.

The heat capacity, C_V is given by:

$$C_v = \left(\frac{\partial E}{\partial T} \right)$$

and hence,

$$C_s = \frac{E_i^{\ 2}}{k_B T^2} e^{-E_i/k_B T} \qquad 3.34$$

Where C_s is the heat Capacity in the superconducting State.

The transition temperature T_c of the system is obtained from the condition that

$$\left(\frac{\partial C_s}{\partial T} \right)_{T=T_c} = 0$$

$$\frac{\partial}{\partial T} \left(\frac{E_i^{\ 2}}{k_B T^2} e^{-E_i/k_B T} \right) = 0$$

$$\frac{E_i^{\ 3}}{k_B^{\ 2} T_c^{\ 4}} e^{-E_i/k_B T} - \frac{2E_i^{\ 2}}{k_B T_c^{\ 3}} e^{-E_i/k_B T} = 0$$

$$\left(\frac{E_i^{\ 3}}{k_B^{\ 2} T_c^{\ 4}} \right) e^{-E_i/k_B T} = \left(\frac{2E_i^{\ 2}}{k_B T_c^{\ 3}} \right) e^{-E_i/k_B T}$$

$$\frac{E_i}{k_B T_c} = 2$$

Or

$$T_c = \frac{E_i}{2k_B} \qquad 3.35$$

CHAPTER FOUR

RESULTS AND DISCUSSIONS

4.1.1 Transition temperature, T_c and Coulomb repulsion, U.

After diagonalizing the Hamiltonian in Equation (3.1) using Bogoliubov transformation, the equations for the energy of state i, E_i, heat capacity, C_V, and transition temperature, T_c are obtained. For high-T_c Cuprates, experimental data suggests that the Fermi energy, ε_f, ranges between ε_f= 0.1eV– 0.3 eV (Saito *et al.*, 1991).For YBCO, ε_f taken to be 0.2 eV (Vladimir, 1992).

The choice of YBCO was due to the excellent experimental heat capacity data available. These data will give a good comparison with the results of this study.

The values of E_i are calculated from Equation 3.31 for t =0.015 eV, 0.025 eV and W=-1.117 eV, -1.177 eV respectively (Kakani, 2007).From Equation 3.35, E_i> 0 values give physically acceptable values of transition temperature in this model. The values of critical temperature T_c corresponding to the values of E_i are calculated from Equation 3.35.When t=0.015 eV and W= -1.117 eV the values of $\bar{U}$, E_i and T_c are calculated for the values of U shown in Table 4.1(a) below. $\bar{U}$=U+W is the effective interaction.

Table 4.1(a): Transition temperature, Energy of state and Coulomb repulsion.

U(eV)	0.75	0.76	0.77	0.78	0.79	0.80	0.81	0.82
$\bar{U}$(eV)	-0.37	-0.36	-0.35	-0.34	-0.33	-0.32	-0.31	-0.30
$E_i x10^{-3}$	0.75	3.25	5.75	8.25	10.75	13.25	15.75	18.25
T_c(K)	4.0	18.7	33.1	47.5	61.9	76.3	90.7	105.1

From Table 4.1(a), the variation of transition temperature T_c with on-site repulsion U for t= 0.015 eV and W= -1.117eV is shown in Figure 4.1 below.

