

**PHASE TRANSITION IN SUPERCONDUCTORS**

**BY**

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## DECLARATION

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## **DEDICATION**

This thesis is dedicated to my loved ones especially my parents Mr. and Mrs. Rop for believing in me and investing in me. To my beloved kids Abigael and Bradley for giving me ample time.

## ABSTRACT

Superconductivity is the disappearance of DC electrical resistance in a material when it is cooled to a certain critical temperature, when a material changes from normal state to superconducting state when it is cooled to a certain critical temperature is known as phase transition. Superconductivity occur when electron-phonon interaction is attractive and this occur when the energy difference between the electronic states involved is less than the phonon energy, and vice versa, that the critical temperature for transition to the superconducting state depends on the isotopic mass. This pointed to the possibility that the superconducting transition involved some kind of interaction with the crystal lattice. This electron-phonon interaction is likely to overcome the Coulomb repulsion and binds the fermions into pairs which then condense and superconduct. In exotic pairing three electrons take part in the superconducting current and that they interact with each other through harmonic forces. Two of these electrons form a bound pair while the third one is a polarization electron which hops from one lattice site to another lattice site of similar symmetry. The polarization electron causes perturbations leading to contraction of  $Cu_p - O_3$  bond. Three types of possible interactions between electrons in the crystal that are believed to cause transition to superconducting phase are explored theoretically using perturbation theory. According to the theory of second quantization, if a perturbation commutes with the rest of the Hamiltonian, it leads to a phase transition. The objective of the study is to investigate the commutability of the three interactions if it can lead to phase transition of a superconductor: The three types of interactions are interaction of electrons through phonons exchange, simultaneous existence of electron-phonon interaction and Coulomb interaction, and exotic pairing of electrons. Thus the interactions commute and can lead to a phase transition, and they can be used to study the properties of superconductors.

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**LIST OF SYMBOLS AND ABBREVIATIONS**

$a_k^+$	Creation operator for the state k
$a_k$	Annihilation operator for the state k
BCS	Bardeen, Cooper and Schrieffer
BEC	Bose-Einstein Condensation
$B$	Magnetic induction
$C_p$	Specific heat capacity
$G$	Gibb's Free energy
$J$	Current density
$K_F$	Fermi wave vector
$H_0$	Unperturbed Hamiltonian
$H$	Magnetic field
$H_1$	Perturbed Hamiltonian
$H_c$	Critical magnetic field
$M$	Magnetic intensity moment
$n_k$	Occupation probability
$R_s$	Superconducting state Resistance



$R_n$	Normal state Resistance
T	Temperature
$T_C$	Critical Temperature
$T_\lambda$	Lambda temperature
$U$	Internal energy
$V_C$	Critical Coulomb repulsion
$V$	Coulomb repulsion
$\sigma$	Electrical Conductivity
$\chi_m$	Magnetic susceptibility
$\lambda$	London penetration depth
$\xi_0$	Coherence length
$\rho$	Resistivity
$\Delta$	Energy gap
${}^3He$	Helium 3
${}^4He$	Helium 4

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God bless you all!

## CHAPTER ONE

### INTRODUCTION

#### 1.1 Background

When temperature of frozen mercury is reduced below its critical temperature of about 4.2 K, its electrical resistance disappeared resulting in the flow of electrical current of the order of  $10^5$  Amperes (Onnes, 1911). This disappearance of electrical resistance was termed superconductivity, and it opened up a new research field that was envisaged to usher in ideal electrical conductors. Later, it was found that a number of pure metals, alloys and doped semiconductors also become superconductors at very low temperatures, which are nowadays called conventional superconductors.

In 1957, an acceptable microscopic theory for superconductivity, based on the concept of pairing of electrons of opposite spins and momenta (time-reversed states) near the Fermi surface, was given by Bardeen, Cooper and Schrieffer and is usually referred as BCS Theory (Bardeen, *et al.*, 1957).

The effective interaction between a pair of electrons (Cooper-pair) results from the virtual exchange of a phonon between the two electrons constituting the pair. Such an interaction is called electron-phonon interaction. The interaction is attractive when the energy difference between the electronic states involved is less than the phonon energy, and vice versa. The important contribution to the interaction energy is given by short rather than long wavelength phonon. The strength of this electron-phonon interaction also reaches peak when the electrons are in the states of equal and opposite momenta and of opposite spins.

It is found that the critical temperature for transition to the superconducting state depends on the isotopic mass (any of two or more forms of a chemical element, having the same number of protons in the nucleus or the same atomic number but having different numbers of neutrons in the nucleus or different atomic weight). This pointed to the possibility that the superconducting transition involved some kind of interaction with the crystal lattice. This supported the concept of electron-phonon interaction (Reynolds *et al.*, 1950; Maxwell, 1950).

Bednorz and Muller (1986) discovered superconductivity in Lanthanum-based cuprate perovskite material, which had a transition temperature of 35 K.

The vanishing of the direct current electrical resistance below the critical transition temperature,  $T_C$  is one of the characteristic properties of a superconductor. Thus, the electrical conductivity,  $\sigma$ , tends to infinity for  $T < T_C$  for superconducting materials.

The current density,  $J$  is given by Ohm's law as:

$$J = \sigma E \quad (1.1)$$

Where  $\sigma$  is the conductivity of the material and  $E$  is the electric field across the conductor. If the current density is finite, then equation (1.1) shows that the conductivity is inversely proportional to the applied electric field, and hence as  $\sigma \rightarrow \infty$ , when  $E \rightarrow 0$  inside a superconductor. The Maxwell's law of electromagnetic induction is given by:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (1.2)$$

Where  $\vec{B}$  is the magnetic field. Thus, if  $E = 0$  inside the superconductor as implied above, then equation (1.2) becomes:

$$\frac{\partial B}{\partial t} = 0 \quad (1.3)$$

On integrating equation (1.3) with respect to time, it gives the value of B as a constant inside the superconductor, i.e.

$$B = \text{Constant} \quad (1.4)$$

Thus, the magnetic field,  $B$ , does not change with time inside a material whose electrical conductivity,  $\sigma$ , is infinite. It is found that the ratio of the resistance  $R_s$  in the superconducting state and that in the normal state  $R_n$  is: (Khanna, 2008)

$$\frac{R_s}{R_n} < 10^{-15} \quad (1.5)$$

When the resistance disappears, there will be no heat dissipative effect and hence circulating electrical current in a superconducting ring can persist for a very long time. The existence of persistent current is a proof of zero resistance.

Several theories have been advanced to describe the transition of materials from the normal state to the superconducting state, but their full understanding and simplification continue to emerge. In this work, three types of possible interactions between electrons in the crystal that are believed to cause transition to superconducting phase are explored theoretically using perturbation theory. The three types of interactions are interaction through phonons exchange, simultaneous existence of electron-phonon interaction and Coulomb interaction, and exotic pairing of electrons.

## 1.2 Statement of the problem

In the study of the phenomena of superconductivity, mainly two types of superconductors exist. One are called conventional superconductors whose properties are explained by the Bardeen-Cooper-Schrieffer Theory (BCS Theory) and the others are called high-temperature superconductors (HTS).As of to-day there is still no definite understanding of what type of interaction between the electrons leads to high-temperature superconductivity. What is common between the BCS Theory and the high- $T_C$  Theories is that the interactions between the electrons play a predominant role in leading to the phenomena of superconductivity. Since the nature of materials that fall under BCS theory is quite different from the nature of materials that can be classified as high  $T_C$  superconductors, the interactions between the electrons in the two cases have to be different. But what seem to be common in the nature of interaction is the electron-phonon interaction. In conventional superconductors or BCS type superconductors, the interaction between a pair of electrons results from the virtual exchange of a phonon between the two electrons constituting the pair. It is found that the critical temperature for transition to the superconducting state in BCS theory depends on the isotopic mass, which hints of a possibility that the transition involves some kind of electron-phonon interaction in the crystal lattice. This electron-phonon interaction is likely to overcome the Coulomb repulsion and binds the fermions into pairs which then condense and super conduct. In exotic pairing two of the electrons form a bound pair while the third one is a polarization electron. The polarization electron causes perturbations leading to contraction of  $Cu_p - O_3$  bond. Thus, theoretical understanding of interactions between electrons is very important in order to show if whether phase transition can take place, and use them to study the properties of superconductors.

### **1.3 Objectives of the study**

#### **1.3.1. General objective**

The general objective of this research is to investigate various types of electrons interactions and show if it can lead to phase transition of a superconductor if they commute.

#### **1.3.2 Specific objective**

The specific objective of this research is;

To show that perturbed and unperturbed Hamiltonian can lead to phase transition of a superconductor if it commutes under the following interactions:

- (i) Electrons interaction via the exchange of phonons using Frohlich Hamiltonian as unperturbed Hamiltonian.
- (ii) Simultaneous existences of electron-phonon interaction and Coulomb interaction using Nakajima Hamiltonian as unperturbed Hamiltonian.
- (iii) Exotic pairing of electrons using Hamiltonian for simple harmonic oscillator as unperturbed Hamiltonian

### **1.4 Justification**

Superconductors have been of great importance since their inceptions in early 20<sup>th</sup> century as a result of their ability to carry large quantities of electric current without heat loss as well as generate strong magnetic field. Thus, electric generators made with superconducting wires are far more efficient than conventional generators wound with copper wire. In addition, a Superconducting Quantum Interference Device (SQUID) is a device capable of sensing a change in a magnetic field over a billion

times weaker than the force that moves the needle on a compass. Thus, varied and practical applications of superconductors are on the rise and theoretical knowledge on their behavior is beneficial for development of newer and cheaper superconductors. One of these characteristics is its ability to undergo a phase transition, and this study gives a simplified theory of analyzing it.



## CHAPTER TWO

### LITERATURE REVIEW

#### 2.1 Introduction

The discovery of liquefied helium by the Dutch physicists Heike Kamerlingh Onnes in 1908 opened up a new field in low-temperature physics and this was a precursor to the discovery of superconductivity three years later (Dirk and Kes, 2010). Superconductivity is the disappearance of electrical resistance in an electric conductor, and since its discovery in 1911 (Onnes, 1911), scientists and engineers have been searching for theoretical understandings and practical applications respectively to date. Various theoretical and experimental studies have been done and published and substantial knowledge and information on superconductivity now exist in literature.

