



# Quantum Phase Transition: Intra and Inter-Band Interaction on D- Wave Superconductivity

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**Abstract:** There are compounds whose structures support superconductivity at high temperatures. They have intra and inter-band interactions which occur within their bands. However there has been no hybrid Hamiltonian developed so far for a lattice structure that can support conduction by both D-waves and other waves on the same Fermi surface. These waves interact or change from one type to another on the same Fermi surface as they travel. The occurrences of interactions within and across bands with different waves lead to variations in transition temperature and resistance. In an attempt to address these effects, theories that have been developed that consider only S-wave which do not adequately account for the differences when compared with experimental observations. Therefore there was need to advance efforts towards formulation of a theory that would explain differences in the characteristics of compounds that have D-waves and other waves on the same Fermi surface. In advancing these efforts a hybrid system has been developed that takes into consideration intra and inter-band interactions that have introduced new interaction dimensions. These efforts have helped in the understanding of how to achieve a high transition temperature superconductor, which a two band hybrid Hamiltonian has been determined for a Fermi surface with varying fermions density and hybridization terms. It is from it that thermodynamic properties have been obtained by use of the Green's function. Where the correlation function has been substituted in the second quantized Hamiltonian form and the energy gap derived. This enabled us to calculate the thermodynamic potential and energy density. These properties have helped not only in the understanding of multi-component type II superconductors, but more so in the development of high transition temperature superconductors needed for magnetic resonance imaging, high speed data transmission and energy transfers. In this research, inter-band interaction has been considered on a new dimension. Consequently a new Hamiltonian has been formulated and thermodynamic properties derived using the Green's function. These properties show the possibility of attaining high transition temperature superconductivity.

**Keywords:** Energy Gap, Phase Transition, Coupling, D-Wave, Hybrid, Superconductivity, Hamiltonian

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## 1. Introduction

Superconductivity has had major breakthroughs in the past; we have had investigations on compounds whose structures support high temperature superconductivity and as consequently has led to a lot of research activities on these compounds. Achieving a high transition temperature superconductor has been at center of focus for long in condensed matter physics. These types of Superconductors have Fermi surfaces that support D-wave and other types of

waves. They are mostly multi element structures where different conduction bands interact to form hybrid energy bands with energy levels that lead to varying band gaps. Of interest in two bands model are the calculations that relate bands. Especially in metal oxides that have energy bands on the Fermi surface overlapping. Cuprite's and iron based are these type of conductors although conduction mechanisms are not understood.

The structure of a compound determines the nature of interactions between its atoms [1]. These atomic interactions

are responsible for the following, electronic energy level splits, close energy spacing levels of compounds especially in solids, continuous energy widths and discrete electronic energy bands. Interactions are also normally affected by electronic energy levels as is the case in two band systems [2]. Body centered  $H_3S$  with rich hydrogen and mediated by phonons form strong light superconductors. A two band model can describe the properties of systems with two groups of electrons e.g. layered compounds. This model can explain many superconducting characteristic anomalies as observed in experiment and also explain how energy states are affected by the inter-band coupling of the condensate making cooper pair receive fluctuating interactions within the valence band widths. This is made more prominent in non-stoichiometric compounds. The influences of interactions in the family of multi component superconductors require a theory that explains the processes that come up due to inter-component couplings. This is because interactions make band gap sizes to vary [1], and lead to changes in the structure especially in non-stoichiometric compounds formed like YBCO [3]. These type two superconductors are multi gap and follow the Bardeen cooper Schrieffer theory but have overlapping energy bands [4]. This is what the superconductivity of a two band model is based on. Reference [5] indicates that the inter-band ladder diagram processes enhance the effect a pair transfer interaction contributes on the effective on-site coulomb energy. However this contribution does not address the differences in the characteristics as observed in experiment. There occurs a transition temperature decrease with increase of oxygen disorder that can be explained using two band model as well as when copper atoms are replaced by non-magnetic dopant like aluminum and zinc.

In the study of the physics of cuprite's [6] and pnictides much attention has been given to two band system interactions. In these cases inter-band coupling is considered the cause of an increase in critical temperature of the condensate and its influence on the transfer of cooper pairs from the stronger to weaker bands [7]. Apart from transfer there occurs scattering where a pair electron with opposite spins is scattered between two bands cross the Fermi level and their Fermi surfaces end up having nesting effects on each other [7]. In these, reference [8] considers two bands on different atoms both at same level of superconductivity and same Fermi surface. As a result a pair of electrons when scattered in between the two orbits result into shielding of the onsite coulombic effects of the atoms on each other. This in the end enhances superconductivity and raises transition temperature. In this same model the bands exchange coulomb interaction across orbits and therefore a Hamiltonian that takes into account all these interactions has been derived [7] and diagonalised. The derivations however do not consider changes in the structure, and also assumes S wave conductivity. The variations in the order parameters are assumed not to occur as estimated in the mean field theory. The location of the Fermi level also determines thermodynamic properties therefore doping or introduction of oxygen changes these properties especially  $T_c$ . This

temperature depends on carrier density that can change the energy band and make it overlap for electronic topological transitions. D waves can overlap with other waves on the same Fermi surface.

There also occur increases in energy bands on Fermi surface that lead to electron state density increase and to additional inter-band electron-electron interaction which contribute to superconductivity.

It is from these that a hybrid system that would account for intra and inter-band interactions was developed to account for the order parameter level interactions, later the greens function was used in determining thermodynamic properties. This has not only enhanced the understanding of two band systems of superconductivity at high transition temperature but has explained the variation of resistance in high transition temperature superconductors.

## 2. Interaction and Coupling between Bands

There are several two band superconductivity factors with hidden aspects that need probing to understand the thermal and quantum criticality that is involved in the transition from an ordered phase induced by a breakdown of basic symmetry and the disordered phase appearing due to phase transition from super to normal conductivity or metals to insulators. This thermal and quantum effects are as a result affected by sheets of Fermi surfaces as is the case in multi-band superconducting materials [9]. The superconductor properties are also controlled by a set of different band condensate states and temperatures that are also dependent on inter-band coupling [10]. In band considerations order parameters which are considered to be a measure of the condensate involve a sum of band pairing amplitudes. Order parameters have amplitudes that depend on the band type and to coupling between them. These make order parameters to fluctuate in relation to the band levels. Coupling affects the way bands interact or influence each other, such that for Singlet pairing supporting S wave there is a unique transition temperature. These temperature changes in relation to coupling as shown multiband compounds. The result leads to conductor formation of independent condensates with different transition temperatures. Changes in a compound's symmetry in multi-element cases have allowed the use of Ginzburg Landau green's function that has spatial gauge invariant derivatives in analysis. This gauge invariant greens function with spatial derivatives has not however been used in considering terms of superconductivity [11]. This if considered can explain the variations in resistivity and reveal other hidden quantum properties of superconductors.

Coupling between different band order parameters can also be achieved by varying the distance between participating layers where (ARPES) reveals multiple bands with extremely small Fermi energies [12]. This affects the acceptance of the influence of external fields and determination of the gap between Fermi level and the next electronic energy level and

by extension internal magnetic field. In this case a conductor can only receive an external magnetic field if there is a vacant energy state. Superconductivity can only quench if kinetic energy of electrons changes but also if the energy gap is occupied by a magnetic field. This is because the energy gap is as a result of loss of dissipative electrons and the development of a coherent electron lattice order parameter.

### 2.1. Dissipative Current

When an external field penetrates or is created internally within a superconductor it introduces energy that is absorbed by fermions and in turn it gives dissipative electron scattering waves. This research considered the effect of electronic energy changes within bands as they interact or shift along a structure on characteristics of D-wave superconductivity. In this case changes in energy gap sizes that are determined by interactions between energy bands, affects dissipative electron scattering wave density (electron causing resistivity). These dissipative currents had not been considered in previous studies though they have had an impact on Meissner effect.

There are variations in the dissipative wave current densities along a non-uniform lattice superconducting structure that need consideration in two band theories. These waves on the Fermi surface affect transition resistance of the superconductor among other properties. This is because of the fact that at temperatures below  $T_c$  heat cannot have dissipative electrons current flow. The causes of variation in resistance along the structure of a compound that super conducts at these levels are field variations and chemical potential changes vary energy gaps. These variations depend on bands to variations of the compounds structure and the number of waves supported on the Fermi surface, therefore the interaction of a band with others varies along the superconductor [11].

In many research papers on two band models of superconductivity especially metal oxides and ceramic Bands of energy on Fermi – surfaces overlap. This in the end results into systems of heavy fermions in which descriptions of properties exhibit two groups of electrons in different layers of compounds. There are however anomalies as observed in experiment, where a two band model with moderate coupling constants lead to high  $T_c$  with two energy gaps.

