THEORETICAL STUDIES ON HIGH TEMPERATURE SUPERCONDUCTIVITY

SURESH V. VETTOOR

THESIS SUBMITTED IN
PARTIAL FULFILMENT OF THE REQUIREMENTS
FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

DEPARTMENT OF PHYSICS
COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY
COCHIN - 682 022

1993

CERTIFICATE

Certified that the work presented in this thesis entitled "Theoretical Studies on High Temperature Superconductivity" is based on the original work carried out by Mr. Suresh V. Vettoor, under my guidance at the Department of Physics, Cochin University of Science and Technology, Cochin - 682 022 and that no part thereof has been included in any other thesis submitted previously for the award of any degree.

V. M. Nandakumaran

Cochin 682 022
September 27, 1993.

Dr. V.M. NANDAKUMARAN
Reader, Department of Physics
Cochin University of Science
and Technology, Cochin 682 022.

DECLARATION

Certified that the work presented in this thesis entitled "Theoretical Studies on High Temperature Superconductivity" is based on the original work done by me under the guidance of Dr. V.M. Nandakumaran, Reader, Department of Physics, Cochin University of Science and Technology, Cochin 682 022, and that no part thereof has been included in any other thesis submitted previously for the award of any degree.

Cochin 682 022
September 27, 1993.

Suresh V. Vettoor

Contents

Preface

This thesis is devoted to an investigation of the Physics of high temperature superconductors based on many body theoretical models. The methods adopted for studying the microscopic Hamiltonians can be grouped as follows.

1. Double time Green's functions and equation of motion method for the evaluation of Green's functions.
2. Functional integral technique for Fermi and Bose systems.
3. Slave boson technique to take care of occupancy constraints in the Hamiltonians when some of the parameters assumes large values.
4. Evaluation of functional integrals using saddle point approximation and fluctuation corrections using $\frac{1}{N}$ expansion techniques.

Ever since its discovery in 1986, few problems in Physics have occupied as many man hours of experimental and theoretical research as the problem of high temperature superconductivity. Experimental efforts are directed towards the synthesis of better samples, preparation of single crystals of the existing high Tc compounds, synthesis of new materials with higher Tc values and preparation of superconductors with desirable physical and chemical properties. Theoretical efforts are directed towards

(1) Understanding the normal state of these materials, (the normal state behaviour of these ceramic oxides are anomalous in several respects).

(2) The mechanism of superconductivity in these materials.

The thesis consists of six chapters. References are given at the end of each chapter. Equation numbers contain information regarding the chapter.

In the introductory chapter various experimental constraints on theoretical investigations are discussed. Towards the end of the chapter, the relevant orbitals and types of excitation which can possibly play a role in superconductivity have been suggested.

In chapter 2 one of the techniques of analyses adopted for the study - functional integral technique is discussed. A brief discussion on the algebra of anticommuting Grassmann variables is given.

Then we discuss how the partition function and Green's function can be set up as a functional integral over complex variables and Grassmann variables. Then how such functional integration are performed is given for the fermi case. The role of slave boson in taking care of constraints in various Hamiltonians is discussed. The original slave boson techniques introduced by Barnes and reinvented by Coleman is given briefly. To throw light on its application in functional integral formalism, the partition function for the single impurity Anderson model is worked out in detail. The slave boson formalism introduced by Kotliar and Ruckenstein and its reformulation in a manifestly spin rotation invariant form is briefly discussed.

To illustrate the power of functional methods, the BCS reduced Hamiltonian is studied using functional integrals. It is shown that the energy gap naturally emerges at the saddle point approximation. Then we briefly discuss variable transformations in functional integrals.

In Chapter 3, an investigation on a microscopic model is discussed. Here the electron-phonon interaction is considered within the frame work of the fluctuating valence of copper atom.

Anderson's lattice Hamiltonian is suitably modified to take this into account. Using Green's function technique, the possible quasiparticle excitation are determined. The energy gap expression is calculated and compared with experiments.

In Chapter 4, taking into account the clearer picture that has evolved regarding the microscopic models of high temperature superconductors, we consider a 2D extended Hubbard model which includes both copper and oxygen orbitals. The direct hopping from oxygen to oxygen is also taken into account. On site repulsion at copper sites is very large. In the low energy sector of the problem, this imposes constraints on hole dynamics. The density of states and hence the low temperature specific heat capacity of high Tc superconductors are calculated in a functional integral formalism using slave boson techniques. The effective single band description is arrived at by obtaining the quasiparticle dispersion relations. The calculated values of density of states are compared with experimental results.

In Chapter 5, the possibility of reducing the extended model to a $t - J$ model Hamiltonian in the large but not infinite U with $t_p = 0$ is emphasized. Previous calculation of the thermodynamic parameters in this model using functional integrals and slave bosons is discussed. Adopting a nonuniform saddle point (periodic one) approximation in the Bose variables, the thermodynamic parameters and density of states at the fermi surface are calculated. The results are compared with previous calculation using a uniform saddle point approximation and also with experimental results. The ground state energy evaluated at the periodic saddle point is compared with that in a uniform saddle point approximation. The much lower ground state energy value in the periodic saddle point case shows that the system is describable in terms of the periodic (nonuniform) saddle point approximation scheme.

In Chapter 6, we give a brief survey of the various ideas which are currently in vogue in the area of high temperature superconductivity theory. Then we discuss the possibility of studying the extended model using a manifestly spin rotation invariant slave boson technique adopting functional integral formation in a periodic saddle point approximation. Parts of the thesis have been previously published in the following journals.

1. Title: Electron-phonon interaction within the framework of the fluctuating valence of copper atoms - A theoretical model for high temperature superconductivity.

Authors: Suresh V. Vettoor and V.M. Nandakumaran

Journal: Modern Physics letters B, Vol.4, No.5 (1990) 325-331.

2. Title: Density of states in high Tc superconductors

Authors: Suresh V. Vettoor and V.M. Nandakumaran

Journal: Physica C 191 (1992) 277-281

Chapter 1

Introduction

1.1

Superconductivity has been one of the challenging subjects since its discovery by Kammerlingh Onnes in 1911. The very low temperature at which this is realised made its large scale technological application economically nonviable except in some special circumstances. The explanation of the phenomenon had remained as a challenge to the ingenuity of many of the leading physicists of the present century . It evaded a correct description for a long time until this was done by Bardeen Cooper and Schrieffer. Thus superconductivity research was directed at the fundamentals and its application progressed at a great pace. There have been speculation regarding high temperature and perhaps room temperature superconductivity.

Signs of realization of this long sought objective appeared in 1986 when Bednorz and Muller discovered new copper oxide superconductors with a $Tc \sim 30k$. This was a great breakthrough. Intense search for higher Tc materials started leading to the synthesis of YBaCuO and Thallium based compounts with Tc as high as 90 K or 125 K. The transition temperature was taken much above the liquid Nitrogen temperature. This is a promising development with far reaching consequences as far as the application side is considered. But the high Tc mechanism still remain as a great challenge to the theoretical community. Even the normal state behaviour of these materials are anomalous in several respects.

In this chapter we present a brief summary of the significant experimental facts about high T_C superconductors and discuss their role in the construction of a proper theory for these systems. We will first have a look at the dominant experimental results in high T_C materials and compare them with conventional low T_C metallic superconductors where necessary

The high T_C superconductors occur in several classes of materials, with Tc varying with doping for each class of materials. The major groups are the 214 Lanthanam, Strontium/Barium Copper Oxide family with T_C =40K and $YBa_2Cu_3O_{7-\delta}$ family with T_C=90K and $Tl_2Sr_2Ca_2Cu_3O_{10}$ with T_C=125K.

All these materials show the following important features.

- They show very small isotope effect
- All of them have Cu-O planar subsystem
- Their Tc is much higher than the conventional strong and weak coupling superconductors.
- They all have related compounds which are antiferromagnetic insulators with rather high Neel temperature.
- The nuclear relaxation rates below Tc in these materials are unusual
- They have extremely small coherence length
- Their dc electrical resistivity is anisotropic with a linear temperature dependence for the a-b plane resistivity.

They have the following features in common with conventional low T_C superconductors.

- Electron pairing is the mechanism for the superconducting transition.
- They have an energy gap in the excitation spectrum with the

  $$\frac{2\Delta}{K_B T_c}$$

  value assuming a larger magnitude compared to the BCS value of 3.52
- The pairs do exist in the singlet spin state and an S-wave orbital angular momentum state
- They show Josephson tunneling and vortex structure found in type-II superconductors.

1.2 Structure and stoichiometry

Compared to the crystal structures encountered in metallic solids , the structure of high Tc materials are complicated. Cu-O planar structure is a common feature of all these high Tc materials. Figure (1.1) shows that these planes, were charge carriers reside are separated from others of similar kind by isolation planes which act as charge reservoirs. These isolation planes contain positive ions La, Ba, Tl, Bi etc.

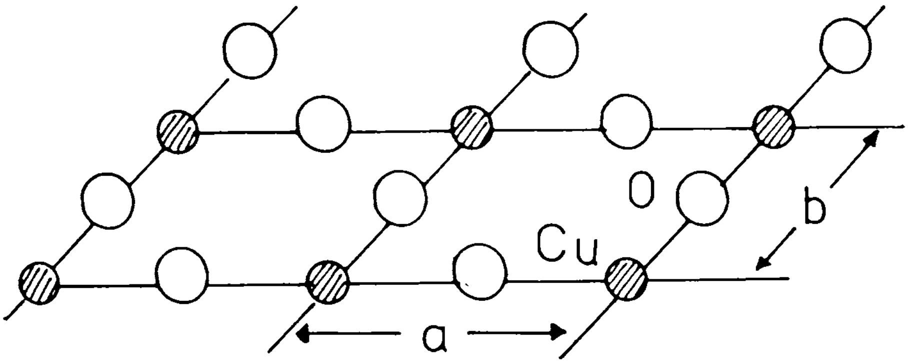
A single Cu-O plane is shown in figure (1.1.a) where square planar bonding of Cu to four Oxygen atoms can be seen. Figure (1.1.b) shows La_2CuO_4 crystal structure. In $La_{2-x}Sr_xCuO_4$ the Cu-O planes are relatively far apart $\sim$ 6.6$\AA$, with two La-O planes between Cu-O planes. In figure (1.1.c) the structure of $YBa_2Cu_3O_{7-\delta}$ is shown. For these materials there are two immediately adjacent Cu-O planes which are nearly 3.2$\AA$ apart. In all high T_C materials the Cu-O distance $\sim$ 1.9$\AA$ is the shortest compared to the other interatomic distances.

In $YBa_2Cu_3O_{7-\delta}$ the Cu-O plane groups are separated from each other by $\sim$ 8.2$\AA$. The metal Oxygen isolation planes that separates the two immediately adjacent Cu-O planes in $YBa_2Cu_3O_{7-\delta}$ are indicated by dashed planes in figure (1.1.c).

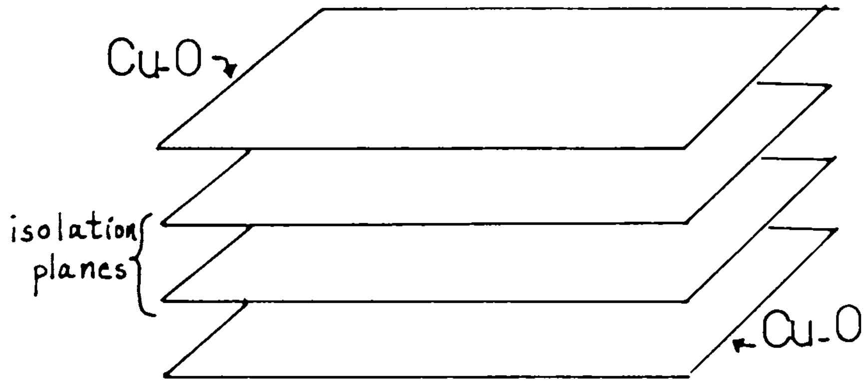
For the high T_C crystal $Tl_2Sr_2Ca_2Cu_3O_{10}$, there are three Cu-O immediately adjacent planes separated by Ca planes. These planes are separated from each other by $\approx$ 3.2$\AA$. These three planes are separated from the next set of three by $\sim$ 11.6$\AA$, with four metal Oxygen isolation planes and (2 Tl-O, & 2 Sr-O) in between such sets.

The high T_C materials are either orthorhombic or tetragonal. For theoretical discussions they can be regarded as tetragonal. Table (1.1) shows the list of high T_C materials, their T_C values and the number of adjacent planes of Cu-O in them. From the table it can be noted that T_C doesn't scale with the number of Cu-O planes. Since the 1-Tl(n) & 2-Tl(n) materials with n > 3 have been synthesised but often their T_C values are not proportionately high. However in each group T_C is correlated with the number of Cu-O planes.

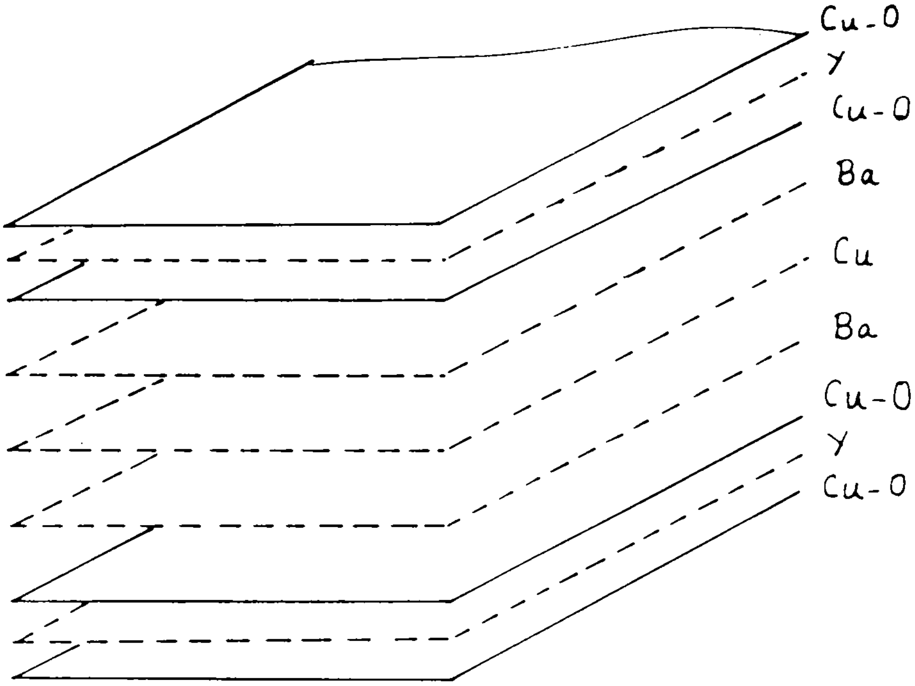
Electrical conduction in these oxides is taking place in the Cu-O planar structures. Superconductivity also seems to have a crucial dependence on their planar character. The crystal structure of La_2CuO_4, $YBa_2Cu_3O_{7-\delta}$,$Tl_2Sr_2Cu_3O_{10}$compounds are shown in figure(1.2), figure(1.3), and figure(1.4) respectively.



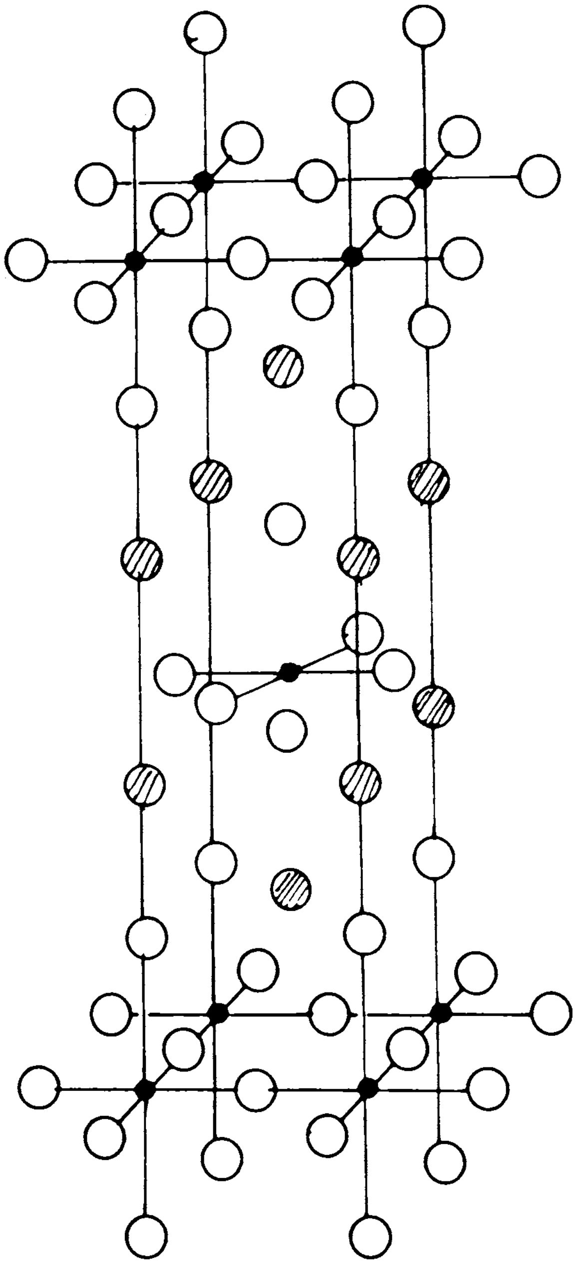
fig(1.1.a)



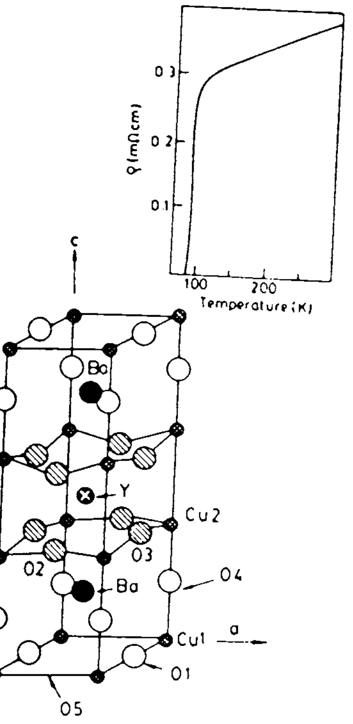
fig(1.1.b)