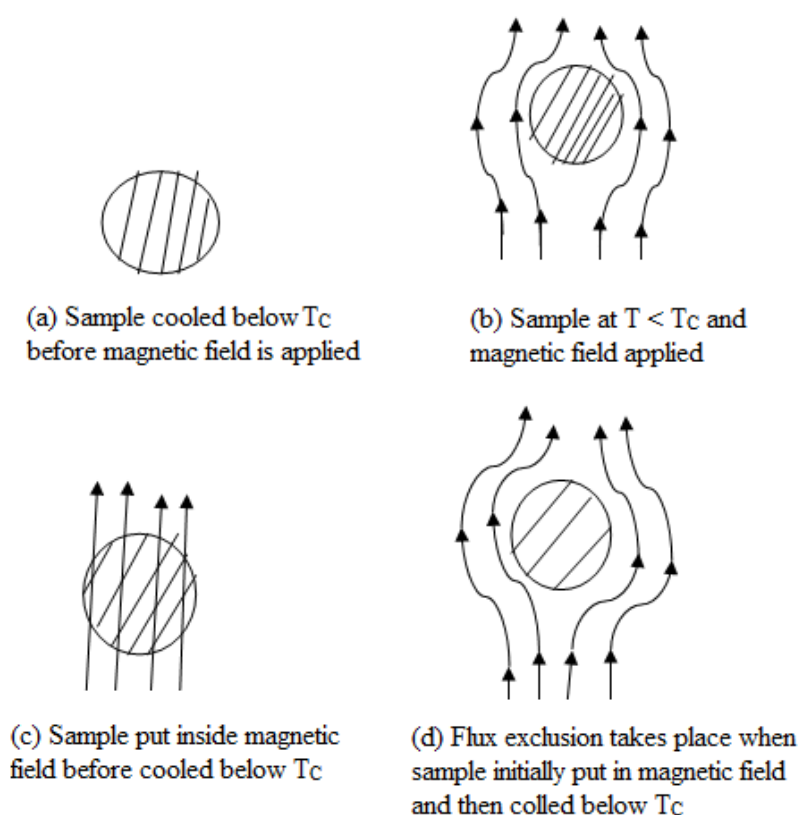
#### 2.2 Superconductivity

A superconductor is a material that loses all electrical resistance to the flow of electric current when it is cooled below a certain temperature, called the critical temperature or transition temperature,  $T_C$ . In addition to suddenly achieving zero resistance at temperatures below  $T_C$ , the superconductor gains other unusual magnetic and electrical properties. Two anomalous properties that a superconductor attains at temperatures below  $T_C$  are:

- a) The transition from finite resistivity,  $\rho_n$  in the normal state above a superconducting  $T_C$  to  $\rho = 0$ , i.e. perfect DC conductivity,  $\sigma = \infty$ , below  $T_C$ ,
- b) The simultaneous change of magnetic susceptibility  $\chi$  from a small positive paramagnetic value above  $T_C$  to  $\chi = -1$ , i.e. perfect diamagnetism below  $T_C$ .

### 2.3 Meissner effect

When a metal is cooled to the superconducting state in a moderate magnetic field, it expels the magnetic field from its interior, regardless of whether there was a field inside or not before cooling below  $T_C$ . This expulsion of magnetic field from the interior of a conductor is referred to as Meissner effect (Meissner and Ochsenfeld, 1933). The sketches in the Fig.2.1 illustrate how Meissner effect is developed in a conductor.



**Figure 2. 1: Formation of Meissner effect in a conductor**

When  $\sigma \rightarrow \infty$ , and the applied magnetic field is small, then the constant value of magnetic field inside the conductor is zero. The superconducting state does not depend on the amount of magnetic field preserved inside the material before it is

cooled below  $T_C$ . The relationship between the magnetic induction,  $B$ , and the magnetic field,  $H$  and the magnetic intensity moment,  $M$  is given by:

$$B = H + 4\pi M \quad (2.1)$$

But, the magnetic susceptibility,  $\chi_M$  is given by:

$$\chi_M = \frac{M}{H} \quad (2.2)$$

Factoring  $H$  on the right hand side of equation (2.1) and using equation (2.2), yields

$$B = H(1 + 4\pi\chi_M) \quad (2.3)$$

Thus, from equation (2.3), if  $B = 0$  inside the material, then  $\chi_M = -\frac{1}{4\pi}$ . This means that for low external magnetic field, the susceptibility of the material is negative and this is the fundamental requirement for a material to be diamagnetic (Khanna, 2008).

When a superconductor is placed in a weak external field  $H$  and cooled below its transition temperature, then the magnetic field is ejected. The Meissner effect does not cause the field to be completely ejected but instead the field penetrates the superconductor but only to a very small distance, characterized by a parameter called London penetration depth,  $\lambda$ . Beyond the length  $\lambda$ , the field decays rapidly to zero. A superconductor with little or no magnetic field within it is said to be in the Meissner state, but this state breaks down when the applied magnetic field is too large, (Khanna, 2008).

## 2.4 Types of Superconductors

Meissner (Meissner and Ochsenfeld, 1933) discovered experimentally that a superconductor has a tendency to exclude magnetic field from its interior.

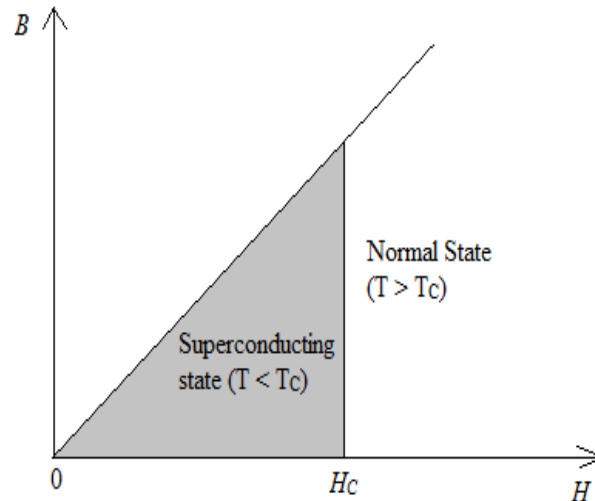
Superconducting materials have the ability to exist either in the normal state or the superconducting state, depending on the external magnetic field they are subjected to. If the magnetic field is increased beyond a critical value  $H_C$ , which is different for different materials, the Meissner effect breaks down. Based on this phenomenon, the superconductors are divided into two classes:

1. Type I superconductors, and
2. Type II superconductors.

#### **2.4.1 Type I superconductors**

Type I superconductors, have a single critical field  $H_C$ , above which all superconductivity is lost. The finite temperature superconductivity is abruptly destroyed when the strength of the applied field rises above a critical value  $H_C$ . Depending on the geometry of the sample, one may obtain an intermediate state consisting of a baroque pattern of regions of normal material carrying a magnetic field mixed with regions of superconducting material containing no field (Landau and Lifschitz., 1984; Callaway and David, 1990).

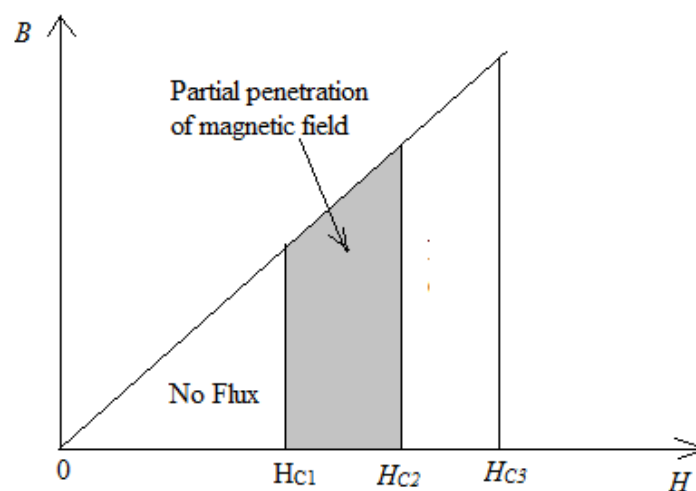
A magnetic field  $H$  is completely excluded from the interior of the specimen when  $H < H_C$  but completely penetrates the sample when  $H > H_C$ . Fig. 2.2 illustrates this behavior.



**Figure 2. 2: Type I Superconductor**

### 2.4.2 Type II superconductors

In type II superconductors, there is a partial penetration of the magnetic field into the sample when the applied magnetic field  $H$  lies between  $H_{C1}$  and  $H_{C2}$ . Small surface super currents may still flow up to an applied field  $H_{C3}$  as long as the current is not too large or a thin surface layer may remain superconducting up to the field  $H_{C3}$ . Beyond  $H_{C3}$  superconductivity is destroyed. Fig.2.3 illustrates this behavior.



**Figure 2. 3: Type II superconductor**

### 2.4.3 Type I and II superconductors

Another important factor, in addition to London penetration depth, in superconductivity is the superconducting coherence length,  $\xi$ . One defines a coherence length  $\xi$  equals to  $\frac{\hbar v_f}{\pi\Delta}$  where  $v_f$  is the Fermi velocity,  $\hbar$  is reduced Planck constant and  $\Delta$  is superconducting energy gap. The ratio of  $\lambda$  to  $\xi$  determines whether a superconductor is type I or type II superconductor. Type I superconductors are those with  $0 < \frac{\lambda}{\xi} < \frac{1}{\sqrt{2}}$  and type II superconductors are those  $\frac{\lambda}{\xi} > \frac{1}{\sqrt{2}}$  (Tinkham, 1996).

## 2.5 Phase Transitions

### 2.5.1 First order phase transition

In a phase change, the change involves a major re-arrangement of structure of the substance, resulting in change of volume, specific heat, entropy, viscosity, etc at the critical temperature  $T_C$ . Since such changes involve energy change produced at a finite amount of heat or the latent heat, then the transition takes place at a constant temperature i.e.  $dT = 0$ .