The conventional superconductor theory was proposed by Bardeen, Cooper and Shrieffer, (BCS) in which the two band situation was not considered though there has been generalized to systems with overlapping bands by [13] that yielded the two band model. The two band model allows for the formation of intra-band and inter-band interactions that couple both bands. In the Surl model, two different energy gaps are used but a single temperature is displayed. In it also superconductivity arises by inter-band interaction terms that couple the bands and lead to singlet pairs between the two bands. In these cases some thermodynamic and magnetic properties are seen as a result of overlapping bands. However several intra and inter-band interaction terms have left out factors such as energy from magnetic fields that are created

or destroyed within conducting compounds, instead consideration is mainly on hybridization coupling and electron hopping terms. These inter-bands pairing in two band models have also been emphasized by researchers in high  $T_c$  superconductors. Where energy bands on the Fermi surfaces overlap and multi gap features are observed. It is these two band character of high  $T_c$  superconductivity is highlighted. The interaction processes done so far are associated with hybridization of oxygen (2p) bands and copper (3d) bands but have no satisfactory physical implication other than a hopping term that transfers single electron (hole) between the bands. A lot therefore need to be done to explain the causes of electron transfers and energy changes. In this model it is only hybridization; the electron mixing or hopping between bands present their influence on normal changes that come along such as the coulomb interactions that are created and anomalous functions that describe the influence are done. Most of these two bands approach however do not consider other bosons of electronic origin (exciton, Plasmon's, etc) that participate in superconductivity however the treatment of the same is similar. Superconductivity is seen as being only an electron phonon interaction mechanism but it has other hidden interactions that come into play that need to be included. This approach therefore needs an exhaustive treatment to bring out some quantum effects.

### 2.2. Carrier Density Effects on Superconductivity

Carrier density is the numbers of electrons/holes that appears in two bands on a Fermi surface. In high transition temperature superconductors, conduction mode is affected by the level of doping or oxygen levels which affects the location or extend of the Fermi surface. This in effect determines the number of energy bands which can be on one Fermi level. This by extension determines thermodynamic and magnetic properties of the superconductor. These aspects are important in a non-phonon superconducting mechanism and more so in cases where transition temperature depends on carrier density and energy band overlap. In the end electronic topological transitions occur that lead to an increase in energy bands on the Fermi surfaces. This increase on bands normally affects the electron –electron state density and to additional inter-band interactions that lead to an onset of superconductivity. This approach goes against the universal BCS theory and lead to dependence on a number of physical characteristics on properties of anisotropic systems; in the approach taken in this research it is shown that the heat capacity depends on intra-band and inter-band interactions that are repulsive and attractive in nature. This is seen in the case of three band models with non-phonon superconductivity  $\text{YbBa}_2$  and  $\text{Cu}_3\text{O}_{7-5}$ , where  $T_c$  depends on carrier density. There is an increase in energy bands on Fermi- surfaces, and electron state density which also change as the lattice elements bond differently on the structure. Lattice bonding differences become similar to defects as superconductivity occurs. Transition temperature  $T_c$  does not depend on the sign of inter-band interaction constant but

instead it works for both cases where repulsion occurs in carriers, as well as electron-phonon mechanisms. All these point to the fact that interactions have an effect on properties of high transition temperature superconductivity, these changes however have not been exhaustively considered and especially for carrier density changes on the Fermi surface with different bands.

There are cases where in superconductivity chemical potential is greater at  $T_c$  for low carrier density. It therefore requires a theory to be developed that will account for superconductivity without constraints on the Fermi – energy for both electron and phonon mechanisms. Chemical potential in some cases depends on the order parameter in the superconducting phase. There can arise low carrier density with electrons pairing across different bands leading to high amplitudes of the order parameter. This enables electron transition of a Cooper pair from one band to another and in the cases where Cooper pairs do not undergo transition, energy changes occur that either increase or reduce Cooper pair sizes.

These order parameter interactions introduce or remove dissipative electrons through creation of fields or allowing changes in chemical potentials. All these developments show that there are aspects in two band theories that need to be developed further in superconductivity without introducing constraints on Fermi – energy levels.

In systems with low carrier density the chemical potential depends on the order parameters sharing a Fermi surface. This in turn determines transition temperature especially in cases that lead to formation of a band at the point  $T=T_c$ . This effect is enhanced by the presence of four order parameters where ( $\Delta_{nm}$ ,  $m=1, 2$ ). On the surface a Hamiltonian is developed for all intra-band and inter-band interactions having an anomalous effect. In this consideration, system properties near  $T_c$  show dependence of  $T_c$  on carrier density for different ratios of  $N_2/N_1$  of electron state densities of the two bands. These Hamiltonian then accounts for all electrons pairing within each band and pairing from different bands. Where in the event that consideration is only done for intra-band pairing and transition of Cooper pair as a whole from one band to another is assumed. Otherwise additional possible onsets of superconductivity on single particles take place, hybridization and all inter-band interaction constants and description of low density of states occurs with a Chemical potential approximately equal to  $T_c$ .

In interactions where creation and annihilation operators are used within a band to calculate energy for a number of electrons that have spin and wave vector  $k$ , an account of all possible electron pairing within and on different bands is done. However Fermi surfaces do not vary and therefore compound structures do not change. The assumption therefore is that the compound is stoichiometric and has no nesting effect on Fermi energy levels.

There are other two band models that take into consideration Hall Effect sign change in a scenario where both hole and electron type carriers exist. There is a model, where two bands exist for YBaCuO and for LaSrCuO, and

when using 33eV photons and clarification is done for existence of two kinds of carriers on Fermi surface using angle resolved photoemission spectra (ARPES). In it is seen evidence of coexistence of electrons and holes with 21 eV photons; it showed coexistence of electron hole like character on Fermi-surface. In this high  $T_c$  superconductivity theories, Kondo type interaction between holes of oxygen (2p) orbital and the localized spins with Cu on (3d) orbital can drive superconductivity only if phonons enhance the strength of this interaction. In this model Kondo lattice models explain heavy fermions' materials superconductivity. It also explains resistivity and magnetic susceptibility in cuprates. The Hall resistivity sign reversal at  $T_c$  is however unexplained using carriers of a single band type. In these two bands sign reversal is used to explain the non-linear resistivity, and the Kondo type interactions are used that do not have pseudo spin gaps.

Superconductivity of heavy fermions carrier density affects, transition temperature resistivity and magnetic susceptibility. An s-d exchange flip interaction occurs where the Hamiltonian has parts with two bands which are carriers with exchange interaction, where the Hamiltonian is formulated that has the creation and annihilation operators for conducting holes /electron. The other part is the interaction between a conducting hole /electron and a localized electron/hole and coulomb interactions between holes/electrons with localized spins.

### 2.3. Hybridized Two Band Superconductors

Yttrium barium copper oxide with the formulae  $YbBa_2Cu_3O_7$  was first used to achieve high temperature superconductivity. It was the first superconductor at  $T_c$  above 77K and became significant for refrigerant use. Superconductivity of  $YbBa_2Cu_3O_{(7-x)}$  is sensitive to the  $x$  value or oxygen content where when  $0 < x < 5$  it super conducts below  $T_c$  and for  $x < 0$  a material super conducts at highest temperatures like 95k. This superconductivity therefore is sensitive to the amount of oxygen. Properties of YBaCuO also depend on its crystallization methods. Its performance as a superconductor depends on crystal grain boundaries determined by annealing and quenching temperature rates. YBaCuO crystallizes in a defect perovskite structure that consists of layers, with each layer having planes of square planer  $CuO_4$  units sharing four vertices. In this model Ba atoms are between  $CuO_4$  ribbons and  $CuO_2$  planes and a reduction in oxygen means formation of non-stoichiometric compound, with  $x=1$  the Cu [1] layer becomes vacant and the structure is tetragonal and therefore becomes insulating which means it does not super conduct. Increasing oxygen atoms changes the structure to an orthorhombic one, with lattice parameters of  $a=3.89\text{\AA}$  and  $c=11.68\text{\AA}$  and optimum superconductivity occurs in these  $O_2$  sites that are maximally occupied.

Evidence shows that conduction occurring in CuO chains act as charge reservoirs that provide carriers to CuO planes. In this type of planes anisotropy is seen in penetration depth and coherence length though coherence length in the a-b

plane is 5 times compared to those along *c* meaning that superconductivity is susceptible to local disruptions, from interfaces or defects on the order of a single unit cell, it is sensitive to degradation from humidity. Grain boundaries can limit critical currents and it is also true that oxide materials are always brittle. If they should be used practically then tapes have to be added to make them flexible. This multi-element compounds introduce inter-band interactions across different waves. There are cases where inter-band coupling components raises critical temperatures of the condensate as shown in derivations in research done by [5]. There are cases where penetration of cooper pairs from a stronger band or a band in superconducting state into a weaker band occurs and induces additional superconductivity with a stronger band actively superconducting in relation to a weaker one. Similarly in the case of multi layered and heavy fermions system there are distinct superconductivity gaps, the weaker band therefore evolves with increased inter-band couplings that are analogous to a phase transition anomaly under applied external field, the field appears around the singularities at phase transition points and these explains why there is a shift in positions that are important for a 1.5 type superconductor [14].