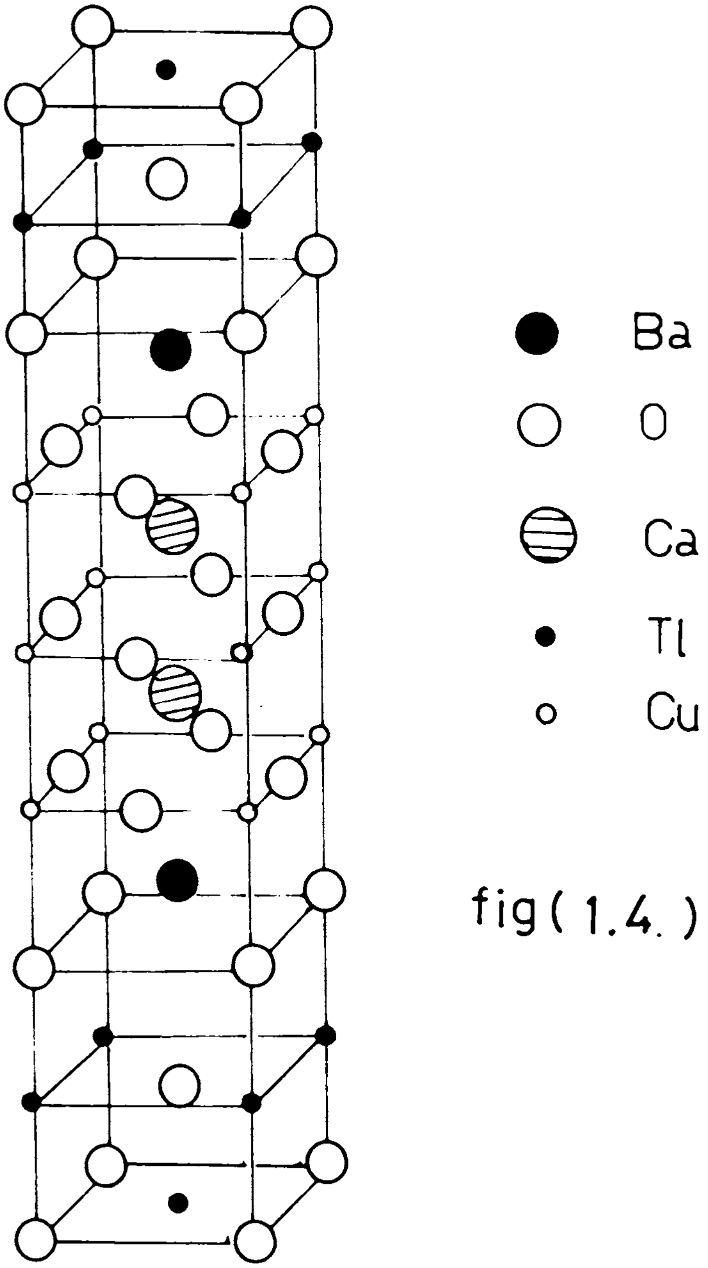
fig(1.1c)


● Cu
▨ La(Sr,Ba)
○ O

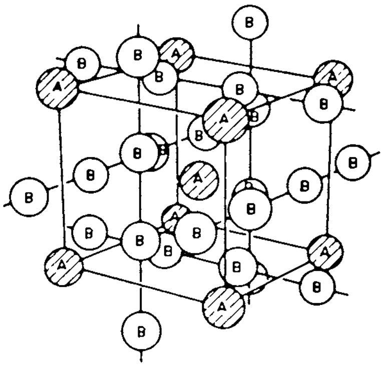
fig(1.2)


0.3
0.2
0.1
ρ(mΩcm)
100
200
Temperature (K)
c
Ba
Y
Cu2
O3
O2
Ba
O4
Cu1
a
O1
b
O5

fig(1.3)



fig(1.4.)



fig(1.5)

Compared to the high T_C materials, most elemental superconductors have the bcc, fcc or hcp structures. Two structures which are more complicated than the metallic structures are those exhibited by Nb_3Ge (Type II superconductors) and $CeCu_2Si_2$ (Heavy fermion superconductors). Nb_3Ge and related materials have the so called A-15 structure shown in figure (1.5). The material is cubic (Space group $Pm\bar{3}n - O_h^3$) with two formula units per unit cell (Z=2). Nb_3Ge belongs to a class of materials denoted generally as A_3B where A can be any of the elements Nb, V, Ti, Zr or other transition metals, and B can be Sn, Al, Ga, Ge, In or Si. Tc is sensitive to the 3/1 stoichiometry with maximum T_C obtained for this ratio. It is generally believed that this sensitivity of T_C to stoichiometry may be associated with a sharp peak in the density of electronic states and near the 3/1 stoichiometry fermilevel is close to the peak.

1.3 The normal state properties

There is a general consensus among theoreticians that a proper understanding of the normal state properties of high T_c materials is a necessary step in constructing any theory for explaining its superconducting behaviour. This is because these materials are showing several unusual normal state properties in the metallic state.

1.3.1 The charge state of various elements in these compounds

In La_2CuO_4, the formal valence states of various atoms have the following values. La exists in +3 valence state. Copper has its outer orbitals $3d^{10}4S^1$. When in +2 valence state, the outer orbital of copper is 3d in character. There is a hole in these 3d orbitals. Hence we have the $3d^9$ outer configuration. This is the case with the insulating state. When hole doped, these additional holes go to the oxygen rather than the Copper orbitals. There are no compounds in which Copper exist in +3 valence state. La_2CuO_4 is an insulator. When La atoms are substituted by Sr it becomes a metal and below the transition temperature T_C, a superconductor. The La atoms exist in +3 valence state whereas Sr is in +2 valence state. This doped compound is a metal in which the charge carriers are holes. Spectroscopic studies [1] show that the holes reside in oxygen 2p orbitals. Simple band theory calculations for the parent compounds show that they should behave as metals. This is because they have a half filled band. The insulating behaviour thus suggests the presence of strong correlation in copper orbitals.

1.3.2 Molecular orbitals

The short Cu-O distance $\sim 1.9\AA$ in the plane indicates a covalent bonding instead of an ionic bonding. Out of the plane Cu-O distance is $\sim 2.4\AA$. This brings us to the conclusion that Cu-O covalent bonding is largely non bonding along the C axis compared to the ab plane Cu-O bond. The ligand fields lift the degeneracy of Cu 3d orbitals.The Cu orbital which is most affected by the ligand environment is the one with $x^2 - y^2$ symmetry. Therefore the relevant orbitals are copper $3d_{x^2-y^2}$, and oxygen Px and Py orbitals in the planes. They have considerable overlaps and hence are the bonding orbitals.

Figure (1.6) shows a Cu-O plane with $d_{x^2-y^2}$ of Cu and Px and Py orbitals of oxygen atoms. Bonding between charge lobes of the orbitals occurs when the orbitals have the same phase. Anti bonding occurs between orbitals of opposite phase. For the molecular orbital shown in figure (1.6.c) there are as many bonding orbitals as there are anti bonding orbitals. Since the bonding and anti bonding energies are approximately the same but opposite in sign, the molecular orbital configuration is non bonding in Figure (1.6.b) shows anti bonding orbital configuration. The energy vs k diagram at the special points on the Brillouin zone are shown in Figure (1.7).

When we consider a unit cell of La_2CuO_4 we find that for every copper atom, there are four Oxygen neighbours in a plane. There are five copper d orbitals-$d_{x^2-y^2}$, d_{z^2} , d_{xy}, d_{yz} and d_{xz}. There are 3 Oxygen orbitals- 2px, 2py and 2pz. This can account for the total number of electrons. The number of orbitals are given by

$$3X4 + 5 = 17$$

. Each orbital can accommodate two electrons and hence there will be 34 electrons for the closed shell structure. But we find that there is a deficiency of 1 electron per formula unit. This deficiency resides in the topmost band-that is the anti bonding bands.

In the atomic state, the ionization energy of an electron from the P orbital of oxygen is larger than that from a Copper 3d orbital. Thus the P orbitals of Oxygen are lower in energy (larger binding energy) than the d orbital of Cu. Therefore the bonding orbital B of figure (1.7) is mostly oxygen p like and the anti bonding orbital AB is mostly Cu $d_{x^2-y^2}$ like.

1.3.3 Electrical resistivity

When discussing the variation of resistivity with temperature in normal metals, it is useful to define the reduced temperature which is the ratio of the temperature to the Debye temperature. The relationship between resistivity and reduced temperature for some simple metals is shown in figure(1.8). For simple metals the resistivity can be divided into a high temperature and a low temperature part. The high temperature part is

$$\rho = A + BT$$

where $T \geq .2\Theta_D$.In this region the quantization of lattice vibrations which causes resistance is not important. Here the Einstein phonon description is applicable. The electron scattering is proportional to the square of the amplitude of lattice vibrations about their equilibrium position [2,3].

The low temperature part of the resistivity is more complicated and it cannot be analysed in classical terms. One has to take into account the quantization of lattice vibration (phonons). The electrical resistivity arises from the scattering of electrons by phonons of the type

$$k + q \rightleftharpoons k'$$

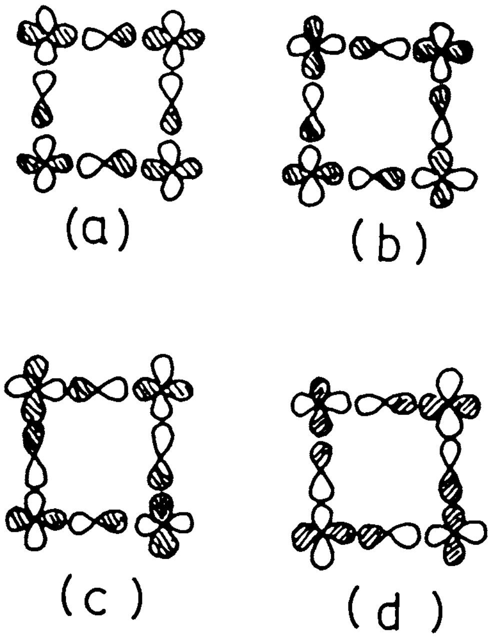
where k and k' are the initial and final wave vector and q is the phonon wave vector . The requirement that q be small and wave vector conservation in the interaction reduces the possible ways the scattering can take place. At low temperatures

$$\rho \propto T^5$$

where $T \ll 0.2\theta_D$

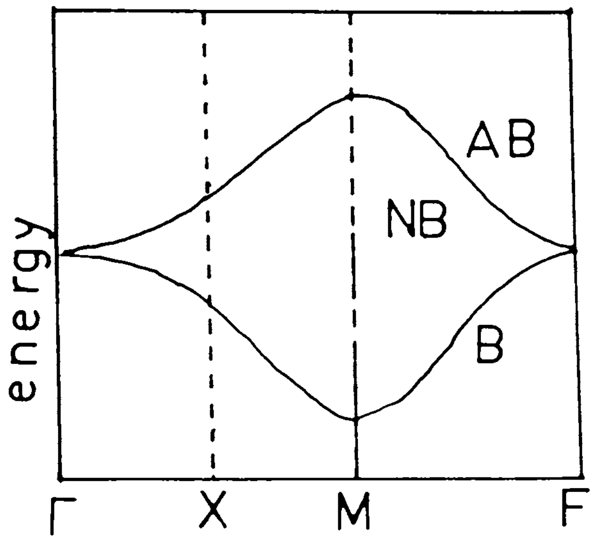
Gruneisen-Block formula extrapolates between the low and high temperature limits. The electrical resistivity is due to deviations of the lattice from perfect periodicity. This deviation can be either due to the lattice vibrations or due to the presence of the impurities or defects.

The deviations from the perfect periodicity due to impurities and defects are static and hence they make a temperature independent contribution to resistivity.


(a) (b) (c) (d)

fig(1.6)

fig.
(1.7)



Thus the low temperature resistivity has the form

$$\rho \approx C + DT^5$$

1.3.4 Electrical resistivity of high Tc superconductors

The electrical resistivity of single crystal $YBa_2Cu_3O_{7-\delta}$ in the C axis direction and in the a-b plane are shown in figure (1.9). ρ_{ab} measured in $YBa_2Cu_3O_{7-\delta}$ shows an approximately linear temperature dependence. The c- axis resistivity shows a semiconductor / non metallic behaviour. However there are measurements that suggests that the C axis resistivity is metallic [4].

In $YBa_2Cu_3O_{7-\delta}$ the ratio $\frac{\rho_a}{\rho_b} = 2.2$. This shows that chain like structures in these materials make a large contribution to the a-b plane conductivity. $YBa_2Cu_3O_{7-\delta}$ has a highly anisotropic resistivity. Anderson and Zou [5] have proposed that the ρ_c data of Tozer etal [6] can be fitted to a functional form.

$$\rho_c(T) = \frac{A}{T} + BT \tag{1.1}$$

Usually in metals, the low temperature resistivity has a temperature dependence given by Block-Gruneisen T^5 law. In transition metals and other alloys with two species of fermions interacting via s-d type coupling we expect the resistivity to have a T^2 dependence given by Baber's law.

Thus we find that the resistivity behaviour in high Tc materials fits into neither of the above schemes. In addition it shows a highly anisotropic behaviour.

The inplane resistivity of high Tc materials have the form $\rho_{ab} = A + BT$. Most of the high Tc materials have $B \sim 1.0\mu\Omega - cm/k$. This suggests the possibility of a common scattering mechanism for the charge transport in the a-b plane. For ordinary metals a linear temperature dependence of resistivity exists for $T \geq .2\Theta_D$ Where Θ_D is the Debye temperature.

1.3.5 Hall effect

Hall measurements enables us to know the nature of charge carriers in a material. These measurements yield parameters specific to the material called Hall coefficient R_H. This is determined by the magnetic field, electric current in an orthogonal direction and the induced voltage in a direction perpendicular to the other two. For carriers in a parabolic band, the free electron model with a band effective mass for the carriers work and the Hall coefficient is given [7] by the relation

$$R_H = -\frac{1}{nec} \tag{1.2}$$

Where e is positive by definition and n is the carrier density. Instead of the Hall coef.we can use the Hall density which is infact the carrier density. For metallic copper this takes the value $\sim 5 \times 10^{22}/cm^3$. If both electrons and holes are present in a parabolic band, the Hall coefficient assumes a much more complicated form.

For materials with complicated band structures even for a single carrier, the Hall coefficient cannot be written in terms of the carrier concentration. Rather it involves a complicated integral over the fermi surface. The above discussion points to the difficulty regarding the interpretation of Hall measurements. This is the case with high Tc oxides especially $YBa_2Cu_3O_{7-\delta}$ compound. Still, for a given material, the Hall Coefficient can point to the effectiveness of doping .

Ong et al [8] studied the change in Hall Constant with Sr doping for the $La_{2-x}Sr_xCuO_4$ system. The positive sign of R_H and $R_H^{-1} \sim x$ contradict the band model. The fact suggests the importance of strong correlations in the problem. Fukuyama and Hasegawa[9] have calculated the Hall Constant in a two dimensional Hubbard model based on strong correlation. Temperature dependant Hall constant is observed in single crystal samples of $YBa_2Cu_3O_{7-\delta}$ [10].

When La_2CuO_4 is doped with Sr, for each substituted Sr one hole will be added to the system. Upto $x = .1$, the Hall number is equal to this number. This value is consistent with that obtained from chemical methods (redox titrations) used to determine the hole concentration. Polycrystalline $YBa_2Cu_3O_{7-\delta}$ have revealed the following properties [11].

- the Hall constant R_H is +ve. That is hole like.
- R_H is very sensitive to the Oxygen content and increases rapidly with increasing Oxygen deficiency δ.
- R_H exhibits a significant temperature dependence.

For 90 K high Tc oxides, the temperature dependence is such that the apparent carrier density $\frac{1}{eR_H}$ varies linearly with T extrapolating to nearly 0 at $T = 0$. (The Hall constants of $La_{2-x}Sr_xCuO_4$ samples are relatively temperature independent).

In 123 single crystals also a temperature dependence similar to that obtained in polycrystalline samples has been reported [12].

The temperature dependence of R_H is one of the puzzling problems. One may jump to the conclusion that the carrier concentration diminishes at low temperatures. However it has been established by measuring superconducting penetration depth by muons [13] that there is no drastic reduction in the carrier concentration.

A two band model is proposed to explain the temperature dependence of R_H. (ie. $R_H \sim T^{-1}$. But in this model several adhoc assumptions are to be introduced to explain the lack of pressure dependence of R_H [14].

The value of Hall coefficient in Thallium compounds and Bismuth compounds are similar to $YBa_2Cu_3O_{7-\delta}$. But their temperature dependence is less and the signs are all +ve (Hole like carriers).

The temperature dependence of R_H found in 123 compounds appears to be an exception rather than a rule. The reason may be the presence of Cu-O chains.

1.3.6 Magnetic order in high Tc materials

. All high Tc compounds have related compounds (Parents) which exists in the insulating phase. In these insulators the Cu ion magnetic moments have three dimensional antiferromagnetic order with rather high Neel Temperature [15]. There are evidences that the antiferromagnetic spin ordering in the ab planes persists above the Neel temperature for three dimensional antiferromagnetic order. Magnetic susceptibility measurements indicate a temperature independent susceptibility in the insulating phase [16]. $YBa_2Cu_3O_{7-\delta}$ has a Neel temperature $T_N \approx 500K$ and La_2CuO_4 has a Neel temperature $T_N \approx 340K$. Figure (1.10) shows the phase diagrams of these materials [17].

In section (1.1) we emphasised the quasi two dimensional behaviour of CuO_2 sheets. The Heisenberg Hamiltonian with nearest neighbour spin-spin interaction has the form.

$$H = \sum_{i,\delta} JS_i.S_{i+\delta} \tag{1.3}$$

With $S = \frac{1}{2}$ Where the sum is over nearest neighbour pairs. When we have antiparallel spin orientation on neighbouring sites,J will satisfy $J > 0$ condition. From the crystal structure one expects that the interplanar interaction with any anisotropic terms will be orders of magnitude smaller than inplane interaction.

Mermin and Wagner theorem shows that a pure two dimensional system described by Heisenberg Hamiltonian cannot exhibit long range order at any non zero temperature [18]. For classical spins the correlation length should diverge exponentially as $T \rightarrow 0$ [19]. Whether this holds for spin $\frac{1}{2}$ systems is not quite well understood. According to P.W. Anderson as T-> 0 a pure 2D spin $\frac{1}{2}$ Heisenberg system would evolve into a paired stage with short range order (the so called "resonating valence bond state") rather than a long range ordered Neel state [20]. Experimental results show that such a situation is absent in the insulating parent materials. In La_2CuO_4 antiferro magnetic order develops as we go below 195K. Detailed measurements show that the three dimensional order is due to the interplanar coupling [21].