When a substance undergoes a change of phase from phase 1 (normal state) to phase 2 (superconducting state), the accompanied latent heat,  $L$  is given by:

$$L_{12} = T_C (S_2 - S_1) \quad (2.4)$$

Where  $S_1$  and  $S_2$  are entropies in phase 1 and 2 respectively. Equation (2.4) shows that there is a discontinuity in entropy since the heat capacity,  $C_P$  is given by:

$$C_P = T \left( \frac{\partial S}{\partial T} \right)_P \quad (2.5)$$

The heat capacity, from equation (2.5), becomes infinity at transition because at  $T = T_C$ ,  $S$  is finite at  $T = 0$ , hence  $c_p \rightarrow \infty$ . Transition for which  $L_{12}$  is finite and  $c_p \rightarrow \infty$  is called first order phase transition (type I superconductor) (Kandie, 2008)

### 2.5.2 Second order phase transition

There are other changes of phase involving the initiation of a different kind of ordering in a crystal lattice, the appearance of superfluid in helium II, super-fluidity of a nuclear system and appearance of the solid and a super-solid  $^4\text{He}$ , superconductivity of such phase changes may involve a change of slope of  $S$  against  $T$  at the transition point not a change of the value. In this case the heat capacity changes discontinuously, but does not become infinite at  $T_C$ . Such changes are called phase changes of the second kind. For such changes, there is no discontinuity in volume ( $V_1 = V_2$ ) or entropy ( $S_1 = S_2$ ) during the transition is called second order phase transition (Type II superconductivity) (Kandie, 2008)

### 2.6 Thermodynamics of superconductors

The Gibbs free energy density of a system when the external magnetic field is changed is given by:

$$G = U - ST + PV \quad (2.6)$$

Differentiating equation (2.6) gives:

$$dG = dU - SdT + TdS + PdV + Vdp \quad (2.7)$$

But  $V = -\frac{B}{4\pi}$  and  $dP = dH$ , and substituting them in equation (2.7) gives:

$$dG = -SdT - \frac{B}{4\pi} dH \quad (2.8)$$

Where  $S$  is the entropy per unit volume. Using equation (2.8) and holding the magnetic field,  $H$  and temperature,  $T$  constant separately yields respectively the entropy  $S$  as:

$$S = -\left(\frac{dG}{dT}\right)_H \quad (2.9a)$$

$$S = -4\pi\left(\frac{dG}{dH}\right)_T \quad (2.9b)$$

If we consider a long superconducting cylinder in a magnetic field that is parallel to the axis of the cylinder and then increase the value of  $H$  from 0 to some value  $H$  at a constant temperature ( $-SdT=0$ ), equation (2.8) becomes

$$G(T, H) - G(T, 0) = -\frac{1}{4\pi} \int_0^H B(H') dH' \quad (2.10)$$

The right hand side of equation (2.10) gives the magnetic work stored per  $\text{cm}^3$  of the material. However, in the normal state  $B = H$  and in the homogeneous superconducting region  $B = 0$ , hence

$$G_n(T, H) - G_n(T, 0) = -\frac{1}{4\pi} \int_0^H H' dH' = -\frac{1}{4\pi} \frac{H^2}{2} = -\frac{H^2}{8\pi} \quad (2.11)$$

And in the superconducting state

$$G_s(T, H) - G_s(T, 0) = -\frac{1}{4\pi} \int_0^H 0 dH' = 0 \quad (2.12)$$

Hence, equation (2.12) gives:

$$G_s(T, H) = G_s(T, 0) \quad (2.13)$$

Since these two phases are in thermodynamic equilibrium at the critical field  $H_c(T)$ ,

then



$$G_s(T, H_c) = G_n(T, H_c) \quad (2.14)$$

Using equations (2.13), we can write

$$G_s(T, 0) - G_n(T, 0) = G_s(T, H) - G_n(T, 0) = G_s(T, H_c) - G_n(T, 0) \quad (2.15)$$

Or

$$G_s(T, 0) - G_n(T, 0) = G_n(T, H_c) - G_n(T, 0) \quad (2.16)$$

Using equation (2.11) in equation (2.16), we get

$$G_s(T, 0) - G_n(T, 0) = -\frac{H_c^2}{8\pi} \quad (2.17)$$

This, equation (2.17), shows that negative condensation energy  $-\frac{H_c^2}{8\pi}$  per unit

volume accompanies the formation of a superconducting state. Subtracting equation

(2.11) from (2.13) and re-arranging the terms, we get,

$$G_s(T, H) - G_n(T, H) = G_s(T, 0) - G_n(T, 0) + \frac{H^2}{8\pi} \quad (2.18)$$

Or

$$G_s(T, H) - G_n(T, H) = -\frac{H_c^2}{8\pi} + \frac{H^2}{8\pi} \quad (2.19)$$

Or

$$G_s(T, H) - G_n(T, H) = -\frac{1}{8\pi} \left[ \{H_c^2(T)\}^2 - H^2 \right] \quad (2.20)$$

Equation (2.20) implies that the superconducting state is indeed the equilibrium state

for all  $H < H_c(T)$ . Using equation (2.9) for the entropy  $S$  and equation (2.20), we get

$$S_s(T, 0) - S_n(T, H) = \frac{1}{4\pi} H_c(T) \frac{dH_c(T)}{dT} \quad (2.21)$$

According to the Nernst theorem,  $S \rightarrow 0$  when  $T \rightarrow 0$ , and from equation (2.21), it follows that

$$\frac{dH_c}{dT} = 0 \quad (2.22)$$

Hence, equation (2.22) shows that  $H_c(T)$  has zero derivative at  $T = 0$ . However, from experiment, equation (2.22) takes the form:

$$\frac{dH_c}{dT} < 0 \quad (2.23)$$

Which implies that  $S_s < S_n$ . The superconducting state is more ordered than the normal state and latent heat  $Q_L$  is given by,

$$Q_L = T(S_s - S_n) = \frac{1}{4\pi} T H_c(T) \frac{dH_c(T)}{dT} \quad (2.24)$$

The empirical relation for the variation of  $H_c(T)$  with the temperature  $T$  is

$$H_c(T) = H_c(0) \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right] \quad (2.25)$$

This gives that at  $T = T_c$ ,  $H_c(T) = 0$  and the  $H_c(T)$  is a maximum at  $T = 0$ . Using these facts in equation (2.14), we get that the latent heat  $Q_L$  vanishes at  $T = 0$  and  $T = T_c$  (since at  $T = T_c$ ,  $H_c(T) = 0$ ).

Finally specific heat is

$$C_H = -T \left( \frac{\delta S}{\delta T} \right)_H \quad (2.26)$$

Using equation (2.9) in equation (2.26) and then substituting for entropy in the expression for the specific heat, we get the expression for  $C_s - C_n$

$$C_s - C_n = \frac{T}{4\pi} \left[ \left( \frac{dH_c}{dT} \right)^2 + H_c \frac{d^2 H_c}{dT^2} \right] \quad (2.27)$$

Now the change in the specific as the specimen undergoes a transition from normal to the superconducting state i.e. the jump in the specific heat at  $T = T_c$  becomes

$$(C_s - C_n)_{T=T_c} = (\Delta C)_{T=T_c} = \frac{T_c}{4\pi} \left[ \left( \frac{dH_c}{dT} \right)_{T=T_c} \right] \quad (2.28)$$

Equation (2.28) is the Rutgers formula. The jump in the specific heat means that the transition is a second order phase transition.

For first order phase transition to occur, there must be constant temperature and constant applied magnetic field; heat must be supplied to the specimen to enable it to make the transition from superconducting to the normal state.

## 2.7 High - $T_c$ superconductivity

Until 1986, it was believed that the BCS theory forbade superconductivity at temperature of about 30K or above. In that year, Bednorz and Muller discovered superconductivity in lanthanum-based cuprate with a transition temperature of 35 K and they won the Noble Prize of physics in 1987 (Bednorz and Muller, 1986) for this discovery.

It was later found by Wu and Chu that replacing the lanthanum with Yttrium raises the critical temperature to 92 K (Wu *et al.*, 1987) which was important because liquid nitrogen could then be used as a refrigerant, since its boiling point is 77 K at

atmospheric pressure. Thus, high  $T_C$  superconductor was defined as one whose critical transition temperature  $T_C$  is greater than 30 K and the superconducting state can be reached by cooling in liquid nitrogen.

The discovery of possible high  $T_C$  superconductivity in Lanthanum-Barium-Copper-oxide (La-Ba-Cu-O,  $T_C=30\text{K}$ ) system was an important and decisive break through in the high  $T_C$  superconductivity research. There was a great success with La-Ba-Cu-O and La-Sr-Cu-O compounds whose transition temperature were more than 90 K. The three main families of mixed oxides that have shown high  $T_C$  superconductivity properties are;

1. Yttrium-Barium-Copper-Oxide (YBa-Cu-O,  $T_C =90\text{K}$ )
2. Bismuth-Strontium-Calcium-Copper-Oxide (Bi-Si-Ca-Cu-O,  $T_C =105\text{K}$ )
3. Thallium-Barium-Calcium-Copper-Oxide (Ti-Ba-Ca-Cu-O,  $T_C =110\text{K}$ )

By March 2007, the World record of high  $T_C$  superconductivity was held by a ceramic superconductor consisting of Thallium, Mercury, Copper, Barium, Calcium, Strontium and Oxygen ( $T_C =138\text{K}$ ). A patent has also been applied for a material with  $T_C =150$  K. Many other cuperate superconductors have been discovered and some of them with their values of  $T_C$  are given below;

Formulae	Highest $T_C$ (K)
YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7.5</sub>	92
Bi <sub>2</sub> Sr <sub>2</sub> CaCu <sub>2</sub> O <sub>8</sub>	90
Bi <sub>2</sub> Sr <sub>2</sub> CaCu <sub>2</sub> O <sub>10</sub>	122

$\text{TL}_2\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$	127
$\text{TLBa}_2\text{CaCu}_2\text{O}_7$	90
$\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_8$	135
$\text{TL}_2\text{Ba}_2\text{CaCu}_3\text{O}_8$	110

Although by now quite a few high  $T_C$  superconductors (HTS) have been discovered, attempt to make HTS was not successful in 1970's. But finally discovered in 1986-1987, and the mechanism of HTS is still not obvious and still continues to be a subject for theoretical study. There is a lot of experimental data on HTS that cannot be explained by BCS theory and the high  $T_C$  theories proposed up to today.