The behavior of gap healing length in this two band system reveals a weak closeness to a superconducting phase transition point. Transition occurs from strong to a weaker band which is taken as the independent system. In analysis, consideration should be on spatial scales of coherency and gap recovery times. The weaker inter-band interactions partially explain the effects on quantities related to a weaker band as an external field associated with order parameters.

In a hybridized two band superconductor Maskalenko and Surl [7] introduced the two band model that accounts for multiple bands in the vicinity of the Fermi- energy and contributes electron pairing in a superconductor, these two band model has also been applied in copper oxide Mg B<sub>2</sub> superconductors. There are also thermodynamic properties of two bands that have also been studied by [7], and intra-band impurity scattering effects on two band superconductors in Mg B<sub>2</sub> was done using Heisenberg theory. In all these, and other studies investigation was on two band superconductor with strong intra-band and weak inter-band electronic scattering rates in the frame work of coupled Usadel equation. In cuprite super conductors it shows magnetic order in the vicinity of the super conducting phase. And Anti-ferromagnetic and ferromagnetic phases occur in heavy fermions' superconductors, and in S wave superconductivity at intermediate temperatures is seen. All these researches point to the fact that internal structure enhances or reduces interactions among superconducting electrons. There is need to explain these effects.

#### 2.4. Charge and Spin Density Waves

There are cases where nesting property of Fermi-surface in low dimensional systems that use the spin wave and the charge density wave states are used in the interplay of superconductivity and magnetrons. Rout in [6], applied the

periodic Anderson model (PAM) for calculating the non-magnetic ground state of heavy fermion systems, in which there are conduction electron bands and other bands referred to as *f*- electron bands where hybridization of conduction and *f* electron bands is done. This leads to a BCS like pairing between the two bands and intra-atomic coulomb interactions of *f*- electrons considered. The Hamiltonian developed in these case was realized by the Hartree Fock approximation with the *f*-electrons band energy composed of bare electron energy and coulomb energy off – electron. The Hamiltonian has two parts, conduction electron and *f*- electron bands that include BCS like pairing bands and a hybridization term. In another study Panda and Rout studied the interplay of charge density wave, Spin density waves and superconductivity in high T<sub>c</sub> superconductor in a low doping phase. The model Hamiltonian for CDW and superconductivity was introduced and a modification done in [6] to obtain a two band superconductor with hybridization. The physical properties of the two band hybridized superconductor that has T<sub>c</sub> zero temperature order parameter gap to T<sub>c</sub> ratio, and isotope effect coefficient were investigated. In these model the conduction electron and *f* electron band BCS like pairing band and hybridization term yielded a Hamiltonian with two band energy terms for quasi particles and interaction terms that include hybridization. But the hybridization done does not account for temperature and resistance variations within the superconductor.

Apart from the above models developed a two band model with two tight binding bands on two different types of orbital and on identical atomic sites has been developed by [6] in which there arises a coulomb exchange like integral.

In this case there exists an inter-band pair transfer interaction where a BCS like pair of two electrons with spin up and down in one band are scattered between the two bands. This interaction is strong if the two bands cross the Fermi level and the Fermi energy has a nesting property. These two electrons also reduce onsite coulomb potential interaction between cooper pairs in the two bands and promote superconductivity which leads to a higher T<sub>c</sub>. A high transition temperature then weakens the isotopic effects this effect however stops once the two bands are both strongly superconducting.

There are other studies done on two band models done by [5] and their research involves two gap interactions where the electron energy in the band relative to (chemical potential) is considered in a given volume of a superconductor and introduces an interaction matrix element of intra-band attraction whereby. When  $\Delta > 0$  or interaction is inter-band meaning that the chemical potential is across overlapping bands.

In these study electron- electron interaction is non zero in the layer where and interaction constants are not dependent on wave vector, it is assumed.

#### 2.5. Band Structures

In electron structure of un-doped compounds La<sub>2</sub>CuO<sub>4</sub> and Nd<sub>2</sub>CuO<sub>4</sub> there are dielectric gaps that are accounted for by

standard band computations that yield a metallic state. However, electron correlations bring about difficulties of the band theory therefore an understanding of these is essential. The dielectric gaps differ by nature for example a large Mott-Hubbard gap that has an occupied band of p-type oxygen states valence band and the empty upper Hubbard band conduction band has an effect on formulations of band theories.

There are two schemes that include strong correlation and lead to a dielectric gap (and to a magnetic moment of  $\approx 0.5$  micrometre per Cu ion) the gap is exchange origin between two fold occupied states.

There are other two band Hamiltonians like the one below

$$H = H_d + H_p + H_{pd} + H_{pp}$$

In which the interaction components have matrix elements of intra-atomic coulomb repulsion by one and different orbitals of oxygen (copper) and also have the Hund exchange integrals, the electrons also hop and there are matrix elements of the p-d and p-p hops to the nearest neighbors of coulomb and exchange interactions of the nearest copper-oxygen neighbors

$U_p$  and  $U_d$ - coulomb interactions on orbital's imply there is p to p hops and inter-atomic p-d, and p-p hops;

At the bottom of the conduction band and valence band are formed at a depth of 6-7 eV by orbital's of oxygen and d orbital's of copper. The other occupied states are lower and the empty ones are higher. Hybridized p-d states of  $\text{CuO}_2$  plane with strong correlation effects are immaterial for the empty and filled bands. As seen in this case the hops occur across bands but there are no interactions across the orbits.

The Hamiltonian of p-d electrons of  $\text{CuO}_2$  has single energies of p and d holes  $U_p$  ( $u_d$ ) and  $V_p$  ( $v_d$ ) matrix elements of intra-atomic coulomb repulsion by one and different orbital's of oxygen (copper), Hund exchange integrals and matrix elements of the p-d and p-p hops between nearest neighbors and  $V$  and  $J$  matrix elements of coulomb and exchange interactions of nearest copper and oxygen neighbors [15].

There are intra-atomic energies with allowance for the Hubbard correlations of coulomb interactions on various orbital's. There is also the interaction and p-p hops within  $d_{x^2-y^2}$  and  $d_{z^2}$  that are essential orbitals for oxygen.

Account is to be taken for correlations in the atomic limits of Hubbard type models, and inter-atomic hops in the band limit.

The lattice here has no overlapping cells and Hubbard operators are constructed on cluster with inter-clusters matrix elements. In a standard Hubbard model the cell has four states in which inter-cluster hops are taken into account by a perturbation theory. Sub lattices depend on occupation numbers, using photoelectron spectroscopy data used and magnetic moment for copper ion. The resultant parameters were no single valued, energy origin is localized resonance level near the top of valence band. Upper conduction band has one state per  $\text{CuO}_2$  layer, double spin degeneracy notwithstanding. For hole representation conduction band has

one hole per  $\text{CuO}_2$  layer. The Fermi layer is inside the gap and ground state is dielectric.

Greater bands are mixed p-d states with different p and d fractions at the top of valence bands are mainly p-orbital's with admixture of  $d_{x^2-y^2}$  of approximately 10% and  $d_{z^2}$  approximately 1% copper states largest dispersion is possessed by p band oxygen hops.

In  $\text{La}_2\text{CuO}_4$ , conduction band is fully occupied by one hole per  $\text{CuO}_4$  layer so that Fermi layer lies inside the gap and on the ground state is a dielectric. The other bands are mixed p-d states, but with different p and d state. Fractions in valence bands have mainly p orbitals and  $\approx 10\%$  of  $d_{x^2-y^2}$  approximately 1%  $d_{z^2}$  States of copper. Dispersion is mainly possessed by p-band made up of oxygen-oxygen hops with 1.2 eV energy [15].

The greatest change occur in charge transfer, the crystal field charges change due to absence of apical oxygen hence  $E_p$  and  $E_d$  shift and only O is renormalized.

The dielectric gap changes and p band due to oxygen to oxygen jumps becoming narrower. A narrow gap appeared in the p-d valence and led to a dip in the density of state in an energy region 1eV lower than the top of the valence band [15].

The conduction bands lower and the top part of the valence band changes by states of  $d_{x^2-y^2}$  of Cu and p states of oxygen. There is 0.6 eV change from  $\text{La}_2\text{CuO}_4$  to  $\text{Nd}_2\text{CuO}_4$  and is of the same order as the contribution of the apical oxygen.

## 2.6. Energy Band Gaps and Fermi Levels

Fermi surfaces enable visualize fullness or occupation of allowed empty lattice bands in k space geometrically, hence theoretically determines electronic properties of a solid. These help know details of electron motion within the lattice. The Fermi level is reached when electrons fill up an empty lattice

All phenomena of interactions affects only electrons that are thermally excited or lie within the range of in width about the Fermi level, the lower electrons are blocked by exclusion.