Doping the insulating materials considerably reduces the Neel temperature and finally the order becomes short range [22]. In the high Tc materials the co-existence of antiferromagnetism at temperatures below Tc is observed for example in $YBa_2Cu_3O_{7-\delta}$. When Y atoms are replaced by rare earth atoms (with local f shell magnetic moments) they have little effects on superconducting Tc. In fact Tc slightly increases, probably due to ionic size effects. This should be contrasted with the conventional superconductors, where magnetic fields tend to destroy superconductivity. The close proximity of antiferromagnetism and superconductivity may be indicative of a common origin.

In $BaBiO_3$ type of superconductors, there is no local magnetic moments and no antiferromagnetism is present. In these materials the Tc is always below 30K. These materials differ from copper oxides in their crystal structure, energy gap behaviour, isotope effect, and coherence length. Thus the fundamental mechanism of superconductivity may be different in these two classes of materials.

1.3.7 Structural phase transitions

In $La_{2-x}Sr_xCuO_4$ there is a structural phase transition from a high temperature tetragonal structure to a lower temperature orthorhombic structure around 180K. The relationship between structural phase transition and superconductivity is not clear.

In 1-2-3 compounds $YBa_2Cu_3O_{7-\delta}$ there is no structural phase transition in the conventional sense as one that occurs at constant composition. But when the material is oxygen deficient it exists in the tetragonal insulating phase. When the material has more oxygen it is an orthorhombic metal and a superconductor. Figure (1.11) shows the variation of cell parameters with doping [23].

1.3.8 Thermoelectric power

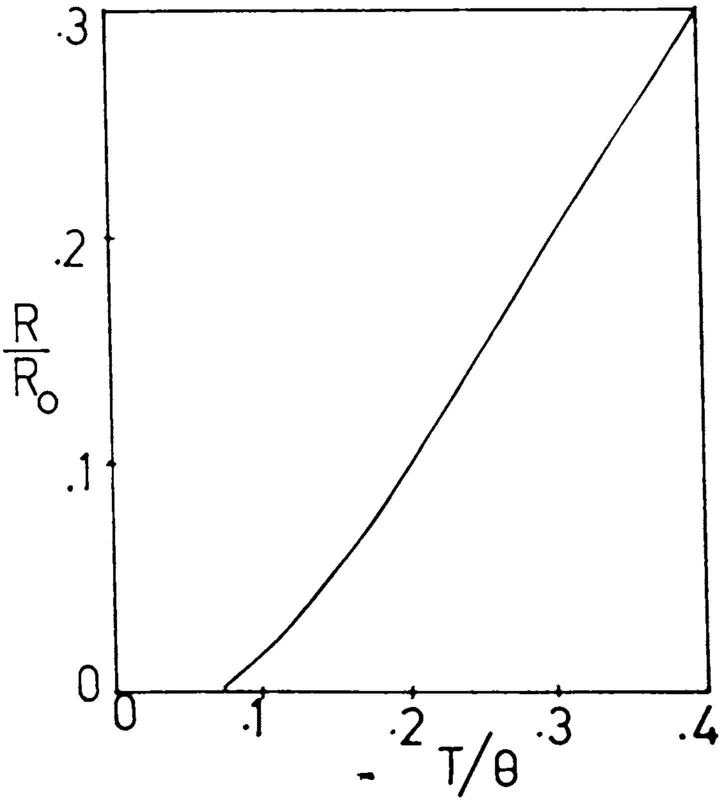
In conventional metals the thermoelectric power (Seebeck coefficient) has a linear temperature behaviour. But in $La_{2-x}Sr_xCuO_4$and $YBa_2Cu_3O_{7-\delta}$ large +ve (hole like) value of temperature independent thermoelectric power has been observed [24,25]. The thermoelectric power in these systems have little magnetic field dependence [26]. This observation could not be explained by some strongly correlated models. The magnitude of the thermopower is very sensitive to oxygen stoichiometry. Anisotropy of thermoelectric power has been observed. In plane thermoelectric power is nearly temperature independent where as the C-axis thermo power is close to a linear T behaviour.

1.3.9 Photoemission spectroscopy

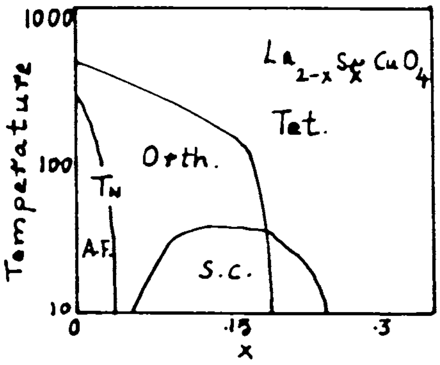
Angle resolved photoemission data are uniquely qualified to answer the question - whether the charge carriers behave as fermi liquids or not. Landau describes a fermi liquid as a system of weakly interacting particles known as quasiparticles. Their behaviour is similar to a system of non interacting fermions. If we consider a fermi liquid, then at 0K the locus of points of K space corresponding to zero energy single particle excitation define what is called a fermi surface. All the electrons in the system must be accommodated within the volume of this surface in momentum space. When quasiparticles exist, they should give rise to a peak in the energy spectrum as the wave vector approaches the fermi surface value. Outside the fermi surface the peak disappears rapidly. Angle resolved photoemission experiments essentially probe different regions of K space and determine whether quasiparticle peaks exist and how it behaves as the fermi surface is approached.

The general conclusion that can be drawn from photoemission measurements is that in the normal state near the fermi energy E_F the material behaves like an ordinary metal [27]. The measured E(k) are consistent with one electron calculations [28].

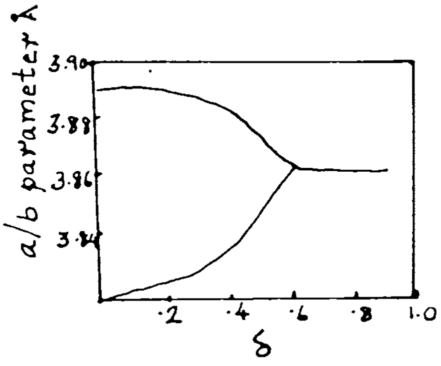
The reverse life time of the electron at energy E in the range below E_F has been



fig(1.8.)



fig(1.10)



fig(1.11)

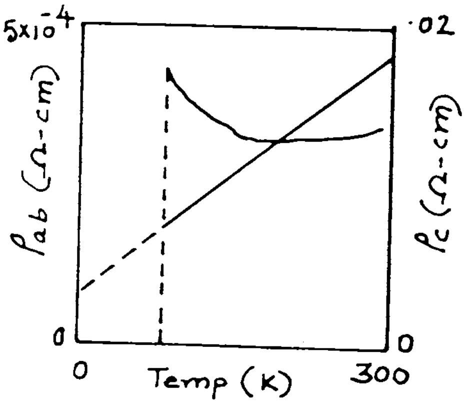
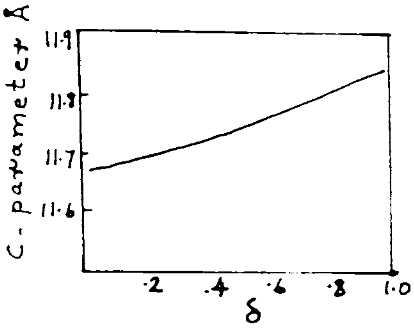


fig.(1.9)



fig(1.11a)

measured. It is linear in $(E - E_F)$ which is to be contrasted with the $(E - E_F)^2$ behaviour in a fermi liquid [29]. For a fermi liquid this is arrived at by phase space considerations and Pauli's exclusion principle [30].

One important theoretical question is the damping rate of electrons near the fermi surface. That is whether

$$\epsilon\tau(\epsilon) \gg 1.0$$

or

$$\epsilon\tau(\epsilon) \ll 1.0$$

as the energy of excitation ϵ goes to zero. $\tau(\epsilon)$ is the life time of the quasiparticle [31]. For a fermi liquid $\epsilon\tau(\epsilon) \rightarrow \infty$ as $\epsilon \rightarrow 0.0$.

while for a Tomonoga Luttinger liquid

$$\epsilon\tau(\epsilon) \propto \epsilon^{\alpha}$$

where $\alpha > 0$ and for the marginal fermi liquid.

$$\epsilon\tau(\epsilon) \propto (|\ln \epsilon|)^{-1}$$

It is clear from the above discussion that the high *Tc* materials are outside the fermi liquid regime in an important respect.

1.4 Superconducting state properties

The high superconducting transition temperature is the most unusual feature of the ceramic oxide superconductors.*Tc* of the materials are related to the number of adjacent Cu-O planar structures.

1.4.1 Cooper pairing in high *Tc* materials

In conventional superconductors, by measuring the magnetic flux trapped in a hollow superconducting cylinder, it was found that this flux is an integral multiple of the fundamental unit, the fluxoid quantum

$$\phi = n\frac{hc}{2e}$$

. where n is an integer. The factor 2 in the denominator shows that the superconducting ground state is composed of paired electrons. In high Tc materials also there is a clear evidence for electron pairing in the superconducting state. Here also there is clear evidence for flux quantization [32].

1.4.2 Nature of the paired state

When we consider a paired state it can be either a singlet spin state or a triplet spin state.The wave function of a pair of electrons can be written as the product of the spin functions and a function of the coordinates. The total wave function must be antisymmetric with respect to the exchange of the two particles of the pair.

If α and β refer to spin up and spin down states of electrons with respect to some axis. Then the spin function for the two particles can be constructed in the following four ways.

1. $\alpha(1)\alpha(2)$
2. $\frac{\alpha(1)\beta(2)+\beta(1)\alpha(2)}{\sqrt{2}}$
3. $\beta(1)\beta(2)$
4. $\frac{\alpha(1)\beta(2)-\beta(1)\alpha(2)}{\sqrt{2}}$

Of the four spin functions, the first three are called triplet state and the fourth one is called a singlet state. In the triplet state under the exchange of particles the spin part of the wave function will not change sign. Therefore the space part should be antisymmetric, under the exchange of particles. In a singlet spin state the spin part is antisymmetric under the exchange of the particles of a pair. Therefore the space part of the wavefunction must be symmetric under the exchange of the particles of the pair. In a singlet state the space part of the wavefunction must be either an S wave or a d wave orbital angular momentum sate. On the other hand in a triplet state the space part must be either a f wave or a p wave.

Josephson tunneling experiments show that the pairs in high *Tc* materials exist in the spin singlet S state [33]. It was shown that Josephson type tunneling will not take place between two superconductors separated by a thin insulator, unless the pair wave functions have the same symmetry in the two superconductors. Tunneling experiments conducted on junctions made out of conventional and high *Tc* materials shows that the pairs in high Tc materials also exists in singlet S state. Even though Josephson tunneling and conventional tunneling experiments lead one to the conclusion that S-wave pairing exists in 1 2 3 compounds, there are many who are not satisfied with these experimental evidences. They are of the view that spin flips can happen in the insulator layers and the conclusion may be wrong.

1.4.3 Non BCS character of high *Tc* materials

In BCS superconductors it is assumed that the pairing interaction is due to electron-phonon coupling. If the pairs are weakly coupled, the superconductors are called weak coupling BCS and if the electron-phonon coupling is rather high, then the pairing is called strong coupling BCS.

In high *Tc* materials the pairing mechanism is still not clear. These materials have Debye temperatures $\sim$ 300k to 450 k. The ratio $\{\frac{Tc}{\theta_D}\}^2$ is very much larger in high *Tc* materials than in conventional metallic superconductors. This excludes a weak coupling phonon mechanism for superconductivity in these materials. The ratio $\frac{2\Delta}{K_B Tc}$ in these materials is rather high (4-8). This is in contrast to the parameter independent BCS value of 3.52 . Energy gap measurements have been carried out by among others- photoemission spectroscopy techniques. The conclusion of photoemission studies is that spin pairing in the Cu-O planes is S-wave like with a small amount of d-wave pairing. There exists a gap anisotropy in these systems. But experimental results in this area are still not leading to a definite result.

1.4.4 Electronic specific heat results

According to the BCS theory $\frac{\Delta c}{\gamma Tc} = 1.43$ where $\Delta C = C_{es} - C_{en}$ and C_{es} is the electronic specific heat capacity in the superconducting state and C_{en} is the electronic specific heat capacity in the normal metallic phase. γ is the Sommerfield constant. The C_{es} and C_{en} values are evaluated at the transition temperature. The above ratio is a parameter independent constant for BCS superconductors. In strong coupled superconductors this ratio is found to be much larger. For high *Tc* materials, the calculation of the above ratio involves difficulties with the estimation of the value of γ in these materials. No definite conclusion can be drawn at this stage.

A linear T behaviour of electronic specific heat capacity has been observed in the high *Tc* materials at low temperatures. This may imply the existence of states within the gap or the absence of a gap of the BCS nature. The linear T low temperature behaviour is consistent with the RVB theory [34].

1.4.5 Nuclear Magnetic Resonance results in high temperature superconductors

In the conventional superconductors the ratio $\frac{T_{1n}}{T_{1s}}$ just below Tc rises. This rise is some- times called coherence peak(Hebel Slichter peak). Here T_{1n} and T_{1s} are the nuclear relaxation times in the normal and superconducting states. For conventional superconductors, the coherence peak could be predicted successfully by the BCS theory.

Experimental investigations in high *Tc* materials show the lack of a coherence peak in the nuclear relaxation rate. This may be an evidence against the BCS mechanism. Large anisotropies in the superconducting gap and spatial inhomogeneities may be the reason for the near absence of coherence peaks. Strong coupling BCS theories also show a reduced coherence peak. Therefore NMR results can not point to the mechanism of superconductivity in these materials in an unambiguous manner.

1.4.6 Isotope effect in high *Tc* materials

According to BCS theory, the transition temperature is given by the relation [35].
$k_BTc = 1.14\hbar\omega_De^{-\frac{1}{NV}}$

where ω_D- the Debye frequency

N-density of states at the fermi surface

V-electron-electron attractive interaction strength

The above expression shows that *Tc* has a nuclear mass dependence via the Debye frequency. i.e.$Tc \propto M^{-\alpha}$ with $\alpha = 1/2$ This prediction of BCS agrees with the experimental values of isotope effect in conventional superconductors.

In the 90k high *Tc* materials there is a near absence of isotope effect. Whereas in $La_{2-x}Sr_xCuO_4$ there is an isotope effect, but at a much reduced level. It should be noted that even in conventional superconducting materials with narrow conduction band, the isotope effect is not a clue to the mechanism. High *Tc* materials being narrow band systems, the absence of isotope effect can not rule out a phonon mechanism.

1.4.7 Magnetic properties of high *Tc* materials

When a superconductor is placed in a magnetic field, and when this is cooled below *Tc*, at *Tc* we find that the magnetic flux is excluded from the specimen. This can take place only if the magnetic field H is less than Hc, the critical field. The materials with a single critical field as described above are called type I superconductors. There are superconductors in which there are two critical fields (1) the upper critical field H_{C_2} (2) the lower critical fieldH_{C_1}.

For $H > H_{C_1}$ the magnetic field penetrates in vortices, and the fluxoid associated with each vortex is one fluxoid quantum. As the external magnetic field is increased, the density of vortices increases until the upper critical field H_{C_2} is reached and the field penetration becomes uniform and the material goes to the normal state. This type of materials are called type II superconductors.

All high *Tc* copper oxide superconductors are of type II character. Below H_{C_1} the external magnetic field is excluded from the bulk of the material by a persistent supercurrent in the surface region. The supercurrent induces a magnetic field which exactly cancells the applied field existing inside the material. The depth of this supercurrent carrying layer is called the penetration depth λ. The external field penetrates into the superconductor in an exponentially decreasing manner. For BCS superconductors the penetration depth λ has a temperature dependence given by the relation

$$\lambda(T) = \lambda(0)\{1 - (\frac{T}{T_C})^4\}^{-0.5} \qquad (1.4)$$

This relation is in good agreement with experimental results in conventional superconductors. This will not hold for p-wave or d-wave superconductors.

Experimental results in all high *Tc* materials [36] shows a behaviour in agreement with the above relation leading to the conclusion that pairing is s-wave and BCS like. There is a clear anisotropy in the penetration depth. The inplane penetration depth is $\lambda_{ab}(0) = 1400\mathring{A}$. Along the c-axis this is about 7000 $\mathring{A}$

1.4.8 Coherence length

Unlike conventional superconductors, the high *Tc* copper oxides have extremely small coherence lengths. The coherence length is a measure of the extent of the superconducting pair wave function in space. For conventional superconductors, ξ the coherence length varies from 500 $\mathring{A}$ to $10^4\mathring{A}$. In superconductors it is possible to define an important dimensionless parameter. It is the ratio of the magnetic penetration depth to the coherence length, called Ginzberg-Landau parameter $k \equiv \frac{\lambda}{\xi}$

If $k > \frac{1}{\sqrt{2}}$ the superconductor is called type II and if $k < \frac{1}{\sqrt{2}}$ it is called type I superconductor [37]. For most elemental superconductors $k \ll 1.0$ and therefore they are type I superconductors. All alloy superconductors eg. Nb_3Ge and high Tc superconductors are type II in character. The k of high Tc superconductor is ~ 100 which falls in the extreme type II limit.

The high Tc superconductors are in the clean limit as their coherence length is much smaller than the electron mean free path ($100 \sim 200\AA$). The coherence length can be estimated from the fluctuation contribution to the specific heat, susceptibility and conductivity. But for high Tc materials the reliable estimation of coherence length is obtained via H_{c_2} the upper critical field. For type II superconductors $H_{c_2} = \frac{\Phi_0}{2\pi\xi^2}$ where Φ_0 is the fluxoid quantum. Using this relation the coherence length in high Tc superconductors are estimated. Coherence length along the c-axis is typically $2 \sim 5\AA$ and in ab plane it is $10 \sim 30\AA$. The following conclusion can be drawn from the small value of coherence length and their anisotropy. Perpendicular to the ab plane the superconducting wave function is essentially confined to the immediately adjacent Cu-O planes at low temperatures. Even the ab plane coherence length exceeds only a few unit cells. This points to the dominance of fluctuations in these systems.

1.5 General conclusions

The Cu-O planar structures are the important subsystems in these ceramic oxides. The conductivity and possibly superconductivity is confined to these structures. The anomalous normal state properties imply that the scattering mechanism in these materials must be quite unlike that in conventional superconductors. Strong correlation in copper orbitals are important to the charge dynamics. Charge carriers are holes and there are holes on copper and oxygen. The model for these systems should include both copper and oxygen orbitals. Copper $3d_{x^2-y^2}$ orbital and the oxygen $2px$ and $2py$ orbitals are the relevant orbitals in the manybody formulation of the problem. There is a strong overlap between $3d_{x^2-y^2}$ orbitals and their neighbouring $2px$ and $2py$ oxygen orbitals.