## **2.8 Anharmonic Apical oxygen vibration in high- $T_C$ superconductors**

There are a number of theories that have been proposed to explain the properties of high- $T_C$  superconductors (Khanna, 2008). The theory of anharmonic apical oxygen vibration in high- $T_C$  superconductors is briefly described here.

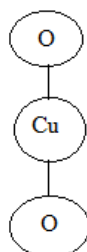
The structure of a high temperature superconductor is closely related to perovskite structure and the structure of these compounds has been described as a distorted, oxygen deficient multi-layered system.

One of the properties of the crystal structure of oxide superconductors is an alternating multi-layer of  $\text{CuO}_2$  planes with superconductivity taking place between these layers. The more the layers of  $\text{CuO}_2$ , the higher the  $T_C$ , but there is no change in  $T_C$  for layers more than three.

The charge carriers are electrons and the pairing mechanism between the electrons is exotic. The electronic pairing in exotic superconductors is such that three electrons

take part in the superconducting current and that they interact with each other through harmonic forces. Two of these electrons form a bound pair while the third one is a polarization electron which hops from one lattice site to another lattice site of similar symmetry (Khanna and Kirui, 2002).

Studies that have been done in photo-induced Raman scattering have confirmed that there exists strong anharmonic nature of apical oxygen vibrations (Mihailovic *et al.*, 1990). When the spectral function of electron-phonon interaction is compared with the phonon spectrum in bismuth compound it is noted that, both low frequency vibrations and high frequency vibrations contribute to the electron-phonon coupling. High frequency vibrations are referred to 'Breathing mode' and low frequency vibrations are called 'Buckling mode'. Fig 2.4 is the apical oxygen atom that contraction when polarization electron causes perturbation.



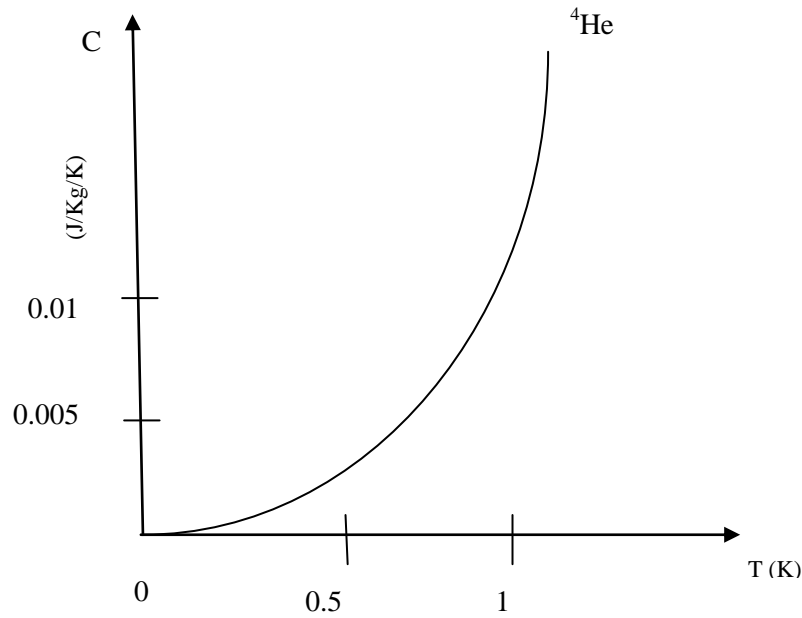
**Figure 2. 4: Apical oxygen atom**

## 2.9 Phase Transition in superconductors and superfluids

Phase transition is of first-order when the latent heat is finite and not equal to zero and are of second-order phase transition when there is a specific heat jump at the transition temperature  $T_C$  .

The well-known superfluid is liquid  $^4\text{He}$  in which there is a discontinuity in the specific heat at the  $\lambda$ -transition temperature. Such a transition is of second-order

phase transition and takes place at  $T_C = T_\lambda = 2.176K$ , and this transition exists also in  $^3\text{He}$ . Again in liquid  $^4\text{He}$  when the specific heat is measured below  $T_\lambda$ ; particularly in the region 0K to 1K, the specific heat varies continuously as shown in Figure 2.5.



**Figure 2. 5: Specific heat capacity**

Thus, if another phase transition takes place in the region  $0 < T < 1K$ , it is not clearly known what kind of phase transition it could be, This is still an open question to be solved theoretically.

There is a possibility of investigating the crossover from a Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein Condensate (BEC) superfluid (Astrakharchik *et al.*, 2004). In these systems the strength of the interaction can be varied over a very wide range by magnetically tuning the two-body scattering amplitude. For positive values of the S-Wave scattering length 'a', atoms with different spins are observed to pair into bound molecules which, at low enough temperatures, form a Bose condensate (Jochim *et al.*, 2003). The molecular BEC state is adiabatically converted into a ultracold Fermi gas

with  $a < 0$  and  $\frac{K_F}{a} \ll 1$  (Bartenstein *et al.*, 2004 and Bourdel *et al.*, 2004) where standard BCS theory is expected to apply. In the cross-over region the value of  $|a|$  can be orders of magnitude larger than the inverse Fermi wave vector  $K_F^{-1}$ . In dilute system, for which the effective range of the interaction  $R_o$  is much smaller than the mean inter particle distance  $K_F R_o \ll 1$ , the energy of the non-interacting Fermi gas is  $\varepsilon_{FG}$  where,

$$\varepsilon_{FG} = \frac{3}{10} \frac{\hbar^2 K_F^2}{m} \quad (2.29)$$



## CHAPTER THREE

### THEORY AND DERIVATIONS

#### 3.1 Introduction

This chapter presents the equations that were used to investigate the mode of electrons interactions in the conductor crystal to explain the transition to the superconducting states.

#### 3.2 Phase transition

In classical thermodynamics, the order of phase transition is determined by a definition given by Ehrenfest (Huang, 1975). Ehrenfest defines a phase transition to be an  $n^{\text{th}}$  order transition if, at the transition point

$$\frac{\partial^n G_1}{\partial T^n} \neq \frac{\partial^n G_2}{\partial T^n} \quad (3.1)$$

And

$$\frac{\partial^n G_1}{\partial p^n} \neq \frac{\partial^n G_2}{\partial T^n} \quad (3.2)$$

Where  $G_1$  and  $G_2$  are the Gibb's free energy in the two phases, whereas all lower derivatives are equal. Apart from the well-known gas-liquid transition, there is one known example of a phase transition that fits into the schemes of Ehrenfest the second order phase transition in superconductivity. With the discovery of different types of superconductors namely , type I superconductors, type II superconductors, BCS superconductors , High Temperature superconductors etc. It is found that in some

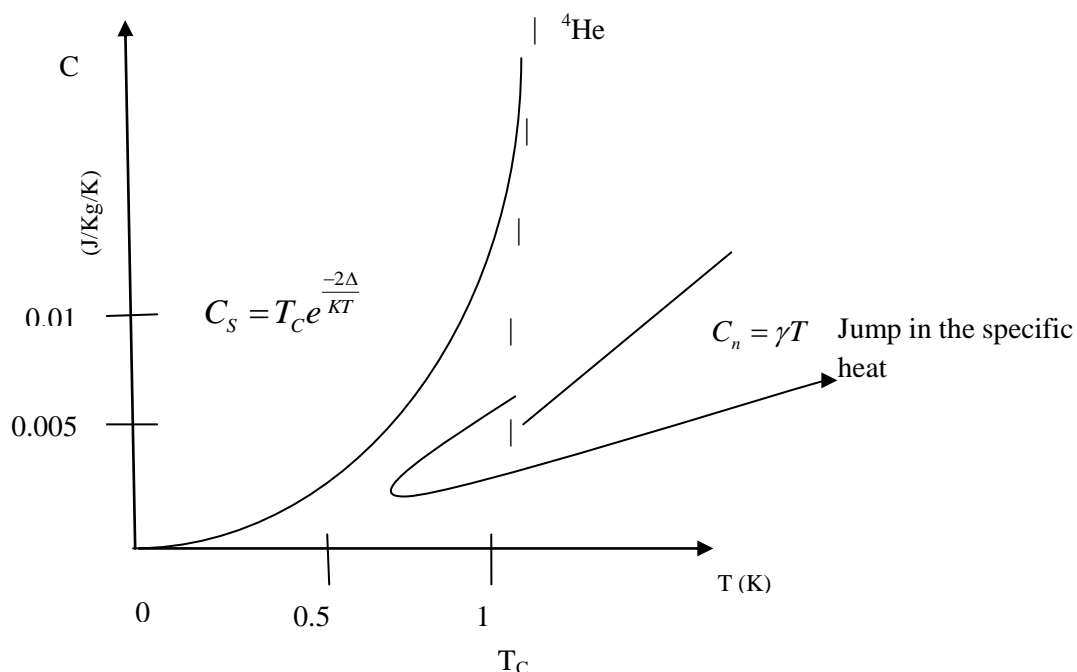
cases the superconducting transition is of the first order and in some cases the superconducting transition is of second order.

In some cases, the variation of specific heat with temperature is used to study the order of phase transition. Since the specific heat is related to the second derivative of  $G$ , these examples cannot be characterized by the behaviours of the higher derivatives of  $G$ , because they do not exist. Thus the Ehrenfest scheme is not the most general classification of the phase transitions.

According to second quantization, if a perturbation commutes with the unperturbed Hamiltonian, it can lead to a phase transition (Fock, 1932). However, it gives no indication of whether the phase transition will be first order or second order. To determine the order of phase transition, we have to use either the Ehrenfest's rule or study the variation of specific heat with temperature. In general in a reversible thermodynamic process involving finite latent heat, the transition is of first-order.