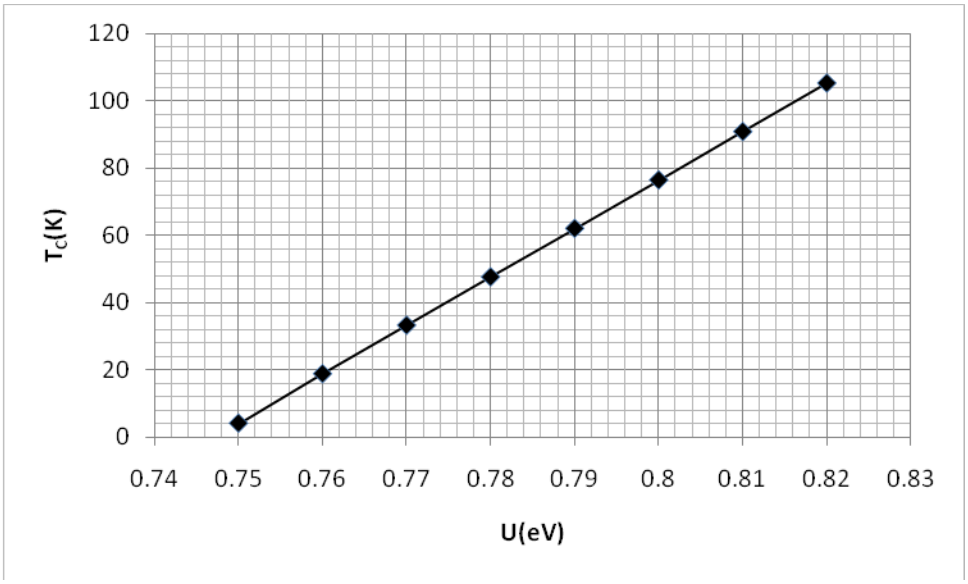

Figure 4.1: Variation of transition temperature T_c with U.

From Figure 4.1, transition temperature increases linearly with U. The values of U was chosen from the condition that E_i> 0 in this model. From Table 4.1(a) when U= 0.81 eV, T_c=90.7 K.

This value is close to the experimental transition temperature of YBCO which is considered in this study.

From Table 4.1(a), the variation of transition temperature T_c with the effective interaction $\bar{U}$ for t=0.015eV and W=-1.177eV is shown in Figure 4.2.

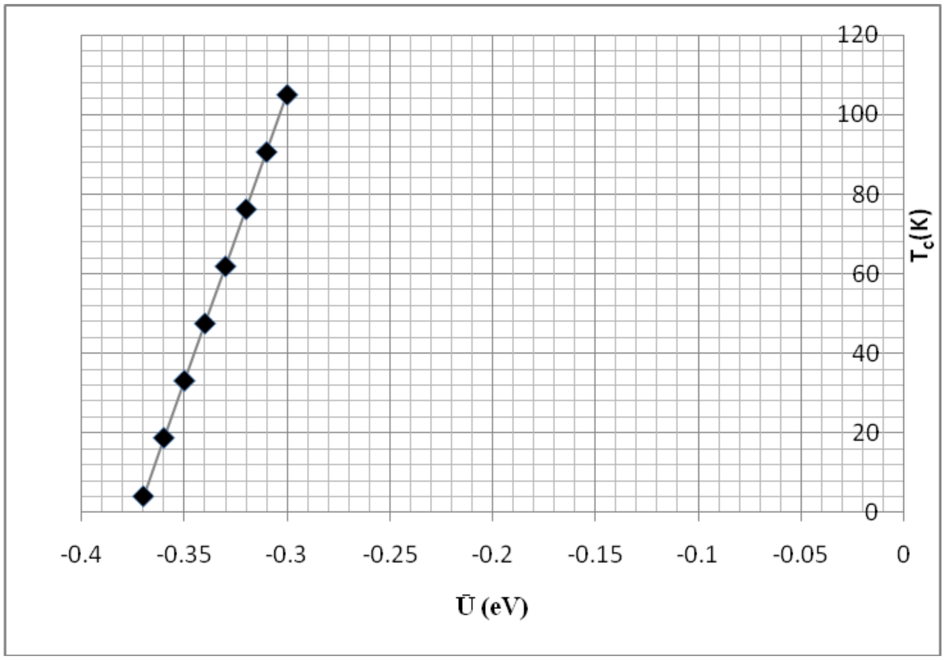

Figure 4.2: Variation of transition temperature T_c with Ū

From Figure 4.2, the transition temperature increases with Ū. The effective interaction Ū is attractive (negative) in this model. This means that the attractive interaction overcomes the on-site coulomb repulsion. When t is increased to 0.025 eV and W=-1.177eV, consequently it leads to an increase in U as shown in Table 4.1(b). For t=0.025 eV, ε_f=0.2 eV and W= - 1.177eV, the values of E_i and T_c are calculated from Equation (3.31) and (3.35) respectively, for the values of U shown in Table 4.1(b).