All high temperature copper oxide superconductors have related parent compounds which have their copper spins ordered in an antiferromagnetic way. This points to the importance of exchange effects in these materials. In the large U limit of the Hubbard-U, the extended model Hamiltonian can be approximately reduced to a $t-J$ model Hamiltonian. The condition is $U \gg t_{pd}$ where t_{pd} is the hopping matrix element between copper and oxygen. In the extended Hubbard model, in addition to U and t_{pd}, nearest neighbour interaction is also included.

The major difficulty in this domain is the deduction of theoretical results by handling the strong correlation in copper orbitals rigorously. But this is a very difficult task and approximations made in the calculation might have significant effects on the results. Therefore comparison of the theoretical results with experiments cannot be done in an unambiguous way.

Superconducting mechanism in these materials is not clear. The most dominant theme for attractive interaction is the repulsion at the copper $3d_{x^2-y^2}$ orbitals. Others are the charge transfer resonances, interlayer mechanism, and phonons with band structure effects. With this brief look at the experimental situation we are concluding this chapter.

TABLE 1.1

Formula	*Tc*(*k*)	*n*
$La_{2-x}Sr_xCuO_4$	38	1
$La_{2-x}Sr_xCu_2O_6$	60	2
$Tl_2Ba_2CuO_6$	$O-80$	1
$Tl_2Ba_2CaCu_2O_8$	108	2
$Tl_2Ba_2Ca_2Cu_3O_{10}$	125	3
$Bi_2Sr_2CuO_6$	$O-20$	1
$Bi_2Sr_2CaCu_2O_8$	85	2
$Bi_2Sr_2Ca_2Cu_3O_{10}$	110	3
$Nd_{2-x}Ce_xCuO_4$	30	1
$YBa_2Cu_3O_7$	92	2
$YBa_2Cu_4O_8$	80	2
$Y_2Ba_4Cu_7O_{14}$	40	2
$TlBa_2CuO_5$	$O-50$	1
$TlBa_2CaCu_2O_7$	80	2
$TlBa_2Ca_2Cu_3O_9$	110	3
$TlBa_2Ca_3Cu_4O_{11}$	122	4
$(Nd, Ce, Sr)CuO_4$	30	1
$Ba_{0.6}K_{0.4}BiO_3$	30	–

1.6 references

1. N.Nucker, J.Fink, J.C Fuggle, P.J Durham and W.M.Temmerman, Phys. Rev.B.37, 5158 (1988)

2. J.M.Ziman, Electrons and phonons, Oxford 1960

3. H.Haken, Quantum field theory of solids, North Holland Publishing Company 1976

4. T.Ito, H.Takagi, S. Ishibashi and S.Uchida, Nature 350, 596 (1991)

5. P.W. Anderson and Z.Zou,Phys. Rev. Lett. 60, 132(1988)

6. S.W. Tozer, A.W. Kleinsasser,T.Penny, D. Kaiser and F.Holtzberg, Phys. Rev. Lett.59, 1768 (1987)

7. C.Kittel, Int. to Solid State Physics, 5th Edn. Wiley Eastern Ltd. (1976)

8. N.P.Ong, Z.Z.Wang, J.Clayhold, J.M.Tarascon, L.H.Greene and W.R.Mc Kinnon, Phys. Rev. B35, 8807(1987)

9. H.Fukuyama and Y.Hasegawa. Physica 148 B, 204(1987)

10. L.Forro, M.Raki, C.Ayache,P.C.E. Stamp,J.Y Henry and J.Rossat-Mignod, Physica C 153-155, 1357 (1988)

11. H.Takagi, T.Ido, S.Ishibashi, M.Uota, S.Uchida and Y.Tokura, Phys.Rev.B 40, 2254 (1990)

12. same as ref 10

13. D.R. Harshman, G.Aeppli, E.J.Ansaldo, B.Batlogg,J.H.Brewer, J.F. Carolan, R.J. Cava, M.Celio. A.C.D. Chaklader, W.N.Hardy, S.R. Kreitzman, G.M. Luke, D.R.Noakes and M.Senba, Phys. Rev.B.36, 2386 (1987)

14. I.D. Parker and R.H. Friend,J.Physics C 21 (1988) L345

15. D.Vaknin, S.K. Sinha, D.E. Moncton, D.C. Johnston, J.M. Newsam, C.R. Safinya and H.E. King Jr., Phys. Rev. Lett.58, 2802 (1987)

16. J.M. Tranquada, A.H. Moudden, A.I. Goldman, P.Zolliker, D.E Cox, and G. Shirane, S.K. Sinha, D.Vaknin, D.C.Johnston, M.S Alvarez, A.J, Jacobson, J.T.Lewandowski, and J.M.Newsam, Phys. Rev.B38, 2477 (1988)

17. J.B. Torrance, A.Bezinge, A.I. Nazzal, T.C. Huang , S.S Parkin, D.T Keane, S.L.La Placa, P.A. Horn and G.A.Held, Phys.Rev.B40, 8872 (1989)

18. N.D.Mermin and H.Wagner, Phys.Rev. Lett.17, 1133 (1966)

19. A.M. Polyakov, Phys.Letters B59, 79 (1975)

20. P.W. Anderson, Mater. Res.Bull.8,153 (1977)

P.W. Anderson, Science 235, 1196 (1987)

21. G.Shirane, Y.Endoh, R.J.Birgeneau, M.A.Kastner, Y.Hidaka, M.Oda, M.Suzuki and T. Murukami, Phys. Rev.Lett. 59, 1613 (1987)

22. R.J.Birgeau, C.Y.Chen, D.R.Gabbe, H.P.Jenssen, M.A.Kastner, C.J.Peters, P.J.Picone, Tineke Thio, T.R. Thurston, H.L.Tuller J.D.Axe, P.Boni and G.Shirane, Phys. Rev. Lett.59, 1329 (1987)

23. C.N.R. Rao, Physics Teacher, April-June 1988

24. S.Uchida, H.Takagi, H.Ishu, H. Eisaki, T.Yabe, S.Tajima and S.Tanaka Jpn. J. Appl. Phys.26. L440 (1987)

25. R.S.Knok, S.E.Brown, J.D. Thomson, Z.Fisk and G.Gruner Physica 148 B, 346 (1987)

26. R.C.Yu, M.J.Naughton, X.Yan , P.M.Chaikin, F.Holtzberg, R.L.Greene J.Stuart and P.Davies, Phys.Rev. B37, 7963 (1988)

27. Barbara Gross Levi, Physics Today 20-22, March 1990

28. J.C.Campuzano, G.Jennings, M.Faiz, L.Beaulaigue, B.W.Veal, J.Z.Liu, A.P.Paulikas, K.Vandervoort, H.Clauo, R.S.List, A.J.Arko, and R.J. Bartlett, Phys. Rev. Lett. 64, 2308 (1990)

29. Same as Ref.27

30. David Pines, "The manybody problem", W.A.Benjamin. Inc. New York 1961

31. Fukuyama, Physica C vol.185-189(1991) Part I,1991

32. C.E.Gough, M.S. Colicough, E.M.Forgan,R.G.Jordan, M.Keene, C.M.Muirhead, A.I.M.Rae, N.Thomas, J.S.Abell, and S.Sutton, Nature 326, 855 (1987)

33. W.A.Little, Science 242, 1390 (1988)

34. G.Baskaran, Int.J.of Modern Physics B, vol.1, 3 and 4 697-719 (1987)

35. J.R.Schrieffer, Theory of superconductivity, W.A.Benjamin, Inc. Publishers (1964) see page 55

36. D.R.Harshman, G.Aeppli, E.J.Ansaldo, B.Batlogg, J.H.Brewer, J.F.Carolan, R.J.Cava, M.Celio, A.C.D. Chaklader, W.N.Hardy, S.R.Kreitzman, G.M.Luke, D.R.Noake and M.Senba, Phys. Rev. B 36, 2386(1987)

37. A.A.Abrikosov, Soviet Phisics, JETP 5, 1174(1957)

Chapter 2

FUNCTIONAL TECHNIQUES

2.1 Introduction

Functional integral techniques provide a powerful approach to several currently active areas of research - for instance the theory of high temperature superconductivity. It provide new ways to organize perturbation theory. The saddle point calculation is a means to do nonperturbative approximation.
Condensed matter physics employs two types of functional integral techniques. (1) Stratanovich-Hubbard transformation [1,2,3] within a conventional treatment of Fock space statistical mechanics and (2) a priori formulation of the partition function and Green's function as path integral over spaces of complex or anticommuting variables. The first class of technique has been applied extensively to the treatments of superconductivity [4], the Ising model [5], the Anderson model[6], and several other condensed matter problems. A Stratanovich-Hubbard transformation replaces the partition function of an interacting system with a Gaussian average partition function for noninteracting system in a time dependent auxiliary field. This provides a method for making mean field approximation and at least in principle allows for the systematic study of fluctuation correction.

Functional integrals of the second class commonly used in field theory, have been applied more sparingly in condensed matter theory. The path integral representation of propagators in quantum mechanics is due to Feynman [7,8,9]. The field theoretical version of path integrals were introduced by Edwards and Peierls [10], Gelfand and Minlos [11] and Mathews and Salam [12]. Functional integral techniques were applied in statistical mechanics by Bell [13] and Edwards [14]. A modern treatment of functional integrals is available in Negalle and Orland [3]

Schulman [15] and V.N. Popov [16].

2.2 Grassmann Algebra and Fock space

In this section we discuss the important features of Grassmann Algebra and how it can be used to characterize the Fock space of Fermions. We approach it along the general lines of Berezin [17] and Itzykson and Zuber [18]. This correspondence between Grassmann variables and Fock space for Fermions is at the basis of the functional integral formulation for the evaluation of the partition function and Green's Function for Fermi system. The study of anticommuting algebras was pioneered by H.Grassmann, a 19th Century German mathematician. First of all we will consider the Grassmann algebra G_2 generated by two anticommuting elements η and $\bar\eta$. They satisfy the anticommuting property

$$\{\eta, \bar\eta\} = \eta\bar\eta + \bar\eta\eta = 0 \tag{2.1}$$

From this it follows that if we put $\bar\eta = \eta$ or $\eta = \bar\eta$, the following relation are implied.

$$\eta^2 = 0, \bar\eta^2 = 0 \tag{2.2}$$

The algebra consists of the set of complex polynomials in η and $\bar\eta$.

$$P(\bar\eta, \eta) = P_{00} + P_{01}\eta + P_{10}\bar\eta + P_{11}\bar\eta\eta \tag{2.3}$$

There will not be any term with P_{ij} where $iorj > 1$. This follows from equation 2.1 and equation 2.2, where the coef. P_{ij} are complex numbers usually written as $P_{ij} \in C$ where C is the complex space. Addition and multiplication of such polynomials are allowed subject to equation 2.1 scalar multiplication by elements of complex space C is allowed. Derivative on G_2 is defined by the following relation.

$$\partial 1 = 0, \partial\eta = 1, \partial\bar\eta = 0, \partial(\eta\bar\eta) = -\partial(\bar\eta\eta) = \bar\eta \tag{2.4}$$

$\partial(\alpha\bar\eta\eta + \beta\bar\eta + \gamma\eta) = -\alpha + \gamma$ where $\alpha, \beta, \gamma \in C$. The derivative $\bar\partial$ is defined in a similar way with an interchange $\partial \to \bar\partial, \eta \leftrightarrow \bar\eta$. It should be noted that $\eta and \bar\eta$ are independent anticommuting variables, just like z and $\bar z$ are independent complex numbers. Integration on G_2 is equivalent to differentiation by definition.

$$\int d\bar\eta P(\bar\eta, \eta) = \bar\partial P(\bar\eta, \eta) \tag{2.5}$$

Multiple integrals are defined as iterated integrals with the innermost integration to be performed first. When the integration is performed according to the rules already defined, the integral evaluation in a multiple integral is given below.

$$\int d\eta d\bar{\eta}(P_0 + P_{00}\bar{\eta} + P_{01}\eta + P_{11}\bar{\eta}\eta = P_{11} \tag{2.6}$$

If the order of integration is reversed

$$\int d\bar{\eta}d\eta(P_{00} + P_{10}\bar{\eta} + P_{01}\eta + P_{11}\bar{\eta}\eta) = -P_{11} \tag{2.7}$$

Now let us consider the effect of change of variables in an integral over Grassmann variables.

Let η, ξ, ω and their barred counterparts form elements of an enlarged Grassmann algebra.

Let the following relation hold among these variables.

$$\bar{\eta} = D_{00}\bar{\xi} + D_{01}\,\xi + \bar{\omega} \tag{2.8}$$

$$\eta = D_{10}\bar{\xi} + D_{11}\,\xi + \omega \tag{2.9}$$

which can be written in matrix form

$$[\eta] = [D][\xi] + [\omega] \tag{2.10}$$

Consider the polynomial $P(\bar{\eta}, \eta)$. Replace $\bar{\eta}$ and η in equation 2.8 and equation 2.9 Then

$$\partial_{\xi}\partial_{\bar{\xi}}[P(\bar{\eta}\eta)] = P_{11}(D(00)D(11) - D(01)D(10)) = P_{11}\det D \tag{2.11}$$

From the equivalence of differentiation and integration

$$\int d\xi d\bar{\xi} P\left(\bar{\eta}\left(\bar{\xi}, \xi, \bar{\omega}, \omega\right), \eta\left(\bar{\xi}, \xi, \bar{\omega}, \omega\right)\right) = P_{11}\det(D) \tag{2.12}$$

From equation 2.6 and equation 2.12, we arrive at

$$\int d\eta d\bar{\eta} P(\bar{\eta}, \eta) = (\det D)^{-1} \int d\xi d\bar{\xi} P\{\bar{\eta}\{\bar{\xi}, \xi, \bar{\omega}\overset{\omega}{\}}, \eta\{\bar{\xi}, \xi, \bar{\omega}, \omega\}\} \tag{2.13}$$

It can be noted that the Jacobian of the transformation $\det D$ enters the denominator rather than the numerator as is the case for a usual integral. This can be generalized to higher dimensional spaces.

$$\eta = (\eta_1, \ldots, \eta_N), \xi = (\xi_1, \ldots, \xi_N), \omega = (\omega_1, \ldots, \omega_N) \tag{2.14}$$

the transformation

$$\begin{pmatrix} \eta_1 \\ \vdots \\ \eta_N \\ \bar{\eta}_1 \\ \vdots \\ \bar{\eta}_N \end{pmatrix} = \begin{pmatrix} D_{2Nx2N} \end{pmatrix} \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_N \\ \bar{\xi}_1 \\ \vdots \\ \bar{\xi}_N \end{pmatrix} + \begin{pmatrix} +\omega_1 \\ \vdots \\ \omega_N \\ \bar{\omega}_1 \\ \vdots \\ \bar{\omega}_N \end{pmatrix} \tag{2.15}$$

gives

$$\prod_{i=1}^{N}(d\eta d\bar{\eta}) = (\det D)^{-1}\prod_{i=1}^{N}(d\xi d\bar{\xi}) \tag{2.16}$$

If D is of the Block diagonal form

$$D = \begin{pmatrix} A_{NxN} & 0 \\ 0 & A^{*}_{NxN} \end{pmatrix} \tag{2.17}$$

then

$$\det D = \mid \det A \mid^2 \tag{2.18}$$

An element P of G_2 satisfying the condition $\partial P = 0$ is called an analytic function on G_2. This leads to the conclusion that every analytic function takes the form

$$f(\bar{\eta}) = f_0 + f_1\bar{\eta} \tag{2.19}$$

where $f_0, f_1 \in C$

Complex conjugation is defined as follows

$$f^{*}(\bar{\eta}) = f_0^{*} + f_1^{*}\bar{\eta} \tag{2.20}$$

where $f_0^{*}, f_1^{*} \in c$ we find that under this operation only the complex coefficients are affected.

Now let us consider a Fock space of a single fermion level with creation operator $c^{\dagger}$ and annihilation operator c. Fock space of the system consists of states $a|0> + b|1>$ where $a, b \in c$.The basis states |0> and |1> have the property

$$c|0> = 0, c^{\dagger} \mid 0 > = |1>, c^{\dagger} \mid 1 > = 0 \tag{2.21}$$

The elements of F may be placed in one to one correspondence with a subset of the Grassmann algebra G_2 generated by two anticommuting elements η and $\bar{\eta}$.

$$a \mid 0 > + b \mid 1 > \longleftrightarrow a + b\bar{\eta} \tag{2.22}$$

The polynomial over G_2 corresponding to the bra vector will be

$$< 0|a^{*}+ < 1|b^{*} \longleftrightarrow a^{*} + b^{*}\eta \qquad (2.23)$$

Let us consider two states belonging to the same Fock space for a single electron say $|f>$ and $|g>$.
This can be written as

$$|f>= f_0|0> +f_1|1>, |g>= g_0|0> +g_1|1> \qquad (2.24)$$

The inner product of these state vectors will be given by

$$g_0^{*}f_0 + g_1^{*}f_1 =< g|f> \qquad (2.25)$$

by equation 2.22 and 2.23 we have established a correspondence between a state of Fock space and an analytic function G_2 The inner product can be achieved provided we define it as

$$< g|f >= g_0^{*}f_0 + g_1^{*}f_1 = \int d\bar{\eta}d\eta e^{-\bar{\eta}\eta}g^{*}(\eta)f(\bar{\eta}) \qquad (2.26)$$

From equation 2.1 and equation 2.2

$$e^{-\bar{\eta}\eta} = 1 - \bar{\eta}\eta = 1 + \eta\bar{\eta} \qquad (2.27)$$

From the above discussion we find that it is possible to construct a Grassmann representation for an arbitrary Fock space. Let us examine what happens to a state vector, when an operator acts on it. Regarding the original vector as a linear superposition of basis vectors, the effect of the linear operator is to change weights of the basis vectors in the linear superposition. The change in the weights defines the linear operator. A Fock space operator can be written as superposition. The change in the weights defines the linear operator

The Fock space operator can be written as

$$\hat{A} = \sum_{n,m=0,1} A_{nm}|n>< m| \qquad (2.28)$$

Where $\hat{A}$ is a complex matrix.
It is easily checked that $\hat{A}$ corresponds to an integral operator in the space of analytic functions on G_2.

$$(\hat{A}f)(\bar{\eta}) = \begin{pmatrix} 1 & \bar{\eta} \end{pmatrix} \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} . = \int d\bar{\xi}d\xi e^{-\bar{\xi}\xi}A(\bar{\eta}, \xi)f(\bar{\xi}) \qquad (2.29)$$