For instance the basis for the thermodynamics description of a superconductor is the assumption that a superconductor in a magnetic field is in a single thermodynamic stable state. When the acting external magnetic field  $H < H_c(0)$ , for  $T < T_c$ , the phase transition at  $H = H_c(T)$  is of the first order, i.e. the latent heat is involved or it is finite. However, the latent heat goes to zero as  $T \rightarrow T_c$  so that the transition at  $T_c$ , when  $H_c(T_c) = 0$  (i.e. when there is no acting external magnetic field) is a second order phase transition. Thus the superconducting transition is of the first order in a finite magnetic field (latent heat is involved), and it is of the second order in the absence of the external magnetic field (latent heat is zero)

The electronic specific heat in the normal state for  $T > T_c$  is roughly given by  $\gamma T$ . In the superconducting state this varies as  $T_c e^{-2\Delta/kT}$ , and it is about three times the normal value  $\gamma T$  and the experimental variation shown in fig.3.1 indicates a second order phase transition like the one in liquid  $^4\text{He}$ .



**Figure 3. 1: Second order phase transition in liquid Helium**

In general, phase transitions are common occurrence in ordinary matter, superconducting and superfluid matter. From experience it would be simplest to characterize a phase transition as the manifestation of a certain singularity or discontinuity in the equation of state and or the specific heat. It is common knowledge that the phenomena of phase transition is a possible consequence of molecular interaction as in matter and superfluid  $^4\text{He}$  and other similar superfluid system and also the interaction between electrons and nucleons leading to superconductivity of different types of materials and the superfluidity of nuclear matter, finite nuclei and neutron stars.

The attempt here is to revisit what kind of interactions can lead to a phase transition in superconductors, use of second quantization and perturbation to determine the type of phase transition can be the milestone of this research. To determine whether the transition is first-order or second-order, either the variation of specific heat with temperature is to be studied or the Ehrenfest's rule has to be used.

### 3.3 Electron-phonon interaction

To explain the phenomena of superconductivity, large number of interactions between the electrons has been proposed. These interactions can be treated as perturbations on the unperturbed Hamiltonian (Frohlich,1950). The first such attempt was due to Frohlich who considered the interaction between the electrons via an exchange of a phonon. The Frohlich Hamiltonian, ( $H_F$ ) is written as:

$$H_F = H_0 + H_{e-ph} \quad (3.3)$$

Where  $H_0$  is the unperturbed Hamiltonian given by

$$H_0 = \sum_k \varepsilon_k C_k^+ C_k + \sum_q \hbar \omega_q a_q^+ a_q \quad (3.4)$$

Here the creation  $C_k^+$  and annihilation  $C_k$  operators refer to electrons and  $a_q$  refer to phonons. The value of  $H_{e-ph}$  is given by:

$$H_{e-ph} = \sum_{k,k'} m_{kk'} (a_{-q}^+ + a_q) C_k^+ C_{k'} \quad (3.5)$$

Where  $m_{kk'}$  is the electron-phonon matrix element, the term  $a_{-q}^+ C_k^+ C_{k'}$  refers to the scattering of an electron from  $k'$  to  $k$  with the emission of a phonon of wave vector number  $q = k' - k$  and the terms  $a_q C_k^+ C_{k'}$  refers to the scattering of an electron from  $k'$  to  $k$  with the absorption of a phonon of wave number  $q = k - k'$ . Now to

understand whether the perturbation  $H_{e-ph}$  will lead to a phase transition, one has to calculate the value of  $[H_0, H_{e-ph}]$  and if it turns out to be zero, then such a perturbation can lead to a phase transition.

The purpose is to understand that if a perturbation does not commute with the unperturbed Hamiltonian, it cannot lead to a phase transition. Since Superconducting transition is a phase transition, such a perturbation cannot be considered. This method helps in the elimination of electronic interaction that cannot lead to Superconducting phase transitions.

### 3.4 Simultaneous existence of electron-phonon and Coulomb interaction

Another Hamiltonian also exists which is called the Nakajima Hamiltonian (Taylor, 1970) and is denoted by  $H_N$ . In this Hamiltonian, in addition to the electron-phonon interaction, the Coulomb interaction between lattice of bare ions has been taken into account. The mutual interaction between the electrons is also added to  $H_N$ , and is given by:

$$H_N = H_F + \sum_{k,k'} (m_{kk'}^i - m_{kk'}) (a_{-q}^+ + a_q) C_k^+ C_k + \frac{1}{2} \sum_{k,k',q} V_q C_{k'+q}^+ C_{k'} C_k \quad (3.6)$$

Where  $V_q$  is the Fourier transformation of the mutual interaction between the electrons.

Now if  $H_F$  is taken as the unperturbed Hamiltonian, then the perturbation  $H_I$  will be the rest of two terms in such a system,  $H_F$  and  $H_I$  have to commute i.e.  $[H_F, H_I] = 0$  if there is to be a phase transition.

### 3.5 Exotic pairing

Another form of interaction between the electron in a superconductor is when the charge carriers are electrons and the pairing mechanism between the electrons is exotic (Cox and Maple, 1995). The electronic pairing in exotic superconductors is such that three electrons take part in the superconducting current and that they interact with each other through harmonic forces (Khanna and Kirui, 2002). Two of these electrons form a bound pair while the third one is a polarization electron which hops from one lattice site to another lattice site of the similar symmetry. Studies that have been done in photo-induced Raman scattering (Mihailovic *et al.*, 1990) have confirmed that there exists strong anharmonic nature of apical oxygen vibrations. When the spectral function of electron-phonon interaction is compared with the phonon spectrum in Bismuth compounds, it is noted that both low frequency vibrations (bucking mode) and high frequency vibration (breathing mode) contribute to the electron-phonon coupling (Khanna, 2008).

It was therefore assumed that the polarization electron causes perturbation with respect to the apical oxygen vibrations leading to the contraction of  $Cu_p - O_3$  bond.

This perturbation is assumed to be of the form:

$$H_1 = \beta x^3 + \gamma x^4 \quad (3.6)$$

Where  $\beta$  and  $\gamma$  may or may not depend on the temperature. The parameter,  $x$  is given by:

$$x = \frac{1}{\alpha\sqrt{2}}(a + a^+) \quad (3.7)$$

Where  $\alpha = \frac{\mu\omega}{\hbar^2}$ , and  $\mu$  is the reduced mass of the pair of electrons,  $\omega$  is the phonon frequency,  $a$  and  $a^\dagger$  are annihilation and creation operators for the electron. Now the unperturbed Hamiltonian  $H_0$  for such a system is,

$$H_0 = \frac{P^2}{2\mu} + \frac{1}{2}\mu\omega^2 x^2 \quad (3.8)$$

For such a system to undergo phase transition, we must have,

$$[H_0, H_1] = 0 \quad (3.9)$$

A large number of high  $T_C$  Superconductors exists whose structures are different from each other, where some of them have layered structures. The role of attractive interlayer and intralayer interactions, in layered high temperature cuprate superconductors have been investigated. The interlayer interactions play an important role in the enhancement of  $T_C$  in layered high  $T_C$  cuprates (Arvind and Kakani, 2008). In fact, both interlayer and intralayer interactions play a significant role, hence we can write the value of the unperturbed Hamiltonian  $H_0$  and that of the perturbed Hamiltonian  $H_1$ , where

$$H_1 = H_{intra} + H_{inter} \quad (3.10)$$

In order that such a system can undergo a phase transition, I have to calculate  $[H_0, H_1]$  and see if it is zero.

In this thesis I will obtain the value of  $[H_0, H_{e-ph}]$  and  $[H_0, H_1]$  using theory of second quantization and see if it will lead to a phase transition.

## CHAPTER FOUR

### RESULTS AND DISCUSSIONS

#### 4.1 Introduction

In this chapter, results and discussions will be presented. The three types of interactions will be shown if it contribute to transition to superconductive state, if they commute.

#### 4.2 Electron-phonon interaction

The Frohlic Hamiltonian,  $H_F$  is given is given in section 3.3 and forms the basis for electron-phonon interaction. We will calculate  $[H_0, H_{e-ph}]$  and if it gives a value of zero, then it can lead to a phase transition, i.e. the electron-phonon interaction can lead to a phase transition.

$$[H_0, H_{e-ph}] = (H_0 H_{e-ph} - H_{e-ph} H_0) \quad (4.1)$$

Replacing  $H_0$  and  $H_{e-ph}$  with the corresponding value, we get;

$$= \left\{ \sum_k \varepsilon_k c_k^\dagger c_k + \sum_q \hbar \omega_q a_q^\dagger a_q \right\} \left\{ \sum_{k,k'} M_{kk'} (a_{-q}^\dagger + a_q) c_k^\dagger c_{k'} \right\} - \left\{ \sum_{k,k'} M_{kk'} (a_{-q}^\dagger + a_q) c_k^\dagger c_{k'} \right\} \left\{ \sum_k \varepsilon_k c_k^\dagger c_k + \sum_q \hbar \omega_q a_q^\dagger a_q \right\} \quad (4.2)$$

Equation (4.2) is broken into two parts; the first term will be;

$$\begin{aligned} & \left\{ \sum_k \varepsilon_k c_k^\dagger c_k + \sum_q \hbar \omega_q a_q^\dagger a_q \right\} \left\{ \sum_{k,k'} M_{kk'} (a_{-q}^\dagger + a_q) c_k^\dagger c_{k'} \right\} \\ &= \sum_k \varepsilon_k c_k^\dagger c_k \sum_{k,k'} M_{kk'} a_{-q}^\dagger c_k^\dagger c_{k'} + \sum_k \varepsilon_k c_k^\dagger c_k \sum_{k,k'} M_{kk'} a_q c_k^\dagger c_{k'} + \sum_q \hbar \omega_q a_q^\dagger a_q \sum_{k,k'} M_{kk'} a_{-q}^\dagger c_k^\dagger c_{k'} + \sum_q \hbar \omega_q a_q^\dagger a_q \sum_{k,k'} M_{kk'} a_q c_k^\dagger c_{k'} \end{aligned} \quad (4.3)$$



The second part will be;

$$\begin{aligned}
& \left\{ \sum_{k,k'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_{k'} \right\} \left\{ \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q \right\} \\
&= \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \sum_k \varepsilon_k c_k^+ c_k + \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \sum_q \hbar \omega_q a_q^+ a_q + \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} \sum_k \varepsilon_k c_k^+ c_k + \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} \sum_q \hbar \omega_q a_q^+ a_q
\end{aligned} \tag{4.4}$$

Now equation (4.1) i.e.  $[H_0 H_{e-ph}]$  will be;

$$\begin{aligned}
&= \left( \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} + \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} \right) - \\
& \left( \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} + \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} \right)
\end{aligned} \tag{4.5}$$

Opening the bracket of equation (4.5) we get;

$$\begin{aligned}
&= \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} + \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} - \\
& \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} - \sum_k \varepsilon_k c_k^+ c_k \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} - \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} - \sum_q \hbar \omega_q a_q^+ a_q \sum_{k,k'} M_{kk'} a_q c_k^+ c_{k'} = 0
\end{aligned} \tag{4.6}$$

Hence electron-phonon interaction can lead to a phase transition.