Fermi surfaces are used for properties like heat capacity but have not been analyzed for symmetry of wave functions on it. Symmetry in a compound specifies distribution of conduction electrons internally and how a foreign ion will scatter conduction electrons especially those far from the nucleus but not S type [3].

Based on the review above there is need to consider several factors in two band models so that the resultant hybrid system has all intra and inter-band interactions especially in compounds that support D- waves. There are several gaps in two band superconductor theories as looked at in the literature review, hybridization like what was done by Rout and Das they left out terms in the Hamiltonian that could explain the inadequacies in the physical properties (transition temperature, order parameter and resistance) [6]. There are no considerations of the nesting properties that come from interactions at Fermi levels as bands overlap on Fermi surfaces. The interactions effect on the order parameter and Hamiltonian are not considered either in this two band

models.

There are also omissions of inter-band impurity scattering effects that have their input on critical transition temperature and critical field.

In Okoye's formulations and computation he did not consider variations in the scattering rates for non-uniform conductors, and in the case of strong to weaker band hopping by charge carriers he does not consider both hole and electron cases. He also assumes that the superconductor has a uniform lattice structure and conduction is by S waves.

The nesting effects of Fermi surfaces in low dimensional systems that lead to spin wave and charge wave densities should be included in a hybrid system, which has D-waves within the effects of other waves. It is also possible that the interactions that affect D wave superconductors can explain experimental anomalies since Fermi surfaces overlap and these introduces intra and inter-band interactions. Fermi surface overlaps affect carrier densities along a superconductor. This definitely affects variation in resistivity and transition temperature and leads to a split in independent condensates. In the case where a weaker band plays an external field to a strong band there are phase transition anomalies in its evolution and as doping level varies compounds, its properties are affected.

### 3. Methodology

An outline of the steps to be followed in order to achieve the expected results was done. The method involved derivation of a hybridized Hamiltonian from first principles and the use of greens function to obtain thermodynamic properties.

#### 3.1. Hybridized Hamiltonian.

The study of two band superconductivity has been done using the greens function [8]. Hubbard Stratonovich approach among other techniques, in all of them a Hamiltonian was developed from what Maskalengo [7] introduced in two band models that takes into account multiple energy bands in the vicinity of the Fermi energy that contribute electron pairing in the copper oxides superconductor.

These Hamiltonians take into account interaction terms that come as a result of electronic band formation that allow both inter-band and intra band couplings. The Hamiltonian development was done using the second quantization formalism from field quantization theories [16]. The derivations of the Hamiltonian of the system, contribution from the kinetic energy of the particles in the two bands and in addition the intra and inter-band interactions were considered [5]. However the inter-band interactions include terms that were not considered previously that contribute to the variations in temperature and resistance, and also brings out some hidden critical quantum effects on temperature. A Hamiltonian similar in form to the one below was developed in order to address some of the aspects of interactions left out. What were considered in analysis were interactions that involved D-wave with other waves on the same Fermi

surface. The Hamiltonian is similar in form to the following components.

$$H=H_0+H_1+H_{01}+H_{00}+H_{11} \quad (1)$$

Where,  $H_0$  and  $H_1$  are kinetic energy terms for the two interacting conduction bands within the Fermi surface.

$H_{01}$ , is the inter-band interaction between the bands that support D-wave and another band in its vicinity.

$H_{00}$  and  $H_{11}$  are the columbic potential energy that comes as a result of intra band interaction terms which introduce changes that affect or enhance superconductivity.

#### 3.2. Specific Heat Capacity

To obtain specific heat capacity differentiation of the thermodynamic potential is done.

$$\frac{c_s}{v} = \frac{\partial}{\partial \Delta} \left( \frac{\Omega_s}{v} \right) \quad (2)$$

The energy density will then be obtained by

$$\frac{E}{v} = \frac{v}{2} \langle H \rangle f(\omega) A(k, \omega) \quad (3)$$

Where

$$\langle H \rangle = \frac{v}{2} \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left\{ \frac{k^2}{2m} + \omega \right\} G^<(k, \omega) \quad (4)$$

And  $G^<(k, \omega)$  is the correlation function,  $A(k, \omega)$  is the spectral function

Where  $G^<(k, \omega) = f(\omega) A(k, \omega)$

The specific heat capacity will be obtained by use of the relation.

$$\frac{\partial E}{\partial T} = C_s \quad (5)$$

And entropy

$$S = \int \frac{C_s}{T} dT \quad (6)$$

#### 3.3. Thermodynamic properties

Graphs of energy versus temperature and specific heat capacity have been drawn and compared with the experimental and other formulations in theoretical work. This has been achieved by using derived equations and values of the constants available, data was then generated, tabulated and graphs drawn for physical interpretation of the properties of the system, MathCAD software was the tool that was used to generate and analyze the data.

Derivations

### 4. Electron Phonon Interaction

A crystal is a complicated much body system of electrons and ions whose properties are determined by coulomb interactions. The Hamiltonian of such a system is composed of two parts, the electronic lattice energy and interaction terms.

The interaction part involves interaction of electrons and

quanta of the lattice vibrations or the phonons. The total Hamiltonian can be written as

$$H=K.E_L+K.E_e+\Omega_l+\Omega_e+\Omega_{cl} \quad (7)$$

The first two terms are K.E of ions and second two terms are contributions from interactions among electrons and ions. The case of superconductivity requires that all these parts combine and interactions mediated by phonons. However phonon energy is smaller than electron energy which is near the Fermi energy.  $\hbar \omega_D \ll \epsilon_f$

The Hamiltonian depends on the ion positions and independent of their motion and the coulomb interactions.

In previous studies a hybridized Hamiltonian was developed and modified to suit two bands with hybridization. This was given as

$$H = \sum_{k,\sigma} \epsilon_K C_{K\sigma}^+ C_{K\sigma} + \sum_{k\sigma} \epsilon_0 f_{k\sigma}^+ f_{k\sigma} + \gamma_0 \sum_{k,\sigma} (f_{k\sigma}^+ C_{K\sigma} + C_{K\sigma}^+ f_{k\sigma}) + U \sum_{i,\sigma} f_{i\sigma}^+ f_{i\sigma} - \Delta \sum_k (C_{k\uparrow}^+ C_{-k\downarrow}^+ + C_{-k\downarrow} C_{k\uparrow}) \quad (8)$$

Where  $C_{K\sigma}^+ (C_{K\sigma})$  and  $f_{k\sigma}^+ (f_{k\sigma})$  are creation and annihilation operators for the two bands and  $\Delta$  is superconducting order parameter. The electron pairing and coulomb interactions involves only electrons in one band only that one is considered to be strongly superconducting and the other weakly,  $\gamma_0$  is the hybridization interaction coefficient between electron band and conduction bands.

$n_i^f = f_{i\sigma}^+ f_{i\sigma}$  is the intra-atomic coulomb interaction between f electrons and is given by  $n_{i\sigma}^f n_{i-\sigma}^f = f_{i\sigma}^+ f_{i\sigma} f_{i-\sigma}^+ f_{i-\sigma} = 2 f_{i\sigma}^+ f_{i\sigma}$  therefore  $f_{i\sigma}^+ f_{i\sigma} = \frac{U}{2} \sum_{i,\sigma} n_{i\sigma}^f n_{i-\sigma}^f$  which when linearized by Hartree Fock approximation becomes  $\approx U \sum_{i,\sigma} n_{i\sigma}^f n_{i-\sigma}^f$  And the Hamiltonian becomes

$$H = \sum_{k,\sigma} \epsilon_K C_{K\sigma}^+ C_{K\sigma} + \sum_{k\sigma} \epsilon_0 f_{k\sigma}^+ f_{k\sigma} + \gamma_0 \sum_{k,\sigma} (f_{k\sigma}^+ C_{K\sigma} + C_{K\sigma}^+ f_{k\sigma}) + U \sum_{i,\sigma} n_{i\sigma}^f n_{i-\sigma}^f - \Delta \sum_k (C_{k\uparrow}^+ C_{-k\downarrow}^+ + C_{-k\downarrow} C_{k\uparrow}) \quad (9)$$

With  $\epsilon_0 = \epsilon_f + U_{n-\sigma}$  being the energy collected that is non-interactive with a modified f electron band level.

The order parameter in consideration is given by

$$\Delta = \frac{V}{2} \sum_k (\langle C_{k\uparrow}^+ C_{-k\downarrow}^+ \rangle + \langle f_{k\uparrow}^+ f_{-k\downarrow}^+ \rangle) \quad (10)$$

In these Hamiltonian the two bands are such that the f electron band is not fully superconducting, it has both intra-band interactions and inter band which acts as an external field to the conduction band. It is from this understanding that a modified two band Hamiltonian is developed in this research such that consideration is done for both bands to be in superconducting state and the order parameter in this case non-homogeneous. This is because order parameters pairing occur across two orbitals on the same Fermi surface thus allowing the D wave to interact across with other waves. The order parameter in these cases can at some instant involve two particle operators that are different in amplitude or may change form and amplitude as it tunnels across the compound whose structure is non uniform and varies due to bonding. These changes also affect the chemical potentials involved.