With Kernel

$$A(\bar{\eta}, \xi) = \sum_{n,m=0,1} \bar{\eta}^n A_{nm} \xi^m \tag{2.30}$$

This representation is inconvenient since we need to know the matrix elements A_{nm}. Most of the Hamiltonians are expressed in terms of creation and annihilation operators and not in the form of projection operators. Therefore it is convenient to derive a representation from the expression for $\hat{A}$ in normal ordered form. In normal ordered form all creation operators are to the left of all annihilation operators. Normal ordering operation is indicated by

$$: cc^\dagger := -c^\dagger c \tag{2.31}$$

What is the action of $\mid 0 >< 0 \mid$ on a general ket $a \mid 0 > +b \mid 1 >$.

$$\mid 0 >< 0 \mid (a \mid 0 > +b \mid 1 >) = a \mid 0 >< 0 \mid\mid 0 > +b \mid 0 >< 0 \mid\mid 1 >= a \mid 0 > \tag{2.32}$$

What is the action of $1 - c^\dagger c$ on the above general ket.

$$(1 - c^\dagger c)(a|0 > +b|1 >) = a|0 > +b|1 > -b|1 >= a|0 > \tag{2.33}$$

Thus the operators $|0 >< 0|$ and $1 - c^\dagger c$ are equivalent for the Fock space of single particle system. $\hat{A}$ can be written as

$$\hat{A} = \sum_{n,m} A_{nm} (c^\dagger)^n |0 >< 0| c^m \tag{2.34}$$

$$\hat{A} = \sum_{n,m} A_{nm} (c^\dagger)^n : e^{c^\dagger c} : c^m \tag{2.35}$$

But already $(c^\dagger)^n$ is acting towards the left and c^m towards the right. Hence there is nothing wrong to write it as

$$\hat{A} = \sum_{n,m} A_{nm} : c^{\dagger^n} e^{-c^\dagger c} c^m : \tag{2.36}$$

$$\hat{A} \equiv \sum_{ij} A^N_{ij} (c^\dagger)^i c^j \tag{2.37}$$

The matrix A^N is trivially known if $\hat{A}$ is specified in normal ordered form. This is the chief benefit of using a normal ordered representation:The quantity $A(\bar{\eta}, \eta)$ is generally hard to calculate, but $A^N(\bar{\eta}, \eta)$ may be found trivially.

$$\hat{A} = \sum_{n,m=0,1} A_{nm} |n >< m| \tag{2.38}$$

$$\hat{A} = A_{00}|0><0| + A_{01}|0><1| + A_{10}|1><0| + A_{11}|1><1| \tag{2.39}$$

$$\hat{A} = A_{00} + A_{01}\eta + A_{10}\bar{\eta} + A_{11}\bar{\eta}\eta \tag{2.40}$$

The general relation between A^N and A is

$$A(\bar{\eta}, \eta) = e^{\bar{\eta}\eta} A^N(\bar{\eta}, \eta) \tag{2.41}$$

The proof of equation 2.41 is given in Appendix A. The Grassmann representation for operator product is also required for future use.

$$(A_1 A_2)^N(\bar{\eta}, \xi) = \int d\bar{\omega} d\omega e^{(\bar{\eta}-\bar{\omega})\omega} e^{(\bar{\omega}-\bar{\eta})\xi} A_1^N(\bar{\eta}, \omega) A_2^N(\bar{\omega}, \xi) \tag{2.42}$$

The proof of equation 2.42 is given in Appendix B. In general

$$A_1^N(\bar{\eta}, \omega) A_2^N(\bar{\omega}, \xi) \neq A_2^N(\bar{\omega}, \xi) A_1^N(\bar{\eta}, \omega) \tag{2.43}$$

They will commute if any one of the operators in the operator product is bilinear in Grassmann variables.

Finally the Grassmann representation for an operator trace is required for use in statistical mechanics.

For an operator $\hat{A}$ on F,

$$\text{Trace}\hat{A} = \int d\eta d\bar{\eta} e^{2\bar{\eta}\eta} A^N(\bar{\eta}, \eta) \tag{2.44}$$

The proof of equation 2.44 is given in Appendix C.

It can be noted that the order of integration is reversed in the trace formula from that in the previous equation. The above derivation for the Fermion case can be generalized to the N Fermion case by making the replacements

$$\eta \longrightarrow (\eta_1, \eta_2, \ldots, \eta_N) \tag{2.45}$$

$$\bar{\eta} \longrightarrow (\bar{\eta}_1, \bar{\eta}_2, \ldots, \bar{\eta}_N) \tag{2.46}$$

$$\int d\eta d\bar{\eta} \longrightarrow \int \prod_{\alpha=1}^{N} d\eta_\alpha d\bar{\eta}_\alpha \tag{2.47}$$

The significant results of this section are summarised in Appendix D.

2.3 Functional integrals for Fermi Hamiltonians

In the present section, we derive the functional integral representations for the partition function and Green's function for a Fermi system. As usual the fermion species is indicated by a Greek superscript on Grassmann element. In any term a repetition of superscripts or subscripts implies sum of all species. The partition function of a second quantized system is written as

$$Z = \mathrm{Trace} e^{-\beta H} \tag{2.48}$$

With β as $\frac{1}{k_B T}$ where k_B the Boltzmann's constant and T the temperature in Kelvin. H is the second quantized Hamiltonian for the system. Consider an arbitrary partition of the interval $[0, \beta]$, $(\tau_0 = 0, \tau_1, \ldots, \tau_N = \beta)$ and let $\Delta\tau_j = \tau_j - \tau_{j-1}$

The partition function may be rewritten as

$$Z = \mathrm{Trace} \prod_{j=1}^{N} e^{-\Delta\tau_j H} \tag{2.49}$$

It is difficult to determine the Grassmann representation of the operator $e^{-\Delta\tau_j H}$. However,the normal ordered representation $: e^{-\Delta\tau_j H} :$ is trivial. It may be obtained by replacing creation and annihilation operators with corresponding Grassmann variables.

$$e^{-\Delta\tau_j H} = e^{-\Delta\tau_j \epsilon_k c_k^\dagger c_k} = 1 - (\Delta\tau_j \epsilon_k - \frac{(\Delta\tau_j \epsilon_k)^2}{2!}) c_k^\dagger c_k \tag{2.50}$$

When $e^{-\Delta\tau_i H}$ is normal ordered.

$$: e^{\Delta\tau_j H} := 1 - \Delta\tau_j \epsilon_k c_k^\dagger c_k + \frac{(\Delta\tau_j^2 \epsilon_k)^2 c_k^\dagger c_k^\dagger c_k c_k}{2!} \tag{2.51}$$

$$: e^{-\Delta\tau_j H} := 1 - \Delta\tau_j \epsilon_k c_k^\dagger c_k \tag{2.52}$$

Thus replacing $e^{-\Delta\tau_j H}$ with its normal ordered form leads to the neglect of terms $\frac{(\Delta\tau_j \epsilon_k)^2}{2!}$. Therefore the error in this replacement is of the order of $(\Delta\tau_j)^2$ when the Hamiltonian itself is normal ordered. It follows that

$$Z = \lim_{\Delta\tau_j \to 0, N \to \infty} \mathrm{Tr}\{\prod_{j=1}^{N} : e^{\Delta\tau_j H} :\} \tag{2.53}$$

A simple Grassmann representation of Z is now possible. Let

$$P \equiv \prod_{j=1}^{N} : e^{-\Delta\tau_j H} : \tag{2.54}$$

Let

$$\begin{aligned} P^N(\bar{\eta}_N, \eta_0) &= (A_1 A_2 \ldots A_N)(\bar{\eta}_N, \eta_0) \\ &= (A_1 B_1)(\bar{\eta}_N, \eta_0) \end{aligned} \tag{2.55}$$

Where

$$B_1 = A_2 A_3 A_4 \ldots A_N \tag{2.56}$$

$$P^N(\bar{\eta}_N, \eta_0) = \int d\eta_{\bar{n}-1} d\eta_{N-1} e^{(\bar{\eta}_N - \eta_{\bar{N}-1})\eta_{N-1}} e^{(\bar{\eta}_{N-1} - \bar{\eta}_N)\eta_0} A_1^N(\bar{\eta}_N, \eta_{N-1}) B_1^N(\eta_{\bar{N}-1}, \eta_0) \tag{2.57}$$

Now consider

$$\begin{aligned} B_1^N(\bar{\eta}_{N-1}, \eta_0) &= (A_2 B_2)^N(\bar{\eta}_{N-1}, \eta_0) \\ &= \int d\bar{\eta}_{N-2} d\eta_{N-2} e^{(\eta_{\bar{N}-1} - \bar{\eta}_{N-2})\eta_{N-2}} \\ &\quad e^{(\bar{\eta}_{N-2} - \bar{\eta}_{N-1})\eta_0} A_2^N(\bar{\eta}_{N-1}, \eta_{N-2}) B_2^N(\bar{\eta}_{N-2}, \eta_0) \end{aligned} \tag{2.58}$$

By making use of the fact that $A_1^N(\bar{\eta}_N, \eta_{N-1})$, $A_2^N(\bar{\eta}_{N-1}, \eta_{N-2})$ etc are bilinear in Grassmann variables and proceeding in the above way through the product of operators, we get

$$P^N(\bar{\eta}_N, \eta_0) = \int (D\bar{\eta} D\eta)^{N-1} e^{-S'} \tag{2.59}$$

Where

$$S' = -\sum_{l=2}^{N} (\bar{\eta}_l^\alpha - \bar{\eta}_{l-1}^\alpha)\eta_{l-1}^\alpha + \sum_{l=1}^{N} \Delta\tau_l H(\bar{\eta}_l^\alpha, \eta_{l-1}^\beta) - (\bar{\eta}_1^\alpha - \bar{\eta}_N^\alpha)\eta_0^\alpha \tag{2.60}$$

and

$$(D\bar{\eta} D\eta)^n = \prod_\alpha \prod_{j=1}^{N-1} d\bar{\eta}_j^\alpha d\eta_j^\alpha \tag{2.61}$$

To each point τ_l on the imaginary time partition we attach a separate set of elements $(\bar{\eta}_l^\alpha, \eta_l^\alpha)$. It can be noted that the creation operators in H are replaced by $\bar{\eta}_l^\alpha$ and destruction operators by η_{l-1}^α. The operator Trace formula given by equation 2.53 becomes

$$\begin{aligned} Z &= \text{Trace}[: \prod_{j=1}^{N} e^{-\Delta\tau_j H} :] \\ &= \int \prod_\alpha d\eta_0^\alpha d\bar{\eta}_N^\alpha e^{2\bar{\eta}_N^\alpha \eta_0^\alpha} P^N(\bar{\eta}_N, \eta_0) \end{aligned} \tag{2.62}$$

The complete exponential given by equation 2.59 becomes

$$\sum_{l=2}^{N} (\bar{\eta}_l^\alpha - \bar{\eta}_{l-1}^\alpha)\eta_{l-1}^\alpha + \bar{\eta}_1^\alpha \eta_0^\alpha + \bar{\eta}_N^\alpha \eta_0^\alpha \tag{2.63}$$

Note that the elements $\bar{\eta}_0^\alpha$ and η_N^α do not appear in equation 2.60. For the sake of conciseness Let

$$\eta_0^\alpha = -\eta_N^\alpha \tag{2.64}$$

Thus expression 2.63 becomes

$$-\sum_{l=1}^{N}\bar{\eta}_l^\alpha(\eta_l^\alpha - \eta_{l-1}^\alpha) + \sum_{l=1}^{N}\Delta\tau_l H(\bar{\eta}_l^\alpha, \eta_{l-1}^\beta) \tag{2.65}$$

It is possible to perform a change of variables in the measure also.

$$\int\prod_\alpha d\eta_0^\alpha d\bar{\eta}_N^\alpha = (-1)^d\int\prod_\alpha d\eta_N^\alpha \bar{\eta}_N^\alpha = \int\prod_\alpha d\bar{\eta}_N^\alpha d\eta_N^\alpha \tag{2.66}$$

The minus sign is removed since the multiplicative factor becomes $(-1)^{2d}$ where d is the number of α values involved. The fundamental relation for Fermi functional integral can be written as

$$Z = \int_\eta e^{-S(\eta)} \tag{2.67}$$

Where

$$\int_\eta \equiv \lim_{N\to\infty}\int(D\bar{\eta}D\eta)^N \tag{2.68}$$

and

$$S(\eta) = \lim_{N\to\infty}\sum_{l=1}^{N}\Delta\tau_l\left(\frac{\bar{\eta}_l^\alpha(\eta_l^\alpha - \eta_{l-1}^\alpha)}{\Delta\tau_l} + H(\bar{\eta}_l^\alpha, \eta_{l-1}^\alpha)\right) \tag{2.69}$$

Where $\eta_0^\alpha = -\eta_N^\alpha$ and H is assumed to be given in normal ordered form. The exponent is called imaginary time action.

The results obtained holds for arbitrary partition of the interval $[0, \beta]$, in particular one may take $\Delta\tau_l = \frac{\beta}{N}$ for all l. The uniform partition has the important advantage that Fourier transform from the imaginary time label to imaginary frequency label is possible.

The partition function of equation 2.67 is completely general in character. It can be noted that the term $H(\bar{\eta}_l^\alpha, \eta_{l-1}^\alpha)$ is off diagonal in the imaginary time label. To make the term containing the Hamiltonian diagonal in the label l we perform the following variable transformation in equation 2.67

$$\begin{pmatrix} \bar{\eta}_l^\alpha \\ \eta_l^\alpha \end{pmatrix} \to \begin{pmatrix} \bar{\eta}_l^\alpha \\ \eta_{l+1}^\alpha \end{pmatrix} \tag{2.70}$$

(This is a valid transformation, since$\bar{\eta}$ and η are independent elements). The new representation for Z is

$$Z = \int_\eta e^{-S} \tag{2.71}$$

$$S = \lim_{N\to\infty} \sum_{l=1}^{N} \Delta\tau_l \left(\frac{\bar{\eta}_l^{\alpha} (\eta_{l+1}^{\alpha} - \eta_l^{\alpha})}{\Delta\tau_l} + H(\bar{\eta}_l^{\alpha}, \eta_l^{\beta}) \right) \tag{2.72}$$

where

$$\int_{\eta} = \lim_{N\to\infty} (-1)^{Nd} \int (D\bar{\eta} D\eta)^{N} \tag{2.73}$$

Arbitrary finite temperature correlation functions are expressed in a form similar to the expression for Z, the partition function .

Correlation functions have the form

$$\frac{\mathrm{Tr}(e^{-\beta H} T_{\tau}(\hat{O}_1(\tau^{(1)}) \hat{O}_2(\tau^{(2)}) \ldots))}{\mathrm{Tr} e^{-\beta H}} \tag{2.74}$$

Where T_{τ} is the time ordering operator, and

$$\hat{O}_1(\tau) = e^{\tau \hat{H}} \hat{O}_1 e^{-\tau \hat{H}} \tag{2.75}$$

The time labels for the operators appearing in correlation functions are denoted by superscripts to distinguish them from imaginary times appearing in the partition of $(0, \beta)$. As a simple example consider the propagator

$$- < T_{\tau} C_{\beta}(\tau^{(2)}) C_{\alpha}^{\dagger}(\tau^{(1)}) > \tag{2.76}$$

Assume $\tau^{(1)} < \tau^{(2)}$ Let the partitioning be

$$(\tau_0 = 0, \tau_1, \tau_2, \ldots, \tau_{n1} = \tau^1, \tau_{n+1}, \ldots, \tau_{n2} = \tau^2, \ldots, \tau_N = \beta) \tag{2.77}$$

This is represented in figure (2.2.2)

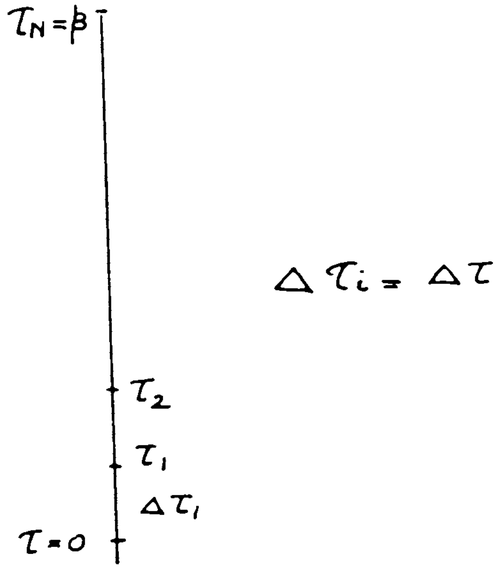
The τ interval contains $\tau^{(1)}$ and $\tau^{(2)}$, the imaginary time label. The correlation function can be written as

$$\mathrm{Trace} e^{-(\beta - \tau^{(2)})H} C_{\beta} e^{-(\tau^{(2)} - \tau^{(1)})H} C_{\alpha}^{\dagger} e^{-\tau^{(1)} H} \tag{2.78}$$

The expression 2.78 may be rewritten by expanding the time evolution operator with the aid of the partition. In the limit of an infinitesimal mesh, the replacement $e^{-\Delta\tau_l H}$ by : $e^{-\Delta\tau_l H}$: is valid. A simple Grassmann representation of $e^{-\Delta\tau_l H}$ becomes possible.

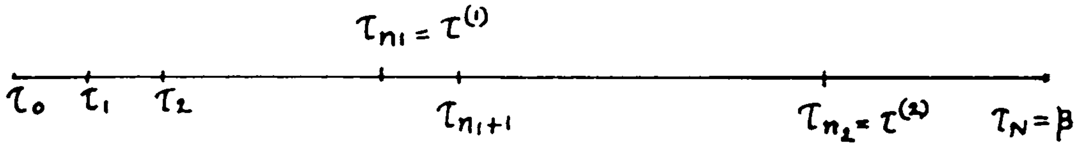
Note that

$$\begin{aligned} :e^{-\Delta\tau_l H} : C_{\alpha} &= : e^{-\Delta\tau_l H} C_{\alpha} : \\ C_{\alpha}^{\dagger} : e^{-\Delta\tau_l H} : &= : C_{\alpha}^{\dagger} e^{-\Delta\tau_l H} : \end{aligned} \tag{2.79}$$



fig(2.2.1)

Partition of the interval [o, β] for the representation of the partition function Z. The intervals $\Delta \tau_j$ may be chosen arbitrarly.



fig(2.2.2)

Thus the correlation function takes the form

$$- < C_\beta(\tau^{(2)})C^\dagger_\alpha(\tau^{(1)}) >= -Z^{-1} \int_\eta e^{-S(\eta)} \eta^\beta(\tau^{(2)}) \bar{\eta}^\alpha(\tau^{(1)}) \tag{2.80}$$

It can be seen that there is no ordering ambiguity in the Grassmann representation in equation 2.80. The reason is that each term in the expression of e^{-S} can contain an even number of Grassmann elements, and hence commutes with any other Grassmann element. Although the formula was derived for $- < C_\beta(\tau^{(2)}C^\dagger_\alpha(\tau^{(1)}) >$, it infact holds for the time ordered quantity $- < T_\tau C_\beta(\tau^{(2)})C^\dagger_\alpha(\tau^{(1)}) >$ The expression for the action in the equation 2.67 is conveniently abbreviated using the continuum notation.

$$S(\eta) = \int_0^\beta d\tau . L(\bar{\eta}^\alpha(\tau), \eta^\beta(\tau)) \tag{2.81}$$

with

$$L(\bar{\eta}^\alpha(\tau), \eta^\beta(\tau)) = \bar{\eta}^\alpha(\tau) \frac{\partial \eta^\alpha(\tau)}{\partial \tau} + H(\bar{\eta}^\alpha(\tau), \eta^\beta(\tau)) \tag{2.82}$$

The above form for the exponent in equation 2.67 and equation 2.80 leads one to interpret 2.67 and 2.80 as path integral in Grassmann functional space.