### 4.3 Simultaneous existence of electron-phonon interaction and coulomb interaction

Nakajima Hamiltonian is denoted as  $H_N$ , in this Hamiltonian, in addition to electron-phonon interaction, the coulomb interaction between a lattices of bare ion has been taken into account. The mutual interaction between the electrons is added to  $H_N$ . Thus the final form of  $H_N$  is written as;

$$H_N = H_F + \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \quad (4.7)$$

Where  $V_q$  is the Fourier transformation of the mutual interaction between the electrons. Now  $H_F$  is taken as the unperturbed Hamiltonian, then the perturbation  $H_1$  will be the rest of two terms in such a system. Now we commute  $H_F$  and  $H_1$

$$[H_F, H_1] \quad (4.8)$$

$$H_F = \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_{k'} \quad (4.9)$$

And

$$H_1 = \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \quad (4.10)$$

So

$$[H_F, H_1] = (H_F H_1 - H_1 H_F) \quad (4.11)$$

$$\begin{aligned} &= \left\{ \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_{k'} \right\} \left\{ \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \right\} \\ &- \left\{ \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \right\} \left\{ \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_{k'} \right\} \end{aligned} \quad (4.12)$$

By considering equation (4.12) into two parts ,the first term i.e.

$$\left\{ \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_{k'} \right\} \left\{ \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \right\} \quad (4.13)$$

But

$$\sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_k = \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k - \sum_{kk'} M_{kk'} a_q c_k^+ c_k \quad (4.14)$$

And

$$\sum_{kk'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_k = \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'} a_q c_k^+ c_k \quad (4.15)$$

Then equation (4.13) becomes

$$\begin{aligned} &= \sum_k \varepsilon_k c_k^+ c_k \left( \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k - \sum_{kk'} M_{kk'} a_q c_k^+ c_k + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \right) \\ &+ \sum_q \hbar \omega_q a_q^+ a_q \left( \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k - \sum_{kk'} M_{kk'} a_q c_k^+ c_k + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \right) \\ &+ \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k \left( \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k - \sum_{kk'} M_{kk'} a_q c_k^+ c_k + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \right) \\ &+ \sum_{kk'} M_{kk'} a_q c_k^+ c_k \left( \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k - \sum_{kk'} M_{kk'} a_q c_k^+ c_k + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \right) \end{aligned} \quad (4.16)$$

Opening the bracket of equation (4.16)

$$\begin{aligned} &= \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k + \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k + \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k \\ &+ \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_k \varepsilon_k c_k^+ c_k \\ &+ \sum_q \hbar \omega_q a_q^+ a_q \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k - \sum_q \hbar \omega_q a_q^+ a_q \sum_{kk'} M_{kk'} a_q c_k^+ c_k \end{aligned}$$

$$\begin{aligned}
& -\sum_q \hbar\omega_q a_q^+ a_q \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_{k'} c_k \sum_q \hbar\omega_q a_q^+ a_q \\
& + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_{k'} + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \\
& - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_{k'} c_k \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \\
& + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_{k'} + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} - \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \\
& - \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_{k'} c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \tag{4.17}
\end{aligned}$$

Considering the second term of equation (4.12)

$$\left\{ \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_{k'} c_k \right\} \left\{ \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar\omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_{k'} \right\} \tag{4.18}$$

But

$$\sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} = \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_{k'} + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} - \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'}$$

Then equation (4.18) gives,

$$\begin{aligned}
& = \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_{k'} \left( \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar\omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \right) \\
& + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \left( \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar\omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \right) \\
& - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \left( \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar\omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \right)
\end{aligned}$$

$$\begin{aligned}
& -\sum_{kk'} M_{kk'} a_q c_k^+ c_k \left( \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'} a_q c_k^+ c_k \right) \\
& + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \left( \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'} a_q c_k^+ c_k \right)
\end{aligned} \tag{4.19}$$

When we open the bracket of equation (4.19);

$$\begin{aligned}
& = \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k \sum_k \varepsilon_k c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k \\
& + \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k \\
& + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_k \varepsilon_k c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_q \hbar \omega_q a_q^+ a_q \\
& + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k \\
& - \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_k \varepsilon_k c_k^+ c_k - \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_q \hbar \omega_q a_q^+ a_q - \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k \\
& - \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k \\
& - \sum_{kk'} M_{kk'} a_q c_k^+ c_k \sum_k \varepsilon_k c_k^+ c_k - \sum_{kk'} M_{kk'} a_q c_k^+ c_k \sum_q \hbar \omega_q a_q^+ a_q \\
& - \sum_{kk'} M_{kk'} a_q c_k^+ c_k \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k - \sum_{kk'} M_{kk'} a_q c_k^+ c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k \\
& + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_k \varepsilon_k c_k^+ c_k + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_q \hbar \omega_q a_q^+ a_q
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k' + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k', \\
\end{aligned} \tag{4.20}$$

Combining equation (4.17) and equation (4.20) gives;

$$\begin{aligned}
& = \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k' + \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k' + \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k', \\
& + \sum_k \varepsilon_k c_k^+ c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k' + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_k \varepsilon_k c_k^+ c_k \\
& + \sum_q \hbar \omega_q a_q^+ a_q \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k' + \sum_q \hbar \omega_q a_q^+ a_q \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k' - \sum_q \hbar \omega_q a_q^+ a_q \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k', \\
& - \sum_q \hbar \omega_q a_q^+ a_q \sum_{kk'} M_{kk'} a_q c_k^+ c_k' + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_q \hbar \omega_q a_q^+ a_q \\
& + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k' \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k' + \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k' \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k' - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k' \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k', \\
& - \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k' \sum_{kk'} M_{kk'} a_q c_k^+ c_k' + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k', \\
& + \sum_{kk'} M_{kk'} a_q c_k^+ c_k' \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k' + \sum_{kk'} M_{kk'} a_q c_k^+ c_k' \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k' - \sum_{kk'} M_{kk'} a_q c_k^+ c_k' \sum_{kk'} M_{kk'}^i a_q c_k^+ c_k', \\
& - \sum_{kk'} M_{kk'} a_q c_k^+ c_k' \sum_{kk'} M_{kk'} a_q c_k^+ c_k' + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_k \sum_{kk'} M_{kk'} a_q c_k^+ c_k', \\
& - \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k' \sum_k \varepsilon_k c_k^+ c_k - \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k' \sum_q \hbar \omega_q a_q^+ a_q - \sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_k' \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_k',
\end{aligned}$$

$$\begin{aligned}
& -\sum_{kk'} M_{kk'}^i a_{-q}^+ c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \\
& -\sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_k \varepsilon_k c_k^+ c_k - \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_q \hbar \omega_q a_q^+ a_q \\
& -\sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} - \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \\
& + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_k \varepsilon_k c_k^+ c_k + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} \\
& + \sum_{kk'} M_{kk'}^i a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \\
& + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_k \varepsilon_k c_k^+ c_k + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_q \hbar \omega_q a_q^+ a_q \\
& + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} + \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} \\
& - \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \sum_k \varepsilon_k c_k^+ c_k - \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \sum_q \hbar \omega_q a_q^+ a_q \\
& - \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \sum_{kk'} M_{kk'} a_{-q}^+ c_k^+ c_{k'} - \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \sum_{kk'} M_{kk'} a_q c_k^+ c_{k'} = 0
\end{aligned} \tag{4.21}$$

Hence electron-phonon interaction with coulomb interaction can lead to phase transition.