When these considerations are taken into account, with

hybridization and gauge invariance. The Hamiltonian for the hybrid system has to allow these considerations and therefore ends up having the following terms.

$$H=H_0+H_1+H_{00}+H_{11}+H_{01} \quad (11)$$

These terms include both intra and inter-band interaction components. The Hamiltonian finally takes the modified form.

$$H = \sum_{k,\sigma} \epsilon_K C_{K\sigma}^+ C_{K\sigma} + \sum_{k\sigma} \epsilon_0 f_{k\sigma}^+ f_{k\sigma} + \gamma_0 \sum_{k,\sigma} (f_{k\sigma}^+ C_{K\sigma} + C_{K\sigma}^+ f_{k\sigma}) + U \sum_{i,\sigma} f_{i\sigma}^+ f_{i\sigma} + U \sum_{i,\sigma} C_{i\sigma}^+ C_{i\sigma} - \Delta \sum_k (C_{k\uparrow}^+ C_{-k\downarrow}^+ + C_{-k\downarrow} C_{k\uparrow}) - \Delta \sum_k (f_{k\uparrow}^+ f_{-k\downarrow}^+ + f_{-k\downarrow} f_{k\uparrow}) - \Delta_c \sum_k (C_{k\sigma}^+ C_{k\sigma} + f_{k\sigma}^+ f_{k\sigma}) \quad (12)$$

Where

$C_{k\sigma}^+, C_{k\sigma}$  and  $f_{k\sigma}^+, (f_{k\sigma})$  Are creation and annihilation operators in two different bands,  $\epsilon_K$  and  $\epsilon_0$  are band energies for the two bands measured from the Fermi energy

$\gamma_0$  Represents hybridization interaction coefficient between bands.

$U \sum_{i,\sigma} f_{i\sigma}^+ f_{i\sigma}$  and  $U \sum_{i,\sigma} C_{i\sigma}^+ C_{i\sigma}$  are the intra-atomic coulomb interaction terms for the two bands approximated using Hartree Fock approximation.  $\gamma_0 \sum_{k,\sigma} (f_{k\sigma}^+ C_{K\sigma} + C_{K\sigma}^+ f_{k\sigma})$  is the interaction coupling terms

$\Delta$  is the effective superconducting order parameter where pairing is within a bands thus conduction electron and other electron bands separately. It is assumed to be non-homogeneous in space, gauge invariant and estimated using the mean field theory approximations.

$\Delta_c$  represents an order parameter where pairing is across bands, it changes as the electrons flow the waves change depending on the structure of the compound.

Therefore there are interactions across bands that come up because they are within range on a Fermi surface and therefore the order parameters varies in size in terms of chemical potential, these changes lead to energy variations at different points. However, these energy fluctuations may be in form of energy fields that excite and scatter electrons and in turn create different energy gaps which absorb or release energy to improve superconductivity or effecting resistivity. The existence of two bands or more on a Fermi surface therefore allows the transfer of electrons and energy across by absorption or release of energy in form of fields. The occurrence of these and the fact that the temperature involved does not allow other forms of energy is a phenomenon that either contributes to increased superconductivity or resistivity of a superconductor. The hybrid Hamiltonian based on these argument then takes the form given by

$$H = \sum_{k\sigma} \epsilon_K C_{K\sigma}^+ C_{K\sigma} + \sum_{k\sigma} \epsilon_0 f_{k\sigma}^+ f_{k\sigma} + \gamma_0 \sum_{k,\sigma} (f_{k\sigma}^+ C_{K\sigma} + C_{K\sigma}^+ f_{k\sigma}) + U \sum_{i,\sigma} f_{i\sigma}^+ f_{i\sigma} + U \sum_{i,\sigma} C_{i\sigma}^+ C_{i\sigma} - \Delta \sum_k (C_{k\uparrow}^+ C_{-k\downarrow}^+ + C_{-k\downarrow} C_{k\uparrow}) - \Delta \sum_k (f_{k\uparrow}^+ f_{-k\downarrow}^+ + f_{-k\downarrow} f_{k\uparrow}) - \Delta_c \sum_k (C_{k\sigma}^+ C_{k\sigma} + f_{k\sigma}^+ f_{k\sigma}) \quad (13)$$

#### 4.1. Greens Function

The greens function is a propagator at finite temperature and is the statistical average of creation and annihilation operators. It can also be given as

$$iG(rt, r't') = \text{Tr}\{\hat{\rho}\tau[\hat{a}(rt)\hat{a}^+(r't')]\} \quad (14)$$

$$\text{Where } \hat{\rho} = \frac{1}{Z} \quad (15)$$

The following are Correlation functions obtained from greens function

$$\begin{aligned} iG^>(rt, r't') &= \text{Tr}\{\hat{\rho}(\hat{a}(rt)\hat{a}^+(r't'))\} \\ iG^<(rt, r't') &= -\text{Tr}\{\hat{\rho}\hat{a}^+(r't')(\hat{a}(rt))\} \end{aligned} \quad (16)$$

These functions represent propagation of a perturbation for fermions in nuclear matter. It is invariant under translations and rotations in space. Consequently it depends on relative distances in space and time and is written as.

$$G(rt, r't') = G(x = |r - r'|, \tau = t - t') \quad (17)$$

Where translational invariance exists it is treated in momentum frequency space by a Fourier transform as

$$G(k, \tau) = \int d^3x e^{-ikx} (G(x, \tau)) \quad (18)$$

And its inverse is

$$G(x, \tau) = \int \frac{d^3x}{(2\pi)^3} e^{ikx} (G(k, \tau)) \quad (19)$$

A correlation function is given written as

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) = \sum_{n,m} \frac{e^{-\beta(E_n - \mu N_n)}}{Z} (\langle n|a_k^+|m\rangle \langle n|a_k|m\rangle +$$

$$\begin{aligned} & (i\hbar\omega_n - \frac{1}{2m}(i\hbar\nabla)^2 + u_x)G(x - x', \omega_n) + i\omega_n - \frac{1}{2m}(-i\hbar\nabla)^2 + u_y)G(y - y', \omega_n) + \gamma_0 \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta(x) \\ & \{f^+(x_\tau, x'_\tau) + f^+(x_\tau, x'_\tau)\} - \Delta(y) \{f^+(y_\tau, y'_\tau) + f^+(y_\tau, y'_\tau)\} - \Delta_c \{G(x - x', \omega_n) + G(y - y', \omega_n)\} = 0 \end{aligned} \quad (24)$$

And the second equation becomes

$$\begin{aligned} & \left\{ \left( i\hbar\omega_n - \frac{1}{2m}(i\hbar\nabla)^2 + u_x - \Delta_c \right) G(x - x', \omega_n) + \left( i\hbar\omega_n - \frac{1}{2m}(i\hbar\nabla)^2 + u_y - \Delta_c \right) G(y - y', \omega_n) + \gamma_0 \int_{-\infty}^{+\infty} A(k, \omega) - \right. \\ & \left. \Delta(x) \{f^+(x_\tau, x'_\tau) + f^+(x_\tau, x'_\tau)\} - \Delta(y) \{f^+(y_\tau, y'_\tau) + f^+(y_\tau, y'_\tau)\} - \Delta_c \{G(x - x', \omega_n) + G(y - y', \omega_n)\} \right\} = 0 \end{aligned} \quad (25)$$

Separated into two bands equations of motion become

$$\left( i\hbar\omega_n - \frac{1}{2m}(i\hbar\nabla)^2 + u_x - \Delta_c \right) G(x - x', \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta(x) (f^+(x_\tau, x'_\tau) + f(x_\tau, x'_\tau)) = 0 \quad (26)$$

$$\left( i\hbar\omega_n - \frac{1}{2m}(i\hbar\nabla)^2 + u_y - \Delta_c \right) G(y - y', \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta(y) (f^+(y_\tau, y'_\tau) + f(y_\tau, y'_\tau)) = 0 \quad (27)$$

Using the transformed relations

$$G(x_\tau, x'_\tau) = (\beta\hbar)^{-1} \sum_n e^{-i\omega_n(\tau-\tau')} G(x - x', \omega_n) \quad (28)$$

And

$$\langle n|a_k|m\rangle \langle n|a_k^+|m\rangle \quad (20)$$

These functions are useful in writing the Hamiltonian that represents a propagation of a disturbance. The order parameter is written as

$$\Delta(x) = g f(x_\tau^+, x_\tau) = -g(\hat{\Psi}_\uparrow(x)\hat{\Psi}_{k\downarrow}(x)) = g(\hat{\Psi}_{\downarrow\uparrow}(x)\hat{\Psi}_{k\uparrow}(x)) \quad (21)$$

And a single particle greens function is written as

$$G(x_\tau, x'_\tau) = -\langle T_\tau [\hat{\Psi}_{k\uparrow}(x_\tau) \hat{\Psi}_{k\uparrow}^+(x'_\tau)] \rangle \quad (22)$$

And can be used to represent the order parameter. All these representations are used in writing the Hamiltonian in terms of the greens function.