2.4 Evaluation of Gaussian integrals in Grassmann variables

Gaussian integrals over complex variables are given in the appendix.This is discussed in several books [19]. Here we will be discussing in detail the evaluation of a general Gaussian integral in Grassmann variables.

Consider the general Gaussian integral

$$I(\bar{\xi}, \xi) = \int (D\bar{\eta} D\eta)^N e^{-\bar{\eta}_n H_{nm} \eta_m + \bar{\eta}_n \xi_n + \bar{\xi}_n \eta_m} \tag{2.83}$$

Summation over repeated indices is implied. To bring the exponent in equation 2.83 to a quadratic form, let us consider the following variable transformation

$$\bar{\eta}_n = \bar{\omega}_n - \bar{\lambda}_n \tag{2.84}$$

$$\eta_n = \omega_n - \lambda_n \tag{2.85}$$

Substituting equation 2.84 and equation 2.85 in equation 2.83, the term containing $\bar{\omega}_n$ and ω_m are grouped and their coefficient is equated to zero, we get the following matrix equation for $\lambda, \xi, \bar{\lambda}, \bar{\xi}$.

$$[H][\lambda] = -[\xi] \tag{2.86}$$

$$[\bar{\lambda}][H] = -[\bar{\xi}] \tag{2.87}$$

Therefore

$$[\lambda] = -[H]^{-1}[\xi] \tag{2.88}$$

$$[\bar{\lambda}] = -[\bar{\xi}][H]^{-1} \tag{2.89}$$

Substituting for $[\lambda]$ and $[\bar{\lambda}]$ and after simplification, the Gaussian integrals becomes

$$I(\bar{\xi}, \xi) = e^{\sum_{nm} \bar{\xi} H^{-1} \xi} \int (D\bar{\omega} D\omega)^N e^{-\bar{\omega} H \omega} \tag{2.90}$$

Then the dummy variables $\bar{\omega}$ and ω are replaced by $\bar{\eta}$, and η Grassmann variables. Thus the integral becomes

$$I(\bar{\xi}, \xi) = e^{\bar{\xi} H^{-1} \xi} \int (D\bar{\eta} D\eta)^N e^{-\bar{\eta} H \eta} \tag{2.91}$$

$$I(\bar{\xi}, \xi) = e^{\bar{\xi} H^{-1} \xi} \int (D\bar{\eta} D\eta)^N \prod_{r,s} (1 + \eta_s \bar{\eta}_r H_{rs}) \tag{2.92}$$

The above form is justified as higher powers of $\eta_s \bar{\eta}_r H_{rs}$ will disappear since $\eta_s^2 = 0 = \bar{\eta_r}^2$

Therefore the integral

$$\int (D\bar{\eta} D\eta)^N \prod_{rs} (1 + \eta_s \bar{\eta}_r H_{rs}) \equiv D(H) = \sum_{P} \int (D\bar{\eta} D\eta)^N \prod_{j=1}^{N} (\eta_j \bar{\eta_{Pj}}) H_{Pjj} \tag{2.93}$$

where the sum extends over all permutations P of the indices$(1, 2, \ldots, N)$

$$\begin{aligned} \int (D\bar{\eta} D\eta)^N \prod_{j=1}^{N} \eta_j \bar{\eta}_{P_j} &= 1 \text{for even permutations} \\ &= -1 \text{for odd permutations} \end{aligned} \tag{2.94}$$

Hence by the definition of the determinant,

$$D(H) = \det H \tag{2.95}$$

and finally

$$I(\bar{\xi}, \xi) = (\det H) \exp[\bar{\xi}_n (H^{-1})_{nm} \xi_m] \tag{2.96}$$

The results derived in this section are essential for the evaluation of Green's function for a fermi Hamiltonian.The results for the Bose and Fermi case are given in appendix E.

2.5 Evaluation of partition function for Fermi and Bose systems

In this section, the partition function for non-interacting Fermi and Bose systems are computed. The Fermi and Bose cases are considered in parallel by the appropriate interpretation of integration and choice of imaginary time boundary condition.

Let the Hamiltonian be of the form

$$H = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \tag{2.97}$$

here the creation and annihilation operators may be either of Fermi or of Bose character.

$$Z = \prod_{\alpha} Z_{\alpha} \tag{2.98}$$

Restricting to a single fermion (Boson) Fock space with Hamiltonian

$$H = \epsilon a^{\dagger} a \tag{2.99}$$

$$Z = \mathrm{Tr.}[e^{-\beta H}] = \lim_{N\to\infty} \int (D\bar{a}Da)^{N} e^{-S_N} \tag{2.100}$$

with

$$S_N = \sum_{l=1}^{N} \bar{a}_l(a_l - a_{l-1}) + \epsilon \sum_{l=1}^{N} \Delta\tau_l \bar{a}_l a_{l-1} \tag{2.101}$$

This can be written as a matrix product

$$S_N = \sum_{i,j} b_{ij} \bar{a}_i a_j \tag{2.102}$$

But

$$S_N = \sum_{l=1}^{N} \bar{a}_l a_l + \sum_{l=1}^{N} (-1 + \epsilon\Delta\tau_l) \bar{a}_l a_{l-1} \tag{2.103}$$

Comparing equation 2.102 and equation 2.103

$$b_{i,i-1} = (-1 + \epsilon\Delta\tau), b_{ij} = 0 \mathrm{when} i \neq j and j \neq i - 1, b_{ij} = 1 \mathrm{when} i = j \tag{2.104}$$

When $i = 1, i - 1 = 0$ the boundary condition $a_0 = \sigma a_N$ where $\sigma = -1$ for fermion and $\sigma = 1$ for Bosons.This leads to a term with $\sigma(-1 + \epsilon\Delta\tau)\bar{a}_1 a_N$ i.e.

$$b_{1N} \neq 0, \mathrm{but}, b_{1N} = \sigma(-1 + \epsilon\Delta\tau) \tag{2.105}$$

Applying the Gaussian integration formula for Grassmann and complex spaces

$$Z = \lim_{N \longrightarrow \infty} [\det(B)]^{-\sigma} \tag{2.106}$$

Evaluating det B

$$\begin{aligned} Z &= \lim_{N \longrightarrow \infty} [1 + (-1)^{N+1} \sigma \prod_{l=1}^{N} (-1 + \epsilon \Delta \tau_l)]^{-\sigma} \\ &= [1 - \sigma \lim_{N \longrightarrow \infty} \prod_{l=1}^{N} (1 - \epsilon \Delta \tau_l)]^{-\sigma} \end{aligned} \tag{2.107}$$

The limiting value of the product is independent of the partition τ_l, but is most simply evaluated for the uniform partition $\tau_l = \frac{l\beta}{N}$, $\Delta \tau_l = \frac{\beta}{N}$ for all l. Then

$$\lim_{N \to \infty} \prod_{l=1}^{N} (1 - \epsilon \Delta \tau_l) = \lim_{N \to \infty} (1 - \frac{\beta \epsilon}{N})^N = e^{-\beta \epsilon} \tag{2.108}$$

Thus

$$Z = (1 - \sigma e^{-\beta \epsilon})^{-\sigma}, = 1 + e^{-\beta \epsilon} \text{Fermi}, = (1 + e^{-\beta \epsilon})^{-1} \text{Bose} \tag{2.109}$$

2.6 Evaluation of propagators for Fermi and Bose systems

The propagator for a noninteracting Fermi or Bose system of the previous section can be written as

$$< T_\tau a(\tau^{(2)}) a^\dagger(\tau^{(1)}) > \equiv G(\tau^{(1)}, \tau^{(2)}) \tag{2.110}$$

Therefore

$$G(\tau^{(1)}, \tau^{(2)}) = -Z^{-1} \lim_{N \to \infty} \int (D\bar{a} Da)^N a(\tau^{(2)}) \bar{a}(\tau^{(1)}) e^{-S_N} \tag{2.111}$$

Assume that $\tau^{(1)}$and $\tau^{(2)}$ occur (in either order) in the partition of $(0, \beta)$ at $\tau_m, \tau_M$with $m < M$ see figure(2. 5.1)

We proceed by evaluating each time step integral separately. For example

$$\begin{aligned} &\int d\bar{a}_1 da_1 \exp\{-\bar{a}_1(a_1 - \sigma(1 - \epsilon \Delta \tau_1) a_N) - \bar{a}_2(a_2 - (1 - \epsilon \Delta \tau_2) a_1)\} \\ &= e^{-\bar{a}_2 a_2} \int d\bar{a}_1 da_1 \\ &\quad e^{-\bar{a}_1 a_1 + \bar{a}_1 \sigma (1 - \epsilon \Delta \tau_1) a_N + \bar{a}_2 (1 - \epsilon \Delta \tau_2) a_1} \end{aligned} \tag{2.112}$$

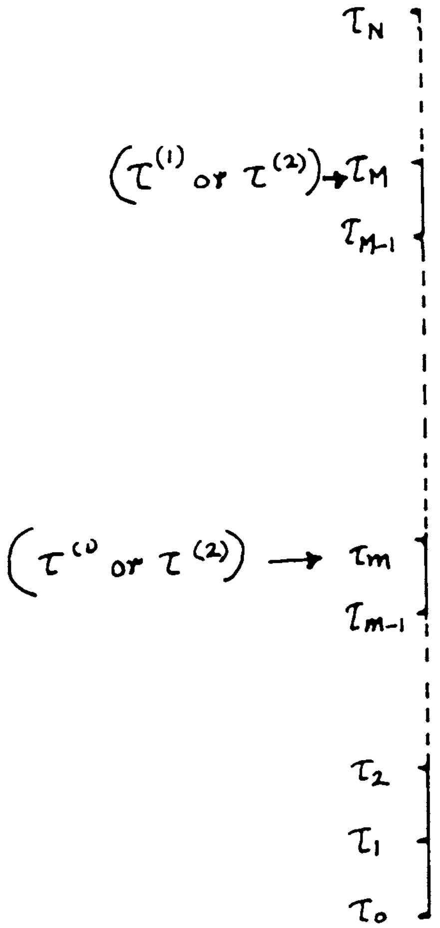

τ_N
$(\tau^{(1)}$ or $\tau^{(2)}) \rightarrow \tau_M$
τ_{M-1}
$(\tau^{(1)}$ or $\tau^{(2)}) \rightarrow \tau_m$
τ_{m-1}
τ_2
τ_1
τ_0

fig (2.5.1)

This becomes on integration with respect to a_1 and $\bar{a}_1$

$$e^{-\bar{a}_2a_2+\sigma(1-\epsilon\Delta\tau_1)(1-\epsilon\Delta\tau_2)\bar{a}_2a_N} \tag{2.113}$$

$$\int d\bar{a}_2 da_2 \exp\{-\bar{a}_2a_2+\sigma\bar{a}_2(1-\epsilon\Delta\tau_1)(1-\epsilon\Delta\tau_2)a_N-\bar{a}_3a_3+\bar{a}_3(1-\epsilon\Delta\tau_3)a_2\} \tag{2.114}$$

Continuing the integration along previous lines,we get

$$\exp\{-\bar{a}_3a_3+\sigma\prod_{j=1}^{3}(1-\epsilon\Delta\tau_j)\bar{a}_3a_N\} \tag{2.115}$$

The result of performing integrals for indices 1 through $m-1$ is just

$$\exp\{-\bar{a}_m a_m+\sigma\prod_{j=1}^{m}(1-\epsilon\Delta\tau_j)\bar{a}_m a_N\} \tag{2.116}$$

The integrals for indices $m+1$ through $M-1$ may also be performed. The result in this case is

$$\exp\{-\bar{a}_M a_M+\prod_{j=m+1}^{M}(1-\epsilon\Delta\tau_j)\bar{a}_M a_m\} \tag{2.117}$$

Finally on performing integrals for indices $M+1\text{through}N_1\text{is}$

$$\exp\{\prod_{j=M+1}^{N}(1-\epsilon\Delta\tau_j)\bar{a}_N a_M\} \tag{2.118}$$

The expression for G becomes

$$\begin{aligned} G &= -Z^{-1}\int\prod_{i=m,M,N} d\bar{a}_i da_i a(\tau^{(2)})\bar{a}(\tau^{(1)})\exp\{-\sum_{i=m,M,N}\bar{a}_i a_i \\ &+ \sigma\prod_{j=1}^{m}(1-\epsilon\Delta\tau_j)\bar{a}_m a_M+\prod_{j=m+1}^{M}(1-\epsilon\Delta\tau_j)\bar{a}_M a_m \\ &+ \prod_{j=M+1}^{N}(1-\epsilon\Delta\tau_j)\bar{a}_N a_M\} \end{aligned} \tag{2.119}$$

Performing integration with respect to $\bar{a}_N$ and a_N we get G as

$$\begin{aligned} G &= -Z^{-1}\int\prod_{i=m,M} d\bar{a}_i da_i a(\tau^{(2)})\bar{a}(\tau^{(1)})\exp\{-\sum_{i=m,M}\bar{a}_i a_i \\ &+ \prod_{j=m+1}^{M}(1-\epsilon\Delta\tau_j)\bar{a}_M a_m+\sigma\prod_{j=1}^{m}(1-\epsilon\Delta\tau_j)\prod_{j=M+1}^{N}(1-\epsilon\Delta\tau_j)\bar{a}_m a_M\} \end{aligned} \tag{2.120}$$

i.e.

$$G = -Z^{-1}\prod_{i=m,M} d\bar{a}_i da_i a(\tau^{(2)})\bar{a}(\tau^{(1)})e^{-\bar{a}Aa} \tag{2.121}$$

Where

$$[a] = \begin{pmatrix} a_m \\ a_M \end{pmatrix} \tag{2.122}$$

$$[\bar{a}] = \begin{pmatrix} \bar{a}_m & \bar{a}_M \end{pmatrix} \tag{2.123}$$

A is a 2x2 matrix with A_{ij} as the matrix elements. Finding $\bar{a}Aa$ and comparing with the exponent in equation 2.120 we find

$$\begin{aligned} A_{11} &= 1 \\ A_{22} &= 1 \\ A_{12} &= -\sigma\prod_{j=1}^{m}(1-\epsilon\Delta\tau_j)\prod_{j=M+1}^{N}(1-\epsilon\Delta\tau_j) \\ A_{21} &= -\prod_{j=m+1}^{M}(1-\epsilon\Delta\tau_j) \end{aligned} \tag{2.124}$$

2.6.1 Case1.Fermions

The exponent in equation 2.120 can be expanded as

$$a(\tau^{(2)})\bar{a}(\tau^{(1)})(1 - A_{11}\bar{a}_m a_m - A_{22}\bar{a}_M a_M - A_{12}\bar{a}_m a_M - A_{21}\bar{a}_M a_m + \frac{A_{11}A_{22}}{2!}\bar{a}_m a_m \bar{a}_M a_M) \tag{2.125}$$

Hence for $\tau^{(2)} < \tau^1$, on simplification equation 2.125 becomes

$$-A_{12}\bar{a}_m a_m \bar{a}_M a_M \tag{2.126}$$

Thus equation 2.121 becomes

$$\begin{aligned} G & \\ &= -Z^{-1}\int\prod_{i=m,M} d\bar{a}_i da_i \bar{a}_m a_m \bar{a}_M aM(-A_{12}) \\ &= \frac{A_{12}}{z} \\ &= -\frac{\sigma}{Z}\prod_{j=1}^{m}(1-\epsilon\Delta\tau_j)\prod_{j=M+1}^{N}(1-\epsilon\Delta\tau_j) \end{aligned} \tag{2.127}$$

Considering uniform partition for the intervals $\Delta\tau_j = \frac{\tau^{(2)}}{m}$ in the first of the products and $\Delta\tau_j = \frac{\beta-\tau^{(1)}}{N-M}$ for the second product. Thus for fermions $\sigma = -1$

$$G = \lim_{N,m,N-M\to\infty} Z^{-1}(1 - \frac{\epsilon\tau^{(2)}}{m})^m(1 - \frac{\epsilon(\beta - \tau^{(1)})}{N-M})^{N-M} \tag{2.128}$$

i.e.

$$G = Z^{-1}e^{-\epsilon\tau^{(2)}}e^{-\epsilon(\beta-\tau^{(1)})} \tag{2.129}$$

Where

$$Z = (1 + e^{-\beta\epsilon}) \tag{2.130}$$

Thus the propagator becomes

$$G(\tau^{(2)}, \tau^{(1)}) = -e^{-(\tau^{(2)}-\tau^{(1)})\epsilon}(\theta(\tau^{(2)} - \tau^{(1)}) - f(\epsilon)) \tag{2.131}$$

where f is the fermi function.