#### 4.4 Exotic pairing of electrons

In exotic pairing three electrons take part in superconducting, two of this electron forms a bond pair while the third one is a polarization electron which hops from one lattice site to another lattice site of the same symmetry. The polarization electron causes perturbation, which was described in section 3.5, using equations (3.6) to

(3.8).For such a system to undergo transition, we commute perturbed and unperturbed Hamiltonian;

$$[H_0, H_1] = \left[ \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 x^2 \right), (\beta x^3 + \gamma x^4) \right] \quad (4.22)$$

Opening the bracket of equation (4.22)

$$[H_0, H_1] = \left\{ (\beta x^3 + \gamma x^4) \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 x^2 \right) - \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 x^2 \right) (\beta x^3 + \gamma x^4) \right\} \quad (4.23)$$

$$\text{but } x^2 = \left\{ \frac{1}{\alpha \sqrt{2}} (a + a^+) \right\} \left\{ \frac{1}{\alpha \sqrt{2}} (a + a^+) \right\} = \frac{1}{\alpha^2 \sqrt{4}} (a + a^+)^2 \quad (4.24)$$

Opening the bracket of equation (4.24) gives;

$$x^2 = \frac{1}{\alpha^2 \sqrt{4}} (aa + aa^+ + a^+a + a^+a^+) \quad (4.25)$$

$$x^3 = \frac{1}{\alpha^3 \sqrt{8}} (aaa + aaa^+ + aa^+a + aa^+a^+ + a^+aa + a^+aa^+ + a^+a^+a + a^+a^+a^+) \quad (4.26)$$

$$x^4 = \frac{1}{\alpha^4 \sqrt{16}} \left( aaaa + aaaa^+ + aaa^+a + aaa^+a^+ + aa^+aa + aa^+aa^+ + aa^+a^+a + aa^+a^+a^+ + a^+aaa + a^+aaa^+ + a^+aa^+a + a^+aa^+a^+ + a^+a^+aa + a^+a^+aa^+ + a^+a^+a^+a + a^+a^+a^+a^+ \right) \quad (4.27)$$

Equation (4.23) will be;



$$= \left\{ \left( \frac{\beta}{\alpha^3 \sqrt{8}} aaa + aaa^+ + aa^+ a + aa^+ a^+ + a^+ aa + a^+ aa^+ + a^+ a^+ a + a^+ a^+ a^+ + \frac{\gamma}{\alpha^4 \sqrt{16}} (aaaa + aaaa^+ + aaa^+ a + aaa^+ a^+ + aa^+ aa + aa^+ aa^+ + aa^+ a^+ a + aa^+ a^+ a^+ + a^+ aaa + a^+ aaa^+ + a^+ aa^+ a + a^+ aa^+ a^+ + a^+ a^+ aa + a^+ a^+ aa^+ + a^+ a^+ a^+ a + a^+ a^+ a^+ a^+) \right) \left\{ \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 aa + aa^+ + a^+ a + a^+ a^+ \right) \right\} - \left\{ \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 aa + aa^+ + a^+ a + a^+ a^+ \right) \left( \frac{\beta}{\alpha^3 \sqrt{8}} aaa + aaa^+ + aa^+ a + aa^+ a^+ + a^+ aa + a^+ aa^+ + a^+ a^+ a + a^+ a^+ a^+ + \frac{\gamma}{\alpha^4 \sqrt{16}} (aaaa + aaaa^+ + aaa^+ a + aaa^+ a^+ + aa^+ aa + aa^+ aa^+ + aa^+ a^+ a + aa^+ a^+ a^+ + a^+ aaa + a^+ aaa^+ + a^+ aa^+ a + a^+ aa^+ a^+ + a^+ a^+ aa + a^+ a^+ aa^+ + a^+ a^+ a^+ a + a^+ a^+ a^+ a^+) \right) \right\} \right\} \quad (4.28)$$

Equation (4.28) is divided into two parts i.e.

$$\left\{ \left( \frac{\beta}{\alpha^3 \sqrt{8}} aaa + aaa^+ + aa^+ a + aa^+ a^+ + a^+ aa + a^+ aa^+ + a^+ a^+ a + a^+ a^+ a^+ + \frac{\gamma}{\alpha^4 \sqrt{16}} (aaaa + aaaa^+ + aaa^+ a + aaa^+ a^+ + aa^+ aa + aa^+ aa^+ + aa^+ a^+ a + aa^+ a^+ a^+ + a^+ aaa + a^+ aaa^+ + a^+ aa^+ a + a^+ aa^+ a^+ + a^+ a^+ aa + a^+ a^+ aa^+ + a^+ a^+ a^+ a + a^+ a^+ a^+ a^+) \right) \left\{ \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 aa + aa^+ + a^+ a + a^+ a^+ \right) \right\} \right\} \quad (4.29)$$

And

$$\left\{ \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 aa + aa^+ + a^+ a + a^+ a^+ \right) \left( \frac{\beta}{\alpha^3 \sqrt{8}} aaa + aaa^+ + aa^+ a + aa^+ a^+ + a^+ aa + a^+ aa^+ + a^+ a^+ a + a^+ a^+ a^+ + \frac{\gamma}{\alpha^4 \sqrt{16}} (aaaa + aaaa^+ + aaa^+ a + aaa^+ a^+ + aa^+ aa + aa^+ aa^+ + aa^+ a^+ a + aa^+ a^+ a^+ + a^+ aaa + a^+ aaa^+ + a^+ aa^+ a + a^+ aa^+ a^+ + a^+ a^+ aa + a^+ a^+ aa^+ + a^+ a^+ a^+ a + a^+ a^+ a^+ a^+) \right) \right\} \quad (4.30)$$

Since  $\frac{\beta}{\alpha^3 \sqrt{8}}$ ,  $\frac{\gamma}{\alpha^4 \sqrt{16}}$ ,  $\frac{p^2}{2\mu}$  and  $\frac{1}{2} \mu \omega^2$  are independent in equation (4.29), we deal

with creation and annihilation operators.

Opening the bracket of equation (4.29) gives;

$$\begin{aligned}
& aaaaa + aaaaa^+ + aaaaa^+a + aaaaa^+a^+ + aaaa^+aa + aaaa^+aa^+ + aaaa^+a^+a + aaaa^+a^+a^+ + \\
& aa^+aaa + aa^+aaa^+ + aa^+aa^+a + aa^+aa^+a^+ + aa^+a^+aa + aa^+a^+aa^+ + aa^+a^+a^+a + aa^+a^+a^+a^+ + \\
& a^+aaaa + a^+aaaa^+ + a^+aaa^+a + a^+aaa^+a^+ + a^+aa^+aa + a^+aa^+aa^+ + a^+aa^+a^+a + a^+aa^+a^+a^+ + \\
& a^+a^+aaa + a^+a^+aaa^+ + a^+a^+aa^+a + a^+a^+aa^+a^+ + a^+a^+a^+aa + a^+a^+a^+aa^+ + a^+a^+a^+a^+a + a^+a^+a^+a^+a^+ + \\
& aaaaaa + aaaaaa^+ + aaaaaa^+a + aaaaaa^+a^+ + aaaaa^+aa + aaaaa^+aa^+ + aaaaa^+a^+a + aaaaa^+a^+a^+ + \\
& aaa^+aaa + aaa^+aaa^+ + aaa^+aa^+a + aaa^+aa^+a^+ + aaa^+a^+aa + aaa^+a^+aa^+ + aaa^+a^+a^+a + aaa^+a^+a^+a^+ + \\
& aa^+aaaa + aa^+aaaa^+ + aa^+aaa^+a + aa^+aaa^+a^+ + aa^+aa^+aa + aa^+aa^+aa^+ + aa^+aa^+a^+a + aa^+aa^+a^+a^+ + \\
& aa^+a^+aaa + aa^+a^+aaa^+ + aa^+a^+aa^+a + aa^+a^+aa^+a^+ + aa^+a^+a^+aa + aa^+a^+a^+aa^+ + aa^+a^+a^+a^+a + aa^+a^+a^+a^+a^+ + \\
& a^+aaaa + a^+aaaa^+ + a^+aaaa^+a + a^+aaaa^+a^+ + a^+aaa^+aa + a^+aaa^+aa^+ + a^+aaa^+a^+a + a^+aaa^+a^+a^+ + \\
& a^+aa^+aaa + a^+aa^+aaa^+ + a^+aa^+aa^+a + a^+aa^+aa^+a^+ + a^+aa^+a^+aa + a^+aa^+a^+aa^+ + a^+aa^+a^+a^+a + a^+aa^+a^+a^+a^+ + \\
& a^+a^+aaaa + a^+a^+aaaa^+ + a^+a^+aaa^+a + a^+a^+aaa^+a^+ + a^+a^+aa^+aa + a^+a^+aa^+aa^+ + a^+a^+aa^+a^+a + a^+a^+aa^+a^+a^+ + \\
& a^+a^+a^+aaa + a^+a^+a^+aaa^+ + a^+a^+a^+aa^+a + a^+a^+a^+aa^+a^+ + a^+a^+a^+a^+aa + a^+a^+a^+a^+aa^+ + a^+a^+a^+a^+a^+a + a^+a^+a^+a^+a^+a^+
\end{aligned}$$

The rest of the operators will give us zero except the following;

$$\left. \begin{aligned}
aaa^+aa^+a^+ &= (n+1)(n+2)^2 & a^+aaa^+aa^+ &= n(n+1)^2 \\
aaa^+a^+aa^+ &= (n+1)^2(n+2) & a^+aaa^+a^+a &= n^2(n+1) \\
aaa^+a^+a^+a &= n(n+1)(n+2) & a^+aa^+aaa^+ &= n^2(n+1) \\
aa^+aaa^+a^+ &= (n+1)^2(n+2) & a^+aa^+aa^+a &= n^3 \\
aa^+aa^+aa^+ &= (n+1)^3 & a^+aa^+a^+aa &= n^3 \\
aaa^+aa^+a^+a &= n(n+1)^2 & a^+a^+aaaa^+ &= (n+1)(n-1)n \\
aa^+a^+aaa^+ &= n(n+1)^2 & a^+a^+aaa^+a &= n^2(n-1) \\
aa^+a^+aa^+a &= n^2(n+1) & a^+a^+aa^+aa &= n(n-1)^2 \\
aa^+a^+a^+aa &= n(n+1)(n-1) & a^+a^+a^+aaa &= n(n-1)(n-2)
\end{aligned} \right\} (4.31)$$