Table 4.1(b): Transition Temperature, Energy of State and Coulomb Repulsion.

U(eV)	0.83	0.84	0.85	0.86	0.87	0.88	0.89	0.90
E_i(eV)x 10^{-3}	0.75	3.25	5.75	8.25	10.75	13.25	15.75	18.25
T_c(K)	4.3	18.7	33.1	47.5	61.9	76.3	90.7	105.1

From Table 4.1(b), the variation of transition temperature T_c with on-site repulsion U for t=0.025 eV and W =-1.177eV is shown Figure 4.3 below.

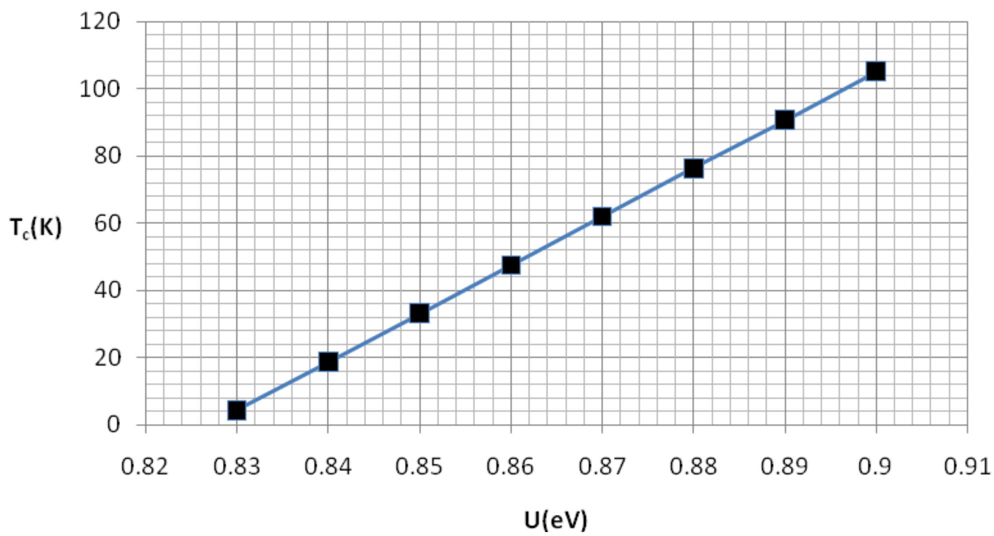

Figure 4.3: Variation of transition temperature T_c with U

From Table 4.1(b), the value of U which gives a transition temperature of 90.7 K is 0.89 eV for t=0.025 eV and W= -1.177eV.This further shows that an increase in interlayer hopping t and interlayer interaction W helps to enhance $T_{c.}$

4.1.2 Heat Capacity

The heat capacity in the superconducting state, C_s is calculated from Equation (3.34) in the temperature domain 10K≤T≤100K.

From Table 4.1(a), the value of U=0.81 eV gives the value of transition temperature as 90.7 K. This is close to the experimental transition temperature of YBCO which is 90K. The value of E_i corresponding to U= 0.81 eV, t=0.015 eV and W= -1.117 eV is 0.01575 eV. Using this value of E_i in Equation (3.34), the heat capacity, C_s, of YBCO is calculated for the temperature range shown in Table 4.2 below.

Table 4.2: Heat Capacity in Superconducting State.

Temperature (K)	$C_s x10^{-6}$(eV/K)
10	0.0003
20	0.08
30	9.1
40	18.8
50	30.3
60	38.5
70	43.7
80	46.2
90	46.9
100	46.0

The variation of heat capacity with temperature in Table 4.2 is shown in Figure 4.4.