2.6.2 Case2.Bosons with $\tau^{(2)} < \tau^{(1)}$

$$G = \frac{-\int\prod_i d\bar{a}_i da_i a_m \bar{a_M} e^{-\bar{a}Aa}}{Z} \tag{2.132}$$

To evaluate the above functional integral over complex variables, we can write the expression $\int\prod_i d\bar{a}_i da_i a_m \bar{a_M} e^{-\bar{a}Aa}$ as

$$\frac{d^2}{d\bar{u_m}u_M}\left(\int\prod_i d\bar{a}_i da_i e^{-\bar{a}Aa+\bar{u}a+\bar{a}u}\right)_{\lim u\to 0} \tag{2.133}$$

Performing the functional integration in equation 2.133 it becomes

$$\frac{d^2}{d\bar{u_m}du_M}\left(\det A)^{-1}e^{\sum_{ij}\bar{u}_i(A^{-1})_{ij}u_j}\right) \tag{2.134}$$

On differentiating with respect to u_M, and then with respect to $\bar{u_m}$ the above expression inside the bracket becomes

$$(\det A)^{-1}\left(e^{\sum_{ij}\bar{u}_i(A^{-1})_{ij}u_j}(A^{-1})_{mM} + e^{\sum_{ij}\bar{u}_i(A^{-1})_{ij}u_j}\sum_j(A^{-1})_{mj}u_j\sum_i\bar{u_i}A^{-1})_{i,M}\right) \tag{2.135}$$

Applying the limit $u_i \to 0$ equation 2.135 becomes

$$\frac{1}{\det A}(e^0)(A^{-1})_{mM} = (\det A)^{-1}(A^{-1})_{mM} \tag{2.136}$$

Thus the propagator G becomes

$$G(\tau^{(1)}, \tau^{(2)}) = -\frac{1}{Z}(\det A)^{-1}(A^{-1})_{mM} \tag{2.137}$$

substituting for Z from equation 2.106

$$G(\tau^{(1)}, \tau^{(2)}) = -(A^{-1})_{mM} \tag{2.138}$$

After some calculations on matrix A,$(A^{-1})_{mM}$ can be obtained.

$$(A^{-1})_{mM} = \frac{\prod_{j=1}^{m}(1-\epsilon\Delta\tau_j)\prod_{i=M+1}^{N}(1-\epsilon\Delta\tau_i)}{(1-\prod_{i=1}^{N}(1-\epsilon\Delta\tau_i))} \tag{2.139}$$

$$\lim_{m,N,N-m\to\infty}(A^{-1})_{mM} = \frac{e^{-\epsilon\tau^{(2)}}e^{-\epsilon(\beta-\tau^{(1)})}}{(1-e^{-\beta\epsilon})} \tag{2.140}$$

Therefore

$$G(\tau^{(1)}, \tau^{(2)}) = -(1-e^{-\beta\epsilon})^{-1}e^{-\beta\epsilon}e^{-(\tau^{(2)}-\tau^{(1)})\epsilon}\text{for}\tau^{(2)} < \tau^{(1)} \tag{2.141}$$

Thus the propagator takes the form

$$G(\tau^{(2)}, \tau^{(1)}) = -e^{-(\tau^{(2)}-\tau^{(1)})\epsilon}(\theta(\tau(2)-\tau^{(1)}) + b(\epsilon)) \tag{2.142}$$

where $b(\epsilon)$ is the Bose function. The above derivation do not directly involve Fermi or Bose commutation relation. These are built into the functional integral schemes themselves. The operator and functional approaches are completely equivalent.

2.7 Functional integrals in the frequency domain

In section 2.5 and section 2.6 we have discussed functional integrals for Fermi and Bose systems in which the interval $(0, \beta)$ is divided into equal intervals with imaginary time labels. The partition function and propagators are evaluated in the limit of the number of such imaginary time steps going to infinity. It is possible to make a Fourier transformation from the imaginary time label to an imaginary frequency label and define the partition function and Green's function in terms of complex variables /Grassmann variables defined for the imaginary frequency case. In the present section we give a rigorous treatment of the conversion between imaginary time label to imaginary frequency label. The continuum limit formal expressions discussed in field theory books [19] can be obtained from this treatment. For the sake of simplicity let us consider a single fermion Fock space with Hamiltonian

$$H = \epsilon a^{\dagger} a \tag{2.143}$$

Where a and $a^{\dagger}$ are creation and annihilation operators. In section 2.5 the partition function for the single fermion case is defined as

$$Z = \lim_{N \to \infty} \int (D\bar{a}Da)^N e^{-S_N} \tag{2.144}$$

With

$$S_N = \sum_{l=1}^{N} \bar{a}_l (a_l - a_{l-1}) + \epsilon \Delta\tau \sum_{l=1}^{N} \bar{a}_l a_{l-1} \tag{2.145}$$

where

$$(D\bar{a}Da)^N = \prod_{j=1}^{N} d\bar{a}_j da_j \tag{2.146}$$

and

$$\Delta\tau = \frac{\beta}{N} \tag{2.147}$$

Consider the evaluation of Z_N for N even (for the sake of simplicity) The choice of uniform partition τ_l allows diagonalisation of the action by Fourier transformation.

$$a_l = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} e^{-i\omega_n \tau_l} a_n \tag{2.148}$$

$$\bar{a}_l = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} e^{i\omega_n \tau_l} \bar{a}_n \tag{2.149}$$

where a_n and $\bar{a}_n$ are new Grassmann elements,

$$\tau_l = l\Delta\tau \text{and}$$

$$\omega_n = (2n+1)\frac{\pi}{\beta} \tag{2.150}$$

It can be noted that N Grassmann variable pairs $(a_l, \bar{a_l})$ map into N new pairs $(a_n, \bar{a_n})$. In subsequent expressions whenever there is summation over n, it implies that the boundary values of n are that in equation 2.148 and equation 2.149.

This new representation preserves the antiperiodic boundary condition .

$$
\begin{aligned}
a_N &= -a_0 \\
\bar{a_N} &= -\bar{a_0}
\end{aligned}
\tag{2.151}
$$

Now let us transform each of the terms in equation 2.145 to the new variables according to the scheme for Grassmann variables.

$$
\begin{aligned}
\sum_{l=1}^{N} \bar{a}_l a_l &= \frac{1}{N}\sum_{n,n'} \bar{a_n} a_{n'} \sum_{l} e^{i(\omega_n-\omega_{n'})\eta} \\
&= \sum_{n} \bar{a_n} a_n
\end{aligned}
\tag{2.152}
$$

The transformation is unitary with Jacobian

$$
J \equiv [\det(\frac{\partial a_l}{\partial a_n})][det(\frac{\partial \bar{a}_l}{\partial \bar{a_n}})] = 1 \tag{2.153}
$$

Likewise

$$
\sum_{l=1}^{N} \bar{a}_l a_{l-1} = \frac{1}{N}\sum_{n,n',l} e^{i\omega_n \eta} e^{-i\omega_{n'}\eta_{-1}} \bar{a_n} a_{n'} \tag{2.154}
$$

$$
\sum_{l=1}^{N} \bar{a}_l a_{l-1} = \sum_{n} \bar{a}_n a_n e^{i\omega_n \Delta\tau} \tag{2.155}
$$

Substituting equation 2.152 and equation 2.155 in equation 2.145

$$
Z = \lim_{N\to\infty} \int (D\bar{a}Da)^N e^{-S_N} \tag{2.156}
$$

where

$$
S_N = \sum_{n} \bar{a}_n [1 - e^{i\omega_n \Delta\tau}(1 - \epsilon\Delta\tau)] a_n \tag{2.157}
$$

Equation 2.157 can be written as

$$S_N = \bar{a}Aa \tag{2.158}$$

A is a diagonal matrix. Hence the functional integral over Fermi variables will be

$$Z = \lim_{N\to\infty} \prod_n \{1 - e^{i\omega_n \Delta\tau}(1 - \epsilon\Delta\tau)\} \tag{2.159}$$

Equation 2.159 can be written as

$$\begin{aligned} Z &= 1 + (-1 + \epsilon\Delta\tau) \sum_n e^{i\omega_n \Delta\tau} \\ &+ (-1 + \epsilon\Delta\tau)^2 \sum_{n>n'} e^{i(\omega_n + \omega_{n'})\Delta\tau} \\ &+ \ldots + (-1 + \epsilon\Delta\tau)^N \prod_n e^{i\omega_n \Delta\tau} \end{aligned} \tag{2.160}$$

The sum $\sum_n e^{i\omega_n \Delta\tau}$ vanishes. The product

$$\prod_n e^{i\omega_n \Delta\tau} = \prod_n e^{i(2n+1)\frac{\pi}{\beta}\frac{\beta}{N}} = 1 \tag{2.161}$$

Thus

$$Z_n = 1 + (1 - \epsilon\Delta\tau)^N \tag{2.162}$$

The partition function becomes

$$Z = \lim_{N\to\infty} 1 + (1 - \frac{\beta\epsilon}{N})^N = 1 + e^{-\beta\epsilon} \tag{2.163}$$

Starting from equation 2.159 we may write the partition function in another way

$$Z = \lim_{N\to\infty} \exp[\sum_n \ln\{1 - e^{i\omega_n \Delta\tau}(1 - \epsilon\Delta\tau)\}] \tag{2.164}$$

This may be written as approximately equal to

$$Z \approx \lim_{N\to\infty} \exp[\sum_n \ln\{\Delta\tau(-i\omega_n + \epsilon)\}] \tag{2.165}$$

This can be written as

$$Z \approx \lim_{N\to\infty} (\Delta\tau)^N \exp[\mathrm{Tr} \ln(-i\omega + \epsilon)] \tag{2.166}$$

Where ω is an NXN diagonal matrix with elements ω_n. The approximation used in equations 2.165 makes Z divergent. This can be avoided by writing the expression in the form of the ratio of two partition functions.

$$\frac{Z}{Z_0} = \exp[\mathrm{Tr} e^{i\omega_0^+}\{\ln(i\omega - \epsilon) - \ln(i\omega)\}] \tag{2.167}$$

where $Z_0 = 1 + e^{-\beta 0} = 2$. The expression in equation 2.167 may be obtained by converting the sum to a contour integral.

For a single boson case a similar expression may be derived.

$$H = \epsilon a^\dagger a \tag{2.168}$$

But in this case Z_0 cannot be defined as in the Fermi case as $(1 - e^{-\beta\epsilon})^{-1}$ diverges for $\epsilon \longrightarrow 0$. To avoid this difficulty we define

$$\begin{aligned} Z &= \mathrm{Tr} e^{-\beta H_0} \mathrm{with} \\ H_0 &= \epsilon_0 a^\dagger a \mathrm{and} \\ \epsilon_0 &> 0 \end{aligned} \tag{2.169}$$

Then the ratio of the partition functions becomes

$$\frac{Z}{Z_0} = \lim_{N \to \infty} \frac{\prod_m [1 - e^{i\nu_m \Delta\tau}(1 - \epsilon_0 \Delta\tau)]}{\prod_m [1 - e^{i\nu_m \Delta\tau}(1 - \epsilon\Delta\tau)]} \tag{2.170}$$

ie.

$$\frac{Z}{Z_0} = \exp\{-\mathrm{Trace} e^{i\nu_0^+}\{2\ln(i\nu - \epsilon) - \ln(i\nu - \epsilon_0)\}\} \tag{2.171}$$

Here $e^{i\nu_0^+}, (i\nu - \epsilon), (i\nu - \epsilon_0)$ are diagonal matrices and $\nu_m = 2\pi m T$ are the Matsubara frequencies in the Bose case.

The frequency space Green's functions are also evaluated along previous lines. Consider for example the Green's function

$$G(\tau) \equiv - < T_\tau a(\tau) a^\dagger(0) > \tag{2.172}$$

For the Fermi(Bose) Hamiltonian

$$H = \epsilon a^\dagger a \tag{2.173}$$

The Fourier transform is just

$$G(i\chi_n) = \int_0^\beta d\tau e^{i\chi_n\tau} G(\tau) \tag{2.174}$$

With

$$\begin{aligned} \chi_n &= \omega_n = (2n+1)\frac{\pi}{\beta}\text{for fermions} \\ &= \nu_n = 2n\frac{\pi}{\beta}\text{for bosons} \end{aligned} \tag{2.175}$$

Consider equation 2.172

$$- < a_\beta(\tau^{(2)}) a^\dagger_\alpha(\tau^{(1)}) > = -Z^{-1} \int_a e^{-S(a)} a^\beta(\tau^{(2)}) \bar{a}^\alpha(\tau^{(1)}) \tag{2.176}$$

Substituting for the variables in terms of their Fourier transforms equation 2.176 becomes

$$G(i\chi_n) = -(Z^{-1}) \int_0^\beta d\tau e^{i\chi_n\tau} \lim_{N\to\infty} \int (D\bar{a}Da)^N \frac{1}{N} \sum_{m,m'} a_m e^{-i\omega_n\tau} \bar{a}_{m'} e^{-S_N} \tag{2.177}$$

Where under the summation sign $e^{i\omega_{m'}0} = 1$ since $\tau^{(1)} = 0$ and $\tau(2) = \tau$ in the present case.

$$G(i\chi_n) = -\frac{1}{Z} \lim_{N\to\infty} \int (D\bar{a}Da)^N \frac{1}{N} \sum_{m,m'} a_m \bar{a}_{m'} e^{-S_N} \int_0^\beta d\tau e^{i(\chi_n - \omega_m)\tau} \tag{2.178}$$

When $\omega_m = \chi_n$ the exponent becomes 0 and the integral over τ becomes β. When $\omega_n \neq \chi_n$ the integral in equation 2.178 vanishes. Therefore equation 2.178 becomes

$$G(i\chi_n) = -\frac{1}{Z} \lim_{N\to\infty} \Delta\tau \int (D\bar{a}Da)^N \sum_{m'} a_n \bar{a}_{m'} e^{-S_N} \tag{2.179}$$

When $m' \neq n$ the functional integral in equation 2.179 vanishes.

$$G(i\chi_n) = -(Z^{-1}) \lim_{N\to\infty} \Delta\tau \int (D\bar{a}Da)^N a_n \bar{a}_n e^{-S_N} \tag{2.180}$$

with

$$S_N = \sum_m \bar{a}_m[1 - e^{i\chi_m\Delta\tau}(1 - \epsilon\Delta\tau)]a_m \tag{2.181}$$

On performing integration for each pair $\bar{a}_m, a_m$ the result is

$$G(i\chi_n) = -\lim_{N\to\infty}(Z^{-1})\Delta\tau \prod_{m\neq n}[1 - e^{i\chi_m\Delta\tau}(1 - \epsilon\Delta\tau)] \tag{2.182}$$

But

$$Z = \prod_m [1 - e^{i\chi_m\Delta\tau}(1 - \epsilon\Delta\tau)] \tag{2.183}$$

Therefore

$$\begin{aligned} G(i\chi_n) &= -\lim_{N\to\infty}\frac{\Delta\tau}{1 - e^{i\chi_n\Delta\tau}(1 - \epsilon\Delta\tau)} && (2.184)\\ &= -\lim_{N\to\infty}\frac{1}{\epsilon - i\chi_n + O(\Delta\tau)} && (2.185)\\ &= -\frac{1}{\epsilon - i\chi_n} && (2.186)\end{aligned}$$

The Green's function for more complex Hamiltonians may be derived in a similar fashion.

2.8 Slave Boson representation for the single impurity Anderson model

In this section we discuss the auxiliary boson (slave boson) technique introduced by Barnes [20] and Coleman [21].It makes use of the Feynman formulation for imaginary time Green's functions. The slave boson formalism introduced in this section is closely related to the conventional manybody techniques based on free particle propagators.

The single impurity Anderson model Hamiltonian [22] has the form

$$H = H_{band} + H_{impurity} + H_{mix} \tag{2.187}$$

$$H_{band} = \sum_{k,M}\epsilon_k n_{k,M} \tag{2.188}$$

where n_{kM} is the number operator for band states. $H_{impurity}$ is written as H_f.

$$H_f = \epsilon_f \sum_M \mid M >< M \mid \tag{2.189}$$

$$H_{mix} = V \sum_{k,M} [c^\dagger_{k,M} \mid 0 >< M \mid + h.c.] \tag{2.190}$$

where $V$is the hybridization parameter, the states$\mid 0 >$ and $\mid M >$ (where Mcan assume values $-j, -j+1, \ldots, j$) represent the empty state and single impurity level. In the limit of U at the impurity level, the only impurity level configuration is the state $\mid 0 >$ or any one among the possible angular momentum states $\mid M >$ .The occupied state degeneracy is just $2j+1$.

The projection operators $\mid M >< 0 \mid$ and $\mid 0 >< M \mid$ present in the hybridization term prevents direct use of diagrammatic techniques based on free fermions.

The infinite U limit of the problem of magnetic impurity may be identified with an equivalent operator acting within a restricted Hilbert space of free particles.

The use of equivalent Hilbert space dates from the work of Abrikosov [23] on the Kondo problem. The additional complications in the Kondo problem is the presence of ionic spin operators. In the scheme introduced by Abrikosov, these operators were replaced by Fermion bilinears acting within a restricted Hilbert space. The fermions which appear in perturbation theory may not be interpreted as physical particles. Hence this approach is called pseudofermion technique. A similar representation for the infinite U Anderson model ,was introduced by Barnes and later by Coleman. In this case, the projection operators are replaced by fermion boson bilinear operators acting within a mixed Hilbert space of fermion and boson states.

$$\mid 0 >< M \mid \rightarrow b^\dagger f_M, \mid M >< 0 \mid \rightarrow f^\dagger_M b, \mid M >< M \mid \rightarrow f^\dagger_M f_M \cdot \tag{2.191}$$

where b and f_M are Bose and Fermi destruction operators. A pseudo-Hamiltonian may be defined on the full Hilbert space;it takes the form

$$H_{pseudo} = H_{band} + H_f + H_{mix} \tag{2.192}$$

where

$$\begin{aligned} H_{band} &= \sum_{k,M} \epsilon_k n_{k,M} && (2.193) \\ H_f &= \epsilon_f \sum_M f^\dagger_M f_M && (2.194) \end{aligned}$$

$$H_{mix} = V\sum_{k,M}(c^{\dagger}_{k,M}b^{\dagger}f_M + h.c.) \tag{2.195}$$

The restricted Hilbert space of physical states is a subspace for which

$$b^{\dagger}b + \sum_M f^{\dagger}_M f_M \equiv Q = 1 \tag{2.196}$$

Now for illustrating the method let us consider the case where $M = 2$, ie. only spin degeneracy is present.Let us represent the auxiliary boson state by$|_b>$ and the two fermion state by $|_{f_1}>$ and $|_{f_2}>$. Therefore the state of the system at an impurity will be represented as a tensor product $|_b> \otimes |_{f_1}> \otimes |_{f_2}>$. They can have 8 different fillings. Operating with equation 2.196 we get the eigen values 0,1,2,2,3,1,1,and 2. Out of the above states with different eigen values the restricted Hilbert space corresponds to the state with eigen value 1.

The states are $|_b\ 1 > \otimes |_{f_1}\ 0 > \otimes |_{f_2}\ 0 >$,$|_b\ 0 > \otimes |_{f_1}\ 0 > \otimes |_{f_2}\ 1 >$, $|_b\ 0 > \otimes |_{f_1}\ 1 > \otimes |_{f_2}\ 0 >$

Now let us return to the general formalism. Within the restricted space,the properties of the pseudo Hamiltonian are identical with that of the initial Hamiltonian. This approach has been called the slave boson or auxiliary technique, since a boson is introduced to represent a system which previously contained only fermions.This is the elementary picture of slave boson formalism.