Considering the Hamiltonian developed in this study and using the greens function in the equation of motion modeled will be written as follows.

$$\begin{aligned} H = & \sum_{k\sigma} \epsilon_k C_{k\sigma}^+ C_{k\sigma} + \sum_{k\sigma} E_0 f_{k\sigma}^+ f_{k\sigma} + \gamma_0 \sum_{k\sigma} (f_{k\sigma}^+ C_{k\sigma} + C_{k\sigma}^+ f_{k\sigma}) + \\ & U \sum_{i\sigma} (f_{i\sigma}^+ f_{i\sigma} + U \sum_{i\sigma} C_{i\sigma}^+ C_{i\sigma}) - \Delta \sum_k (C_{k\uparrow}^+ C_{-k\downarrow} + C_{-k\downarrow} C_{k\uparrow}) - \\ & \sum_k (f_{k\uparrow}^+ f_{-k\downarrow} + f_{-k\downarrow} f_{k\uparrow}) - \Delta_c \sum_k (C_{k\sigma}^+ C_{k\sigma} + f_{k\sigma}^+ f_{k\sigma}) \end{aligned} \quad (23)$$

The Fourier transformed greens functions 18 and correlation functions 20 are substituted in the Hamiltonian 23. These form two equations after substituting these relations and allowing operators to act on the Fourier transformed greens function and writing

$H\psi = E\psi$  as  $-E\psi + H\psi = 0$  Equation after applying operators becomes

$$f^+(x_\tau, x'_\tau) = (\beta\hbar)^{-1} \sum_n e^{-i\omega_n(\tau-\tau')} f^+(x-x', \omega_n) \quad (29)$$

Where  $\omega_n = (2n+1)\frac{\pi}{\beta\hbar}$  and

$$\Delta^*(x) = -g \langle \hat{\psi}_\uparrow^+(x) \hat{\psi}_\uparrow^+(x) \rangle = g f^+(x_\tau, x'_\tau) = \frac{g}{\beta\hbar} \sum_n e^{-i\omega_n \tau} f^+(x, \omega_n) \quad (30)$$

The Fourier transforms are

$$G(x, \omega_n) = (2\pi)^{-3} \int d^3k e^{ikx} G(k, \omega_n) \quad (31)$$

$$f^+(x, \omega_n) = (2\pi)^{-3} \int d^3k e^{ikx} f^+(k, \omega_n) \quad (32)$$

The two equations 26 and 27 formed respectively become

$$(i\hbar\omega_n + (\frac{\hbar k^2}{2m}) + u_x - \Delta_c)G(k, \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta(x)f^+(k, \omega_n) = \hbar \quad (33)$$

And

$$(i\hbar\omega_n + (\frac{\hbar k^2}{2m}) + u_y - \Delta_c)G(k, \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta(y)f^+(k, \omega_n) = 0 \quad (34)$$

The equations are obtained as shown below

$$(i\hbar\omega_n + (\frac{\hbar k^2}{2m}) + u_x - \Delta_c)G(k, \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta(x)f^+(k, \omega_n) = \hbar \quad (35)$$

$$(i\hbar\omega_n + (\frac{\hbar k^2}{2m}) + u_x - \Delta_c)f^+(k, \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta^*(x)G(k, \omega_n) = 0 \quad (36)$$

Equating ax to  $(i\hbar\omega_n + (\frac{\hbar k^2}{2m}) + u_x - \Delta_c)$

And substituting in 35 and 36 then the two equations become

$$a_x G(k, \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta(x)f^+(k, \omega_n) = \hbar \quad (37)$$

$$a_x f^+(k, \omega_n) - \gamma_0 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) - \Delta^*G(k, \omega_n) = 0 \quad (38)$$

Solving simultaneously by multiplying 37 by  $a_x$  and 38 by  $\Delta(x)$

$$a_x^2 G(k, \omega) - a_x \gamma_0 - \Delta(x)a_x f^+(k, \omega) = a_x \hbar \quad (39)$$

$$a_x \Delta(x) f^+(k, \omega) - |\Delta(x)|^2 G(k, \omega) = 0$$

Adding the two equations and solving them

$$a_x^2 G(k, \omega) - |\Delta(x)|^2 G(k, \omega) = a_x \hbar + a_x \gamma_0 - \Delta(x) \gamma_0$$

$$G(k, \omega) = \frac{a_x \hbar + a_x \gamma_0 - \Delta(x) \gamma_0}{a_x^2 - |\Delta(x)|^2}$$
(40)

$$\Delta^*(x) a_x G(k, \omega) - \Delta^*(x) \gamma_0 - |\Delta(x)|^2 f^+(k, \omega) = \hbar$$
(41)

$$a_x^2 f^+(k, \omega) - a_x \Delta^*(x) G(k, \omega) = 0$$

Adding the equations

$$a_x^2 f^+(k, \omega) - a_x \gamma_0 - \Delta^*(x) \gamma_0 - |\Delta(x)|^2 f^+(k, \omega) = \Delta^*(x) \hbar$$

$$f^+(k, \omega) = \frac{\Delta^*(x) \hbar + \Delta^*(x) \gamma_0}{a_x^2 - |\Delta(x)|^2}$$
(42)

The gap equation is given by

$$\Delta^*(x) = \frac{g}{\beta \hbar} \sum_n \int e^{-i\omega_n} f^+(x, \omega)$$
(43)

The gap equation appears when a substance or the material attains superconducting state and disappears when the material is in normal state. And on substituting  $f^+(k, \omega)$  gap equation becomes

$$\Delta^*(x) = \frac{g}{\beta \hbar} \sum_n \int \frac{d^3 k}{(2\pi)^3} \left( \frac{\Delta^*(x)(\hbar + \gamma_0)}{a_x^2 - |\Delta(x)|^2} \right)$$
(44)

$$1 = \frac{g}{\beta \hbar} \sum_n \int \frac{d^3 k}{(2\pi)^3} \frac{\hbar + \gamma_0}{a_x^2 - |\Delta(x)|^2}$$

After dividing on both sides by  $\Delta(x)$

$$1 = \frac{g}{\beta \hbar} \sum_n \int \frac{d^3 k}{(2\pi)^3} \left( \frac{\hbar}{a_x^2 - |\Delta(x)|^2} + \frac{\gamma_0}{a_x^2 - |\Delta(x)|^2} \right)$$

$$1 = \frac{g}{(2\pi)^3} \sum_n \int \frac{d^2 k}{\beta (a_x^2 - |\Delta(x)|^2)} + \frac{g}{\beta \hbar} \sum_n \int \frac{d^3 k}{(2\pi)^3} \frac{\gamma_0}{a_x^2 - |\Delta(x)|^2}$$
(45)

$$= \frac{g}{(2\pi)^3} \int \frac{d^3 k}{2a_x} \tanh\left(\frac{1}{2} \beta a_x\right) + \frac{g \gamma_0}{(2\pi)^3 \hbar} \int d^3 k (2a_x)^{-1} \tanh\left(\frac{1}{2} \beta a_x\right)$$

On introducing the approximation

$$(2\pi)^{-3} \int d^3k \dots \approx N(0) \int d\varepsilon \dots \tag{46}$$

$$1 = gN(0) \int_0^{\hbar\omega_D} \frac{d\varepsilon}{E_k} \tanh\left(\frac{\beta E_k}{2}\right) + gN(0) \frac{\gamma_0}{\hbar} \int \frac{d\varepsilon}{a_x} \tanh\left(\frac{\beta a_x}{2}\right) \tag{47}$$

Substituting (44) into gap equation (42) and using standard integrals it becomes

$$\frac{1}{N(0)g} = \int_0^z \frac{dz}{z} \tanh z = [\ln z \tanh z]_0^z - \int_0^z dz \ln z \operatorname{sech}^2 z \tag{48}$$

$$\approx [\ln z] - \int_0^\infty dz \ln z \operatorname{sech}^2 z \tag{49}$$

$$\frac{1}{N(0)g} = \ln z + \ln 4e^\gamma = \ln(z \times 4e^\gamma) \text{ With } z = \frac{\hbar\omega_D}{2k_B T_C} = \frac{\hbar\omega_D}{2} \beta \tag{50}$$

$$K_B T_C = \hbar\omega_D 2e^\gamma e^{\frac{-1}{N(0)g}} \tag{51}$$

Using  $\left(\sum_n \frac{1}{\beta((\hbar\omega_n)^2 + E_k^2)}\right) = \frac{1}{2E_k} \tanh\left(\frac{1}{2} \beta E_k\right)$