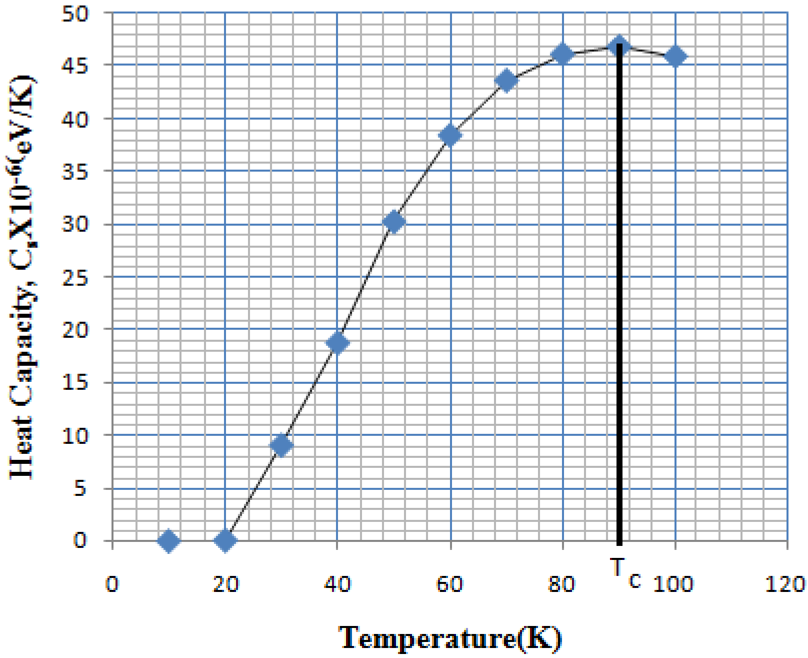

Figure 4.4: Variation of heat capacity with temperature.

From Figure 4.4, for T<Tc, the graph increases exponentially with temperature. The shape of heat capacity graph for superconducting phase C_s indicate specific heat jump at $T=T_c$ typical of superconducting state. From Figure 4.4, the transition temperature is around 90K which is equal to the experimental value of YBCO.

From Equation (3.31), when t = 0.015 eV, W=-1.117eV and U=0.81 eV then E_i =0.01575 eV, the value of T_c calculated from Equation (3.35) is given by,

$$T_c = \frac{E_i}{2k_B}$$

$$= \frac{0.01575}{2x0.868\,x10^{-4}}$$

= 90.7K

This calculated value of T_c compares well with the value of T_c from Figure 4.4 which is around 90K.

The heat capacity for the normal state C_n is calculated using the formula (Varshney et. al., 2003).

$$C_n = \gamma T \tag{4.1}$$

Where γ is the specific heat coefficient (Sommerfeld gamma)

= 3.0 x 10^{-26} J/K^2, or 1.87 x 10^{-7} eV/K^2, (Plakida, 1995).

The heat capacity, for the normal state, C_n is calculated using Equation (4.1) for the temperature range shown in Table 4.3.

Table 4.3: Heat Capacity for the Normal State.

Temperature(K)	C_n x 10^{-6}(eV/K)
10	1.9
20	3.7
30	5.6
40	7.5
50	9.4

Table 4.3 (continuation)

Temperature(K)	C_nX10^{-6}(eV/K)
60	11.2
70	13.1
80	14.9
90	16.8
100	18.7
110	20.6
120	22.4
140	26.2
150	28.1
160	29.9
170	31.8
180	33.7
190	35.5
200	37.4
210	39.3
220	41.2
230	43.0

From Table 4.2 and 4.3, the comparison between specific heat capacity C_s for the superconducting state and C_n for the normal state is shown in Figure 4.5.