Since  $\frac{\beta}{\alpha^3\sqrt{8}}$ ,  $\frac{\gamma}{\alpha^4\sqrt{16}}$ ,  $\frac{p^2}{2\mu}$  and  $\frac{1}{2}\mu\omega^2$  are independent, we deal with creation and

annihilation operator in equation (4.30). Opening the bracket of equation (4.30),

gives;

$$\begin{aligned}
& aaaaa + aaaaa^+ + aaaa^+ a + aaaa^+ a^+ + aaa^+ aa + aaa^+ aa^+ + aaa^+ a^+ a + aaa^+ a^+ a^+ + aaaaa + aaaaa^+ + \\
& aaaaa^+ a + aaaaa^+ a^+ + aaaa^+ aa + aaaa^+ aa^+ + aaaa^+ a^+ a + aaaa^+ a^+ a^+ + aaa^+ aaa + aaa^+ aaa^+ + aaa^+ aa^+ a + \\
& aaa^+ aa^+ a^+ + aaa^+ a^+ aa + aaa^+ a^+ aa^+ + aaa^+ a^+ a^+ a + aaa^+ a^+ a^+ a^+ + aa^+ aaa + aa^+ aaa^+ + aa^+ aa^+ a + aa^+ aa^+ a^+ + \\
& aa^+ a^+ aa + aa^+ a^+ aa^+ + aa^+ a^+ a^+ a + aa^+ a^+ aa^+ + aa^+ aaaa + aa^+ aaaa^+ + aa^+ aaa^+ a + aa^+ aaa^+ a^+ + aa^+ aa^+ aa + \\
& aa^+ aa^+ aa^+ + aa^+ aa^+ a^+ a + aa^+ aa^+ a^+ a^+ + aa^+ a^+ aaa + aa^+ a^+ aaa^+ + aa^+ a^+ aa^+ a + aa^+ a^+ aa^+ a^+ + aa^+ a^+ a^+ aa + \\
& aa^+ a^+ a^+ aa^+ + aa^+ a^+ a^+ a^+ a + aa^+ a^+ a^+ a^+ a^+ + a^+ aaaa + a^+ aaaa^+ + a^+ aaa^+ a + a^+ aaa^+ a^+ + a^+ aa^+ aa + a^+ aa^+ aa^+ + \\
& a^+ aa^+ a^+ a + a^+ aa^+ a^+ a^+ + a^+ aaaaa + a^+ aaaaa^+ + a^+ aaaa^+ a + a^+ aaaa^+ a^+ + a^+ aaa^+ aa + a^+ aaa^+ aa^+ + a^+ aaa^+ a^+ a + \\
& a^+ aaa^+ a^+ a^+ + a^+ aa^+ aaa + a^+ aa^+ aaa^+ + a^+ aa^+ aa^+ a + a^+ aa^+ aa^+ a^+ + a^+ aa^+ a^+ aa + a^+ aa^+ a^+ a^+ a + a^+ aa^+ a^+ a^+ a^+ + \\
& a^+ a^+ aaa + a^+ a^+ aaa^+ + a^+ a^+ aa^+ a + a^+ a^+ aa^+ a^+ + a^+ a^+ a^+ aa + a^+ a^+ a^+ aa^+ + a^+ a^+ a^+ a^+ a + a^+ a^+ a^+ a^+ a^+ + a^+ a^+ aaaa + \\
& a^+ a^+ aaaa^+ + a^+ a^+ aaa^+ a + a^+ a^+ aaa^+ a^+ + a^+ a^+ aa^+ aa + a^+ a^+ aa^+ aa^+ + a^+ a^+ aa^+ a^+ a + a^+ a^+ aa^+ a^+ a^+ + a^+ a^+ a^+ aaa + \\
& a^+ a^+ a^+ aaa^+ + a^+ a^+ a^+ aa^+ a + a^+ a^+ a^+ aa^+ a^+ + a^+ a^+ a^+ a^+ aa + a^+ a^+ a^+ a^+ aa^+ + a^+ a^+ a^+ a^+ a^+ a + a^+ a^+ a^+ a^+ a^+ a^+
\end{aligned}$$

The rest will be zero except the following;

$$\left. \begin{aligned}
aaaa^+ a^+ a^+ &= (n+1)(n+2)(n+3) & a^+ aaaa^+ a^+ &= n(n+1)(n+2) \\
aaa^+ aa^+ a^+ &= (n+1)(n+2)^2 & a^+ aaa^+ aa^+ &= n(n+1)^2 \\
aaa^+ a^+ aa^+ &= (n+1)^2 (n+2) & a^+ aaa^+ a^+ a &= n^2 (n+1) \\
aaa^+ a^+ a^+ a &= n(n+1)(n+2) & a^+ aa^+ aaa^+ &= n^2 (n+1) \\
aa^+ aaa^+ a^+ &= (n+1)^2 (n+2) & a^+ aa^+ aa^+ a &= n^3 \\
aa^+ aa^+ aa^+ &= (n+1)^3 & a^+ aa^+ aa^+ a &= n^3 \\
aa^+ aa^+ a^+ a &= n(n+1)^2 & a^+ aa^+ a^+ aa &= n^2 (n-1) \\
aa^+ a^+ aaa^+ &= n(n+1)^2 & a^+ a^+ aaaa^+ &= n(n-1)(n+1) \\
aa^+ a^+ aa^+ a &= n^2 (n+1) & a^+ a^+ aa^+ aa &= n(n-1)^2 \\
aa^+ a^+ a^+ aa &= n(n-1)(n+1) & a^+ a^+ a^+ aaa &= n(n-1)(n-2)
\end{aligned} \right\} (4.32)$$

Combining equation (4.31) and equation (4.32) we get;

$$\begin{aligned}
& (n+1)(n+2)(n+3) + (n+1)(n+2)^2 + (n+1)^2 (n+2) + n(n+1)(n+2) + (n+1)^2 (n+2) + (n+1)^2 + n(n+1)^2 + \\
& n(n+1)^2 + n^2 (n+1) + n(n-1)(n+1) + n(n+1)(n+2) + n(n+1)^2 + n^2 (n+1) + n^2 (n+1) + n^3 + n^3 + (n+1)(n-1)n + \\
& n^2 (n-1) + n(n-1)^2 + n(n-1)(n-2) - (n+1)(n+2)(n+3) - (n+1)(n+2)^2 - (n+1)^2 (n+2) - n(n+1)(n+2) - \\
& (n+1)^2 (n+2) - (n+1)^2 - n(n+1)^2 - n(n+1)^2 - n^2 (n+1) - n(n-1)(n+1) - n(n+1)(n+2) - n(n+1)^2 - n^2 (n+1) - \\
& n^2 (n+1) - n^3 - n^3 - (n+1)(n-1)n - n^2 (n-1) - n(n-1)^2 - n(n-1)(n-2) = 0
\end{aligned} \tag{4.33}$$

Hence exotic pairing can lead to a phase transition.

## CHAPTER FIVE

### CONCLUSIONS AND RECOMMENDATIONS

#### 5.1 Conclusions

By considering electron-phonon interactions, simultaneous existences of electron-phonon interaction and Coulomb interaction between a lattice of bare ions and exotic pairing, and using the theory of second quantization, it has been shown that such interactions leads to a phase transitions because of the commutation of perturbed and unperturbed Hamiltonian. This has been shown in equation (4.6) for electron-phonon interaction, equation (4.21) for simultaneous existences of electron-phonon interaction and Coulomb interaction and equation (4.33) for exotic pairing.

#### 5.2 Recommendations

Having theoretical understanding of interactions between electrons in electron-phonon interactions, simultaneous existences of electron-phonon interaction and Coulomb interaction, and exotic pairing that it can lead to a phase transition, it can be used to study the properties of superconductors and nature of phase transition can be studied.

Theory of second quantization may be used to study whether interlayer and intralayer interactions in layered high temperature cuprate superconductors, can lead to phase transition.

The corresponding Hamiltonian can be written such that the interaction terms between the electrons in the  $CuO$  plane and that perpendicular to it, the two interactions will have different magnitudes and their effect on the nature of phase transition can be studied.

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## APPENDIX

A state with no particles or unoccupied state is called a vacuum state and is written as  $|0\rangle$ . A state with  $n$  particles will be written as  $|n\rangle$ . The relation between  $|n\rangle$  and  $|0\rangle$  is given by,

$$|n\rangle = \frac{(a^+)^n |0\rangle}{(n!)^{1/2}}$$

Where  $(n!)^{1/2}$  is for normalization.

If a destruction operator 'a' operates on  $|0\rangle$ , since there is nothing to destroy in the vacuum state, we will get

$$a|0\rangle = 0$$

Now if a creation operates on  $|n\rangle$ , we get

$$\begin{aligned} a^+ |n\rangle &= \frac{1}{(n!)^{1/2}} (a^+)^{n+1} |0\rangle \\ &= \frac{(n+1)^{1/2}}{[(n+1)!]^{1/2}} (a^+)^{n+1} |0\rangle \\ &= (n+1)^{1/2} \frac{(a^+)^{n+1} |0\rangle}{[(n+1)!]^{1/2}} \\ &= (n+1)^{1/2} |n+1\rangle \end{aligned}$$



This shows that when a creation operator  $a^+$  acts on a state  $|n\rangle$  that has  $n$  particles, we get a new state with the next integer, i.e.  $n+1$  particle state written as  $|n+1\rangle$ . The matrix element between the two states  $n$  and  $n'=n+1$  will be,

$$\begin{aligned}\langle n'|a^+|n\rangle &= \langle n'|(n+1)^{\frac{1}{2}}|n+1\rangle \\ &= (n+1)^{\frac{1}{2}}\langle n'|n+1\rangle \\ &= (n+1)^{\frac{1}{2}}\delta_{n',n}\end{aligned}$$

Using commutation laws, it can be shown that,

$$\begin{aligned}a|n\rangle &= \frac{n^{\frac{1}{2}}(a^+)^{n-1}}{(n!)^{\frac{1}{2}}}|0\rangle \\ &= \frac{n(a^+)^{n-1}|0\rangle}{(n)^{\frac{1}{2}}[(n-1)!]^{\frac{1}{2}}} \\ &= n^{\frac{1}{2}}|n-1\rangle\end{aligned}$$

The matrix element between the two states  $n$  and  $n'=n-1$  will be,

$$\begin{aligned}\langle n'|a|n\rangle &= \langle n'|n^{\frac{1}{2}}|n-1\rangle \\ &= n^{\frac{1}{2}}\langle n'|n-1\rangle \\ &= n^{\frac{1}{2}}\delta_{n',n-1}\end{aligned}$$

This shows that the destruction operator  $a$  lowers the particle number (or quantum number) by unity. Thus operating on the Eigen functions in sequence gives,

$$a^+ a |n\rangle = a^+ n^{1/2} |n-1\rangle$$

$$= n^{1/2} a^+ |n-1\rangle$$

$$= n^{1/2} n^{1/2} |n\rangle$$

$$= n |n\rangle$$

Hence the eigen value of  $a^+ a = n$