The gap equation becomes

$$\frac{1}{gN(0)} = \int \frac{d\varepsilon}{a_x} \tanh\left(\frac{1}{2} \beta a_x\right) + \frac{\gamma_0}{k} \int \frac{d\varepsilon}{a_x} \tanh\left(\frac{1}{2} \beta a_x\right) \tag{52}$$

On integration equation 52 becomes

$$= [\ln a_x \tanh a_x]_0^{a_x} - \int_0^{a_x} da_x \ln a_x \operatorname{sech}^2 a_x \tag{53}$$

By partial integration

$$a_x = \frac{\hbar\omega_D}{2k_B T_C} \approx \ln a_x - \int_0^\infty da_x \ln a_x \operatorname{sech}^2 a_x \tag{54}$$

$$da_x \ln a_x \operatorname{sech}^2 a_x = \left[ \frac{d}{dn} \int_0^\infty da_x a_x^{n-1} \operatorname{sech}^2 a_x \right]_{n=1} = -\ln 4e^4 \tag{55}$$

$$\approx \ln a_x + \frac{4e^\gamma}{\pi} + \frac{\gamma_0}{\hbar} \left( \ln a_x + \frac{4e^\gamma}{\pi} \right) \in \left( a_x \times \frac{4e^\gamma}{\pi} \right) + \frac{\gamma_0}{\hbar} \in \left( a_x \times \frac{4e^\gamma}{\pi} \right)$$

From these relations  $\frac{1}{N(0)g} = \left( a_x \times \frac{4e^\gamma}{\pi} + \frac{\gamma_0}{\hbar} \in \left( a_x \times \frac{4e^\gamma}{\pi} \right) \right) \in \left( a_x \times \frac{4e^\gamma}{\pi} \right) \left( a_x \times \frac{4e^\gamma}{\pi} \right)^{\frac{\gamma_0}{\hbar}}$  and

$$e^{\frac{1}{N(0)g}} = \frac{(\hbar\omega_D)^{1+\gamma_0} \times (2)^{1+\gamma_0} e^{1+\gamma_0}}{(K_B T_C)^{1+\gamma_0} \times \pi^{1+\gamma_0}} \tag{56}$$

$$(K_B T_C)^{1+\gamma_0} = \frac{(\hbar\omega_D)^{1+\gamma_0} \times (2)^{1+\gamma_0} (e^\gamma)^{1+\gamma_0}}{\pi^{1+\gamma_0}} e^{-\frac{1}{N(0)g}}$$

$$= \frac{(\hbar\omega_D \times 2e^\gamma)^{1+\gamma_0}}{\pi} e^{-\frac{1}{N(0)g}}$$

$$(K_B T_C)^{1+\gamma_0} \approx (1.13 \hbar\omega_D)^{1+\gamma_0} e^{-\frac{1}{N(0)g}} \tag{57}$$

Zero temperature gaps  $\Delta(t = 0) \equiv \Delta_0$  and  $\Delta = 2\hbar\omega_D e^{\frac{-1}{N(0)g}}$  then

$\frac{\Delta}{K_B T_C} = \pi e^{-\gamma} \approx 1.76$  Where  $\gamma = (\gamma_0 + 1)$  applying in equation (55)

$$\frac{\Delta}{K_B T_C \times (K_B T_C)^{\frac{\gamma_0}{\hbar}}} = \frac{2\hbar\omega_D e^{\frac{-1}{N(0)g}}}{\frac{\hbar\omega_D 2e^\gamma}{\pi} \times \left(\frac{\hbar\omega_D 2e^\gamma}{\pi}\right)^{\frac{\gamma_0}{\hbar}} \times e^{\frac{-1}{N(0)g}}} \tag{58}$$

$$= \left( \frac{\pi}{eV} \right) \times \frac{\frac{\gamma_0}{\pi \hbar}}{(\hbar \omega_D 2eV) \frac{\gamma_0}{\hbar}}$$

And therefore

$$\frac{\Delta}{K_B T_C \times (K_B T_C) \frac{\gamma_0}{\hbar}} = 1.76 \times \frac{\frac{\gamma_0}{\pi \hbar}}{(\hbar \omega_D 2eV) \frac{\gamma_0}{\hbar}} = 1.76 \left( \frac{1.76}{2\hbar \omega_D} \right) \frac{\gamma_0}{\hbar} = 1.76 \times \left( \frac{0.88}{\hbar \omega_D} \right) \frac{\gamma_0}{\hbar} \quad (59)$$

#### 4.2. Thermodynamic Functions

Thermodynamic functions are obtained from the relations below (Alexander & Walecka, 2002)

$$\begin{aligned} \Omega_s - \Omega_n &= \int_0^1 \partial \lambda \lambda^{-1} \langle \lambda H_1 \rangle \\ &= -\frac{1}{2} \int_0^g \frac{\partial g}{g} \int d^3 k g \langle H_1 \rangle \\ &= V \int_0^g dg \frac{d\left(\frac{1}{g}\right)}{dg} \Delta^2 \\ &= -V \int_0^g dg \int \left( \frac{1}{g} \right)^2 \Delta^2 \end{aligned} \quad (60)$$

Change of variables leads to  $\Delta$

$$\Omega_s - \Omega_n = V \int_0^\Delta d\Delta \left( \Delta \right)^2 \frac{d\left(\frac{1}{g}\right)}{d\Delta} \quad (61)$$

Applying

$$\begin{aligned} 1 &= \frac{g}{\beta \hbar} \sum_n \int \frac{d^3 k}{(2\pi)^3} \left( \frac{\hbar}{a_x^2 - |\Delta(x)|^2} + \frac{\gamma_0}{a_x^2 - |\Delta(x)|^2} \right) \\ 1 &= \frac{g}{(2\pi)^3} \sum_n \int \frac{d^2 k}{\beta (a_x^2 - |\Delta(x)|^2)} + \frac{g}{\beta \hbar} \sum_n \int \frac{d^3 k}{(2\pi)^3} \frac{\gamma_0}{a_x^2 - |\Delta(x)|^2} \\ &= \frac{g}{(2\pi)} \int \frac{d^3 k}{2a_x} \tanh\left(\frac{1}{2} \beta a_x\right) + \frac{g \gamma_0}{(2\pi)^3 \hbar} \int d^3 k (2a_x)^{-1} \tanh\left(\frac{1}{2} \beta a_x\right) \\ \frac{1}{g} &= \frac{1}{(2\pi)} \int \frac{d^3 k}{2a_x} \tanh\left(\frac{1}{2} \beta a_x\right) + \frac{\gamma_0}{(2\pi)^3 \hbar} \int d^3 k (2a_x)^{-1} \tanh\left(\frac{1}{2} \beta a_x\right) \\ \frac{1}{g} &= \left( 1 + \frac{\gamma_0}{\hbar} \right) \frac{1}{(2\pi)} \int \frac{d^3 k}{2a_x} \tanh\left(\frac{1}{2} \beta a_x\right) \end{aligned} \quad (62)$$

$\frac{1}{g}$  in terms of  $\Delta(T)$  and substituting into the equation

$$\frac{\Omega_s - \Omega_n}{V} = \left(1 + \frac{Y_0}{h}\right) N(0) \Delta^2 \int_0^{\hbar\omega_D} \frac{d\varepsilon}{E} \tanh\left(\frac{1}{2}\beta a_x\right) - \frac{4N(0)}{\beta} \int_0^{\hbar\omega_D} d\varepsilon \frac{\text{Incosh}\left(\frac{1}{2}\beta a_x\right)}{\cosh\left(\frac{1}{2}\beta a_x\right)} \left(1 + \frac{Y_0}{h}\right) \left\{ \frac{\Delta^2}{g} - 4 \frac{N(0)}{\beta} \int_0^{\hbar\omega_D} d\varepsilon \left[ \ln(1 + e^{-\beta a_x}) + \frac{1}{2} \beta [a_x - \varepsilon] + \frac{4N(0)}{\beta} \int_0^{\hbar\omega_D} d\varepsilon \ln(1 + e^{-\beta \varepsilon}) \right] \right\} \quad (63)$$

Then

$$\frac{\Omega_s - \Omega_n}{V} = \left(1 + \frac{Y_0}{h}\right) \left\{ -\frac{1}{2} N(0) \Delta^2 - N(0) \Delta^2 \ln \frac{\Delta_0}{\Delta} - 4N(0) K_B T_C \int_0^{\hbar\omega_D} d\varepsilon \ln(1 + e^{-\beta a_x}) + \frac{1}{3} \pi^2 N(0) \right\} \quad (64)$$