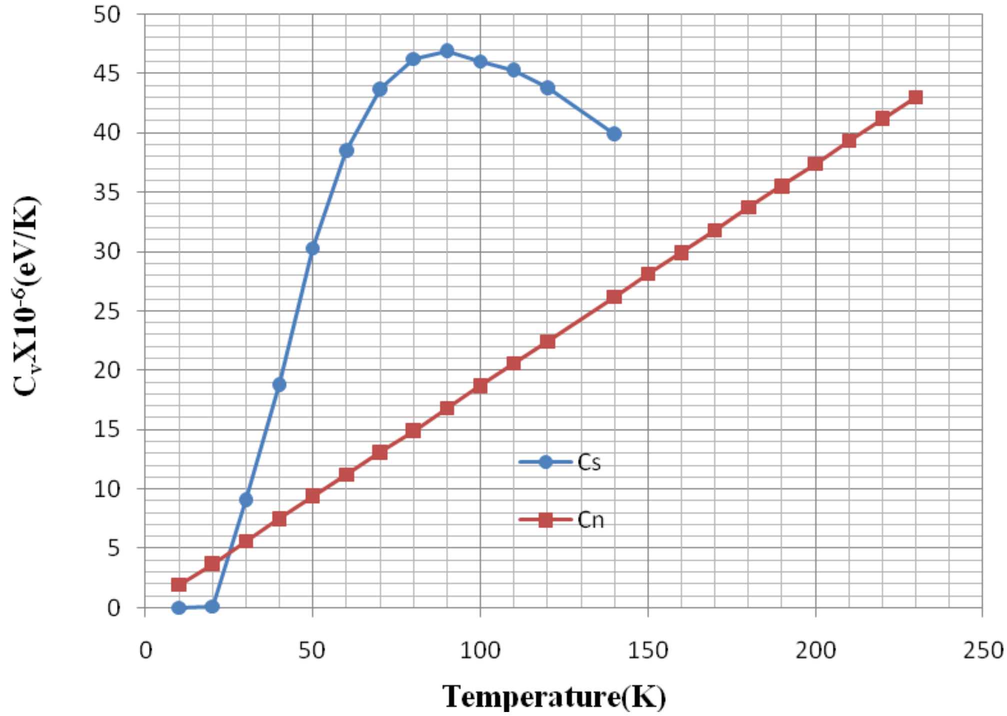

Figure 4.5: Variation of C_n and C_s with temperature.

When T_c = 90.7K, C_n= 16.96 x 10^{-6} eV/atom-K,

From Figure 4.5, at T = T_c, C_s = 46.9 x 10^{-6} eV/atom-K,

Hence $\frac{C_s}{C_n} = 2.76$

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATIONS

The presence of square planer Cu-O layer in the high T_c Cuprates clearly establishes the importance of interlayer interaction. In a bilayer or multilayer Cuprate the separation between adjacent CuO_2 planes within the unit cell is smaller than the adjacent layers in a single layer system; therefore it is natural to include interlayer interactions in multilayer Cuprates. The one-band, two-layer model with intra and interlayer interactions considered in this study for Yttrium Barium Copper Oxide can be generalized to multilayer systems.

For t=0.015eV and W= -1.117eV, the transition temperature increases linearly with on-site Coulomb repulsion as shown in figure 4.1. The transition temperature obtained for t=0.015eV, W=-1.117eV and E_i= 0.01575 eV was 90.7K. When t is increased to 0.025eV and W=-1.177eV, the transition temperature obtained was 90.7K. It was found that the transition temperature increases linearly with the effective interaction, $\bar{U}$ as shown in figure 4.2.This study therefore reveals that the interlayer and intralayer interactions play a significant role in enhancing transition temperature in layered Cuprates.

The variation of heat capacity in the superconducting state with temperature increases exponentially for $T<T_c$, it suffers a jump at T_c=90.7K as shown in figure 4.4. The ratio of heat capacity in the superconducting state to that of the normal state at $T=T_c$ is 2.76. This compares well with the experimental value of 2.43 (Hazen, 1990).

It is recommended that this model be extended to study the role of interlayer and intralayer interactions in transition temperature and heat capacity of Mercury-based Cuprates such as $H_gBa_2Ca_2Cu_2O_8$ and $H_gBa_2Ca_2Cu_3O_x$ which have transition temperature of 135K and 133K respectively.

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