$T \ll T_C \ll \Theta \ll T_F$  is assumed

$$N_s \approx N_n \text{ For } T \leq T_C$$

$$\frac{\Omega_s}{V} = \frac{\Omega_n(T=0)}{V} \left\{ -\frac{1}{2} N(0) \left[ 1 + 2 \ln \frac{\Delta_0}{\Delta} - 4N(0) K_B T \int_0^{\hbar\omega_D} d\varepsilon \ln(1 + e^{-\beta a_x}) \right] \right\} \left(1 + \frac{Y_0}{h}\right) \Delta^2 \quad (65)$$

$$\frac{\Omega_s}{V} \approx \frac{\Omega_n(T=0)}{V} \left\{ -\frac{1}{2} N(0) \Delta_0^2 - 2N(0) \left( \frac{2\pi\Delta_0}{\beta^3} \right)^{\frac{1}{2}} e^{-\beta\Delta_0} \right\} \left(1 + \frac{Y_0}{h}\right) \quad (66)$$

$$\frac{C_s}{V} = \frac{\partial}{\partial \Delta} \left( \frac{\Omega_s}{V} \right) = \left(1 + \frac{Y_0}{h}\right) 2N(0) \Delta_0 K_B (2\pi)^{\frac{1}{2}} \left( \frac{\Delta_0}{K_B T} \right)^{\frac{1}{2}} e^{\frac{-\Delta_0}{K_B T}} \rightarrow 0 \quad (67)$$

$$\frac{C_s}{V} = \frac{3}{2} \pi^2 N(0) K_B^2 T + \left(1 + \frac{Y_0}{h}\right) 2N(0) \Delta_0 K_B (2\pi)^{\frac{1}{2}} \left( \frac{\Delta_0}{K_B T} \right)^{\frac{1}{2}} e^{\frac{-\Delta_0}{K_B T}} T \quad (68)$$

## 5. Results and Discussion

### 5.1. Specific Heat Capacity

The equation for specific heat after substituting constants the values of specific heat capacity in response to temperature change are obtained and a characteristic graph drawn.

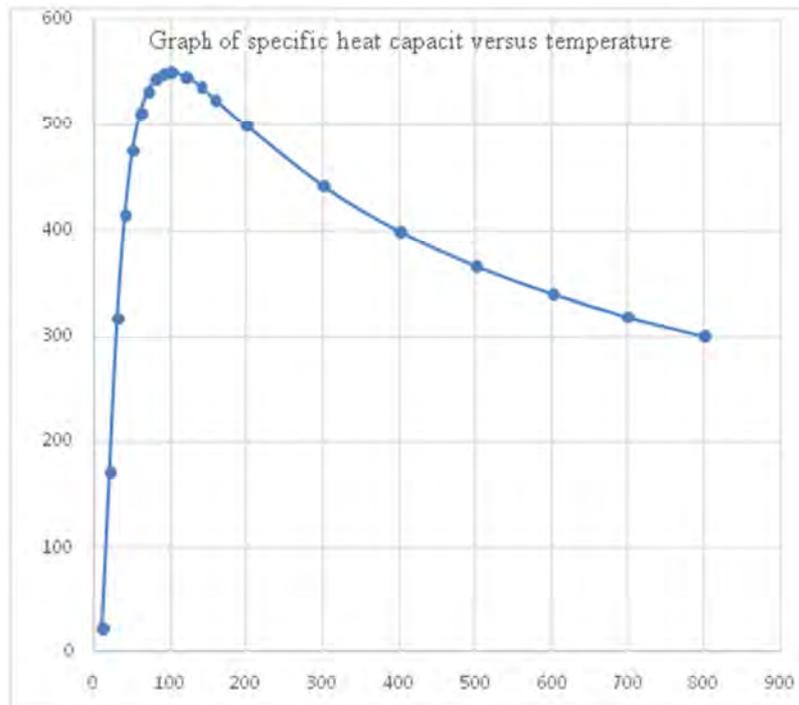


Figure 1. Graph of heat capacity against temperature for both superconducting and normal states.

In this figure there is a jump in heat capacity at the maxima which corresponds to the transition temperature as expected, thus in superconducting state heat capacity is at the peak. The temperature at which this occurs is high enough intimating a possible high temperature superconductivity.

A graph of temperature against density of states is drawn using Microsoft excel as shown below.

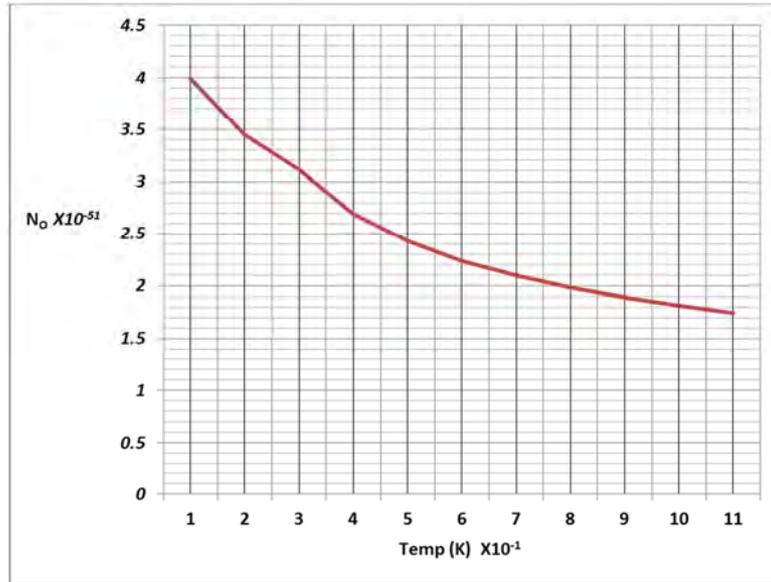


Figure 2. A graph of temperature against density of states

5.2. Discussion

In this research the two band superconductors has been done for high temperature superconductors. A Hamiltonian was developed for a compound that is composed of copper oxides and other atomic structures. The system considered has both d waves and others used for conduction.

It is assumed that the conduction waves are on the same Fermi surface. The waves therefore form energy gaps within reach of each other as they begin superconducting. Therefore the waves allow interactions that affect each other. The waves allow interactions affecting each other. The nature of the compounds also allow the formation of Fermi surfaces that enhance higher temperature superconductivity.

The Hamiltonian formed has been used to find thermodynamic properties. The greens function has been employed to find the gap equation that eventually was used to calculate transition temperature, specific heat capacity and entropy of the system. For different values of the coupling constant different graphs have been obtained in figure 1. This shows that coupling which is as a result of interaction plays an important role in determination of superconductivity transition temperature. This also has a direct link to the density of states. This is because the number of electrons used for conduction in a given compound determines the transition temperature. A higher number will require more energy to be removed to attain superconducting states. A smaller number changes state faster as shown in the graph of figure 2. In the graph the transition temperature is higher if

Temperature and density of states:

The equation of density of states was used in plotting temperature against density of states. The variation of temperature against density of states was done.

density will be higher but for conductivity to be at higher rates the channels should be increased by having several waves involved in conduction. Apart from number of wave’s phonon interactions across waves minimizes the columbic forces effects on the electrons involved.

In superconductivity states the entropy of the system is expected to be constant and at very low or near zero. This is proved as shown in the graph of entropy against temperature in figure. 3. Therefore the Hamiltonian formulated rightly represents a system in superconducting state. This is in agreement with experiment and predictions from other studies done on a similar field.

The graph of specific heat capacity against temperature shows heat capacity reduces as transition temperature increases. it agrees with the predictions in other researches. This is because in superconducting state heat capacity should be lower. This facilitates formation of cooper pairs and reduces dispersive currents. Higher specific heat capacity will allow heat as a n energy source and this will mean the compound will not super conduct. In this specific heat capacity it is evident that coupling has a direct effect on the number of waves on the Fermi surface. This in turn determines the superconducting state and transition temperature. For the case of single band conduction on the Fermi surface interactions among the fermions involved increase and columbic forces play a bigger role. This in turn increase or reduce transition temperature. Therefore with proper formulation a high temperature superconductor can be achieved.

## 6. Conclusion

The two band hybrid system superconductor has been studied and by use of greens function thermodynamic properties have been derived. The main focus was on D-waves interacting with waves on the same Fermi surface. This is the different as opposed to the other studies that focused mainly on s waves. In this research we have developed a Hamiltonian that accounts for interaction across and internally on bands. A hybrid system was developed with various coupling constants representing interaction. The Hamiltonian has both intra and inter band interaction terms. Interacting terms have both D-waves and other waves on the same Fermi surface because the compounds in consideration have elements with different waves on them. The case where there is no restriction to S waves brings a characteristic that favors transition at higher temperatures. Hybridization can breed a higher temperature transition superconductor as indicated by the characteristic graphs that indicate a higher temperature resulting from the coupling constants that are as a result of interaction. Transition temperature also depends on coupling and by extension the structure of the compounds and the waves on the Fermi surfaces.

The interactions have accounted for effects not previously considered and in this case the order parameters variations as the waves either transformed to fit the compounds different waves. The order parameter amplitudes on high temperature compounds reduce or change in size by absorbing or releasing energy into the system. This energy is in form of fields that introduce dispersion currents or electrons or absorb energy to enhance superconductivity. Therefore various sections of a superconductor can enhance or resist due to the type of waves anchored at that point or section, this explains the variations in resistance within superconductors.

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