2.9 Derivation of $O(1/N^2)$ partition function for the single impurity Anderson model

Large N technique in condensed matter theory originated with their application to the problem of magnetic impurity in a nonmagnetic host. The possibility of considering the orbital degeneracy as an expansion parameter was suggested by Anderson [24]. This was applied to the magnetic impurity problem by T.V. Ramakrishnan [25].In this section we give a detailed derivation of the partition function for the single impurity Anderson model in a large N functional integral formalism [26].

The partition function for the Anderson model discussed in section 2.8 may be written as

$$Z = \text{trace}(e^{-\beta H}) \tag{2.197}$$

where H is the pseudo Hamiltonian introduced in section 2.8.

$$\begin{aligned} H &= \sum_{k,M} c^{\dagger}_{kM} c_{kM} + \epsilon_f \sum_{M} f^{\dagger}_{M} f_{M} \\ &+ V\sum_{k,M}(c^{\dagger}_{k,M} f_{M} b^{\dagger} + b f^{\dagger}_{M} c_{kM}) \end{aligned} \tag{2.198}$$

where $c^{\dagger}_{kM}$ and $f^{\dagger}_{M}$ are the fermion creation operators for conduction electrons and impurity electrons.$b^{\dagger}$and$b$ are the creation and annihilation operators for slave bosons. The impurity degeneracy $N = 2j + 1$ where j is the orbital angular momentum quantum number.

The Hamiltonian given by equation 2.198 is acting on a restricted subspace of the original Hilbert space, which satisfies the condition given by equation 2.196. The trace operation may be extended to the full Hilbert space if an operator delta function which projects out the $Q = 1$ subspace is inserted. Such an operator can be written as

$$\int_{-\frac{\pi}{\beta}}^{\frac{\pi}{\beta}} \frac{\beta d\lambda}{2\pi} e^{-i\beta\lambda(Q-1)} \tag{2.199}$$

Regarding Q as aC number we can perform the integration and equation 2.199 becomes

$$-\frac{\beta}{2i\beta(Q-1)\pi}[e^{-i\beta(Q-1)\frac{\pi}{\beta}} - e^{i\beta(Q-1)\frac{\pi}{\beta}}] = \frac{\sin(Q-1)\pi}{(Q-1)\pi} \tag{2.200}$$

$$\lim_{Q\to 1} \frac{\sin(Q-1)\pi}{(Q-1)\pi} = 1 \tag{2.201}$$

For $Q \neq 1$,Q can take values 2,3 upto $2j+1$ in which case equation 2.200 becomes zero. Thus we find that the integral given by equation 2.199 behaves like a delta function. When Q is an operator it becomes an operator delta function.

therefore

$$Z = \text{Trace}[\int_{-\frac{\pi}{\beta}}^{\frac{\pi}{\beta}} \frac{\beta d\lambda}{2\pi} e^{-i\beta\lambda(Q-1)} e^{-\beta H}] \tag{2.202}$$

where H is given by equation 2.198

The restriction of the Trace operation to a subspace of the Hilbert space is affected by the operator delta function

$$Z = \int_{\frac{\pi}{\beta}}^{\frac{\pi}{\beta}} \frac{\beta d\lambda}{2\pi} e^{i\beta\lambda} \text{Trace}[e^{-\beta(H+i\lambda Q)}] \tag{2.203}$$

put

$$H + i\lambda Q = H(\lambda) \tag{2.204}$$

Since the Trace is now performed over the full Hilbert space of Fermi and Bose states,a relatively simple functional integral representation of the partition function is possible.

$$\begin{aligned} H(\lambda) &= \sum_{k,M} \epsilon_k c^\dagger_{kM} c_{kM} + (\epsilon_f + i\lambda) \sum_M f^\dagger_M f_M + i\lambda b^\dagger b \\ &+ V \sum_{k,M} (c^\dagger_{kM} f_M b^\dagger + b f^\dagger_M c_{kM}) \end{aligned} \tag{2.205}$$

Now Z becomes a functional integral over complex and Grassmann variables.

$$Z = \text{Trace}[e^{-\beta H(\lambda)}] = \int_{c,f,b} e^{-S} \tag{2.206}$$

where

$$\begin{aligned} S &= \sum_{l=1}^{N} [\bar{c}_l^{kM}(c_l^{kM} - c_{l-1}^{kM}) + \bar{f}_l^M(f_l^M - f_{l-1}^M) + +\bar{b}_l(b_l - b_{l-1})] \\ &+ \sum_{l=1}^{N} \Delta\tau[\epsilon_k \bar{c}_l^{kM} c_{l-1}^{kM} + (\epsilon_f + i\lambda)\bar{f}_l^M f_{l-1}^M + i\lambda \bar{b}_l b_{l-1}] \\ &+ \sum_{l=1}^{N} \Delta\tau V[\bar{b}_l \bar{c}_l{}^{kM} f_{l-1}^M + b_{l-1} \bar{f}_l^M c_{l-1}^{kM}] \end{aligned} \tag{2.207}$$

This form is inconvenient to manipulate because of the asymmetric time step indices in the interaction term. This may be remedied by the following transformation.

$$\begin{pmatrix} \bar{f}_l^M \\ f_l^M \end{pmatrix} \to \begin{pmatrix} \bar{f}_{l-1}^M \\ f_{l+1}^M \end{pmatrix} \tag{2.208}$$

The action becomes

$$\begin{aligned} S &= \bar{c}_l^{kM}(c_l^{kM} - c_{l-1}^{kM}) + \bar{f}_{l-1}^M(f_{l+1}^M - f_l^M) + \bar{b}_l(b_l - b_{l-1}) \\ &+ \Delta\tau[\epsilon_k \bar{c}_l^{kM} c_{l-1}^{kM} + (\epsilon_f + i\lambda)\bar{f}_l^M f_{l-1}^M + i\lambda \bar{b}_l b_{l-1} \\ &+ V(\bar{b}_l \bar{c}_l^{kM} f_l^M + b_l \bar{f}_l^M c_l^{kM})] \end{aligned} \tag{2.209}$$

where summation over l label is implied. After making a parameter rescaling $V \to \frac{V}{\sqrt{N}}$ and introducing Fourier transform of the Grassmann and complex variables.

$$Z = \int_{c,f,b} e^{-S} \tag{2.210}$$

$$\begin{aligned} S &= -\sum_n \Delta\tau e^{i\omega_n\Delta\tau} G_\Delta^{-1}(i\omega_n, \epsilon_k)\bar{c}_n^{kM} c_n^{kM} \\ &- \sum_n \Delta\tau e^{-i\omega_n\Delta\tau} G_\Delta^{-1}(i\omega_n, \epsilon_f + i\lambda)\bar{f}_n^M f_n^M \\ &- \sum_m \Delta\tau D_\Delta^{-1}(i\nu_m, i\lambda)\bar{b}_m b_m \\ &+ \Delta\tau\frac{V}{\sqrt{N}}\sum_{n,n'}(\bar{b}_{n-n'}\bar{c}_{n'}^{kM} f_n^M + b_{n-n'}\bar{f}_n^M c_{n'}^{kM}) \end{aligned} \tag{2.211}$$

$$G_\Delta^{-1}(i\omega_n, \epsilon_k) = -\frac{(e^{-i\omega_n\Delta\tau} - 1)}{\Delta\tau} - \epsilon_k \tag{2.212}$$

$$G_\Delta^{-1}(i\omega_n, \epsilon_f + i\lambda) = -\frac{(e^{-i\omega\Delta\tau} - 1}{\Delta\tau} - (\epsilon_f + i\lambda) \tag{2.213}$$

$$D_\Delta^{-1}(i\nu_m, i\lambda) = -\frac{(1 - e^{i\nu_m\Delta\tau})}{\Delta\tau} - i\lambda e^{i\nu_m\Delta\tau} \tag{2.214}$$

The last two terms in equation 2.211 contain Grassmann variables, which are not in the diagonal form. To bring them to the diagonal form we make variable transformations defined by

$$\bar{\gamma}_n^{kM} = \bar{c}_n^{kM} - \frac{V}{\sqrt{N}} e^{-i\omega_n\Delta\tau} G_\Delta(i\omega_n, \epsilon_k)\sum_{n'} b_{n'-n}\bar{f}_{n'}^M \tag{2.215}$$

$$\gamma_n^{kM} = c_n^{kM} - \frac{V}{\sqrt{N}} e^{-i\omega_n\Delta\tau} G_\Delta(i\omega_n, \epsilon_k)\sum_{n'} \bar{b}_{n'-n} f_{n'}^M \tag{2.216}$$

The partition function is given by

$$Z = \int_{-\frac{\pi}{\beta}}^{\frac{\pi}{\beta}} d\lambda \int_{\gamma,f,b} e^{-S} \tag{2.217}$$

where S is given by

$$\begin{aligned} S &= -\Delta\tau\sum_n e^{i\omega_n\Delta\tau} G_\Delta^{-1}(i\omega_n, \epsilon_k)\bar{\gamma}_n^{kM}\gamma_n^{kM} \\ &- \Delta\tau\sum_n e^{-i\omega_n\Delta\tau} G_\Delta^{-1}(i\omega_n, \epsilon_f + i\lambda)\bar{f}_n^M f_n^M \\ &+ \Delta\tau\frac{V^2}{N}\sum_{n,n',n''} e^{-i\omega_{n'}\Delta\tau} G_\Delta(i\omega_{n'}, \epsilon_k)\bar{b}_{n''-n'} b_{n-n'}\bar{f}_n^M f_{n''}^M \\ &- \Delta\tau\sum_m \bar{b}_m b_m D_\Delta^{-1}(i\nu_m, i\lambda) \end{aligned} \tag{2.218}$$

Doing the integration over γ and f Grassmann variables

$$\frac{Z}{Z_{band}} = \int_{-\frac{\pi}{\beta}}^{\frac{\pi}{\beta}} \frac{\beta d\lambda}{2\pi} e^{i\beta\lambda}(1 + e^{-\beta(\epsilon_f + i\lambda)})^N \int_b e^{-S} \tag{2.219}$$

where

$$S = -N\text{Trace}\left(\ln[I - V^2 \sum_k G(\epsilon_k + i\lambda) X G(\epsilon_k) X^\dagger]\right) - \beta \sum_m \bar{b}_m b_m D_0^{-1}(i\nu_m, i\lambda) \tag{2.220}$$

$$G(\epsilon_k)_{nn'} \equiv G_k(i\omega_n)\delta_{nn'} = \frac{\delta_{nn'}}{(i\omega_n - \epsilon_k)} \tag{2.221}$$

$$G(\epsilon_f + i\lambda)_{nn'} \equiv G_f^\lambda(i\omega_n)\delta_{nn'} = \frac{\delta_{nn'}}{(i\omega_n - \epsilon_f - i\lambda)} \tag{2.222}$$

$$D_0(i\nu_m, i\lambda) \equiv D_0^\lambda(i\nu_m) = \frac{1}{i\nu_m - i\lambda} \tag{2.223}$$

$$X_{nn'} = b_{n-n'} \tag{2.224}$$

$$\int_b \equiv \int \prod_m d\bar{b}_m db_m = \int \prod_m \frac{d(\text{Re}b_m) d(\text{Im}b_m)}{\pi} \tag{2.225}$$

where ω_n and ν_m are the Fermi and Bose Matsubara frequencies. In equation 2.223 the Bose propagator is written with subscript 0. We reserve the notation D^λ for the dressed Bose propagator.

Now let us derive the expression for $Z^{(1)}$ and $Z^{\frac{1}{N}}$. The quantity NV^2 is to be treated as a constant of $O(1)$. To obtain terms of order $O(1)$, we retain terms of order $\bar{b}_m b_m$in the action S.

Terms of quartic and higher order,which follow from the expansion of the logarithm enter with coef. of $O(\frac{1}{N^l})$ where $l \geq 1$. Thus $S^{(1)}$ becomes

$$S^{(1)} = -\beta \sum_m \mid b_m \mid^2 \left(D_0^{-1}(i\nu_m, i\lambda) - \Pi^\lambda(i\nu_m)\right) \tag{2.226}$$

where $\Pi^\lambda(i\nu_m)$ can be obtained by expanding the logarithm to the lowest order and then explicitly writing out the frequency trace.Expanding the logarithm term in equation 2.220

$$- NV^2 \sum_k G(\epsilon_f + i\lambda) X G(\epsilon_k) X^\dagger \tag{2.227}$$

$$\sum_m \beta \frac{NV^2}{\beta} \sum_{k.n} G_f^\lambda(i\omega_n + \nu_n)) G_k(i\omega_n) b_m \bar{b}_m \tag{2.228}$$

Combining equation 2.223 with the term

$$- \beta \sum_m \mid b_m \mid^2 D_(0)^{-1}(i\nu_m, i\lambda) \tag{2.229}$$

$$S^{(1)} = -\beta \sum_m [D_0^{-1}(i\nu_m, i\lambda) - \Pi^\lambda(i\nu_m)] \mid b_m \mid^2 \tag{2.230}$$

where

$$\Pi^\lambda(i\nu_m) = \frac{NV^2}{\beta} \sum_{k,n} G_f^\lambda(i(\omega_n + \nu_m)) G_k(i\omega_n) \tag{2.231}$$

On performing frequency sum in equation 2.231 using contour integral technique the right hand side becomes

$$\Pi^\lambda(i\nu_m) = NV^2 \sum_k \frac{(f(\epsilon_k) - f(\epsilon_f + i\lambda))}{(i\nu_m - i\lambda)} \tag{2.232}$$

where$f(\epsilon_k)$and $f(\epsilon_f + i\lambda)$ are fermi functions.When Gaussian integrals over the fluctuating complex variables $b(\nu_m)$ are performed at this order of approximation, we get

$$\int_b e^{-S^{(1)}} = \exp[-\sum_m \ln \beta(i\nu_m - i\lambda)] \exp[-\sum_m \ln(1 - \Pi^\lambda(i\nu_m) D_0^\lambda)] \tag{2.233}$$

The sum $\sum_m \ln(i\nu_m - i\lambda\beta)$ can be written as a frequency sum.

$$\frac{1}{2\pi i} \int_c \frac{dz \ln(z - i\lambda\beta)}{(e^z - 1)} \tag{2.234}$$

Making a coordinate shift, we get expression 2.234 as

$$\frac{1}{2\pi i} \oint_c \frac{dz \ln z}{e^{i\beta\lambda + z} - 1)} \tag{2.235}$$

Here the contour is taken as shown in figure (2.8.1)

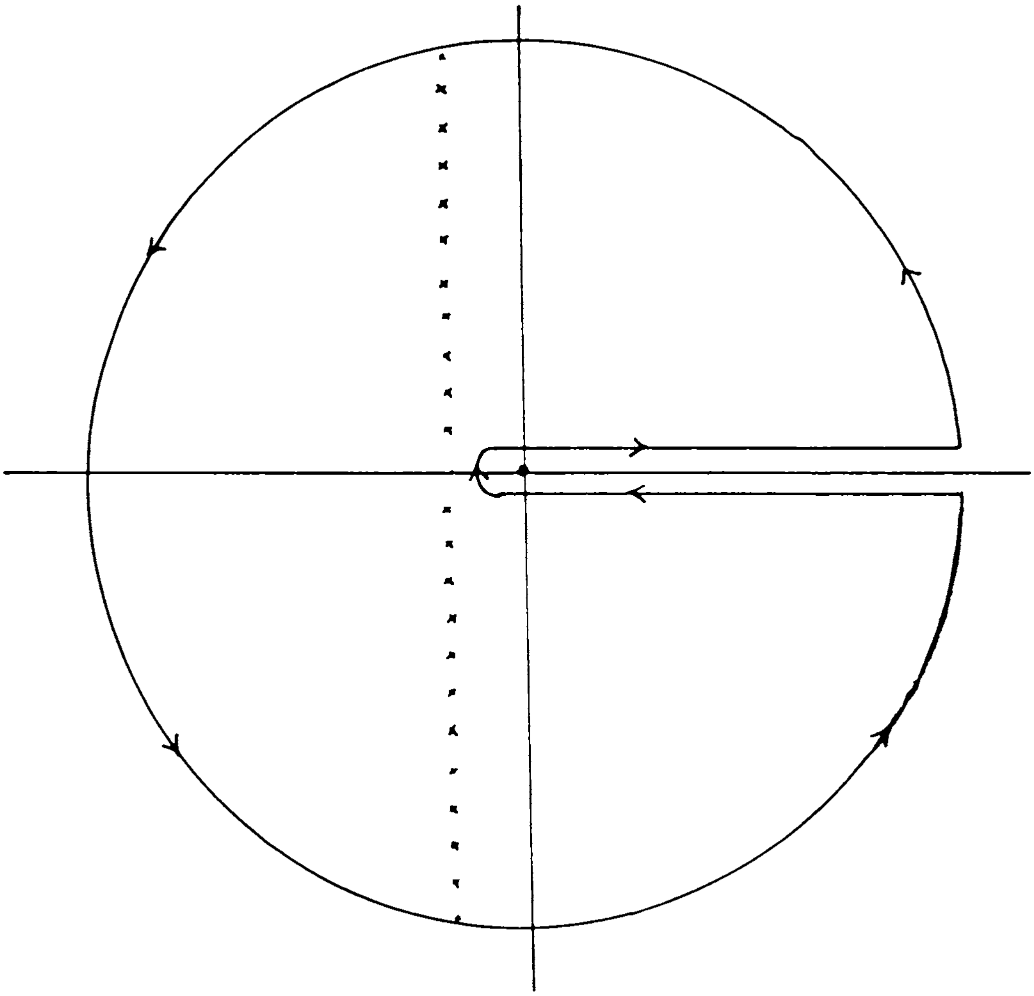


fig (2.8. 1)

Going over to polar coordinates, after simplification the contribution from the contour parallel to the X-axis in the integral in equation 2.235 becomes

$$\int_0^\infty -\frac{dx}{(e^{x+i\lambda\beta}+1)} \tag{2.236}$$

When the integration is performed

$$-\ln(e^{i\lambda\beta}-e^{-x})\,|_0^\infty = -\ln(e^{i\lambda\beta})+\ln(e^{i\lambda\beta}-1)=\ln(1-e^{-i\lambda\beta}) \tag{2.237}$$

Along the arc the contribution to the integral is vanishingly small.

Thus we get equation 2.233as

$$\int_b e^{-S^{(1)}} = (1-e^{-i\lambda\beta})^{-1}\exp\{-\sum_m \ln[1-D_0^\lambda(i\nu_m)\Pi^\lambda(i\nu_m)]\} \tag{2.238}$$

The sum over the discrete variable m in equation 2.238 may be transformed to an integral over the contour Γ_1 surrounding the imaginary axis in figures (2.8.2a, 2.8.2b, 2.8.2c)

The frequency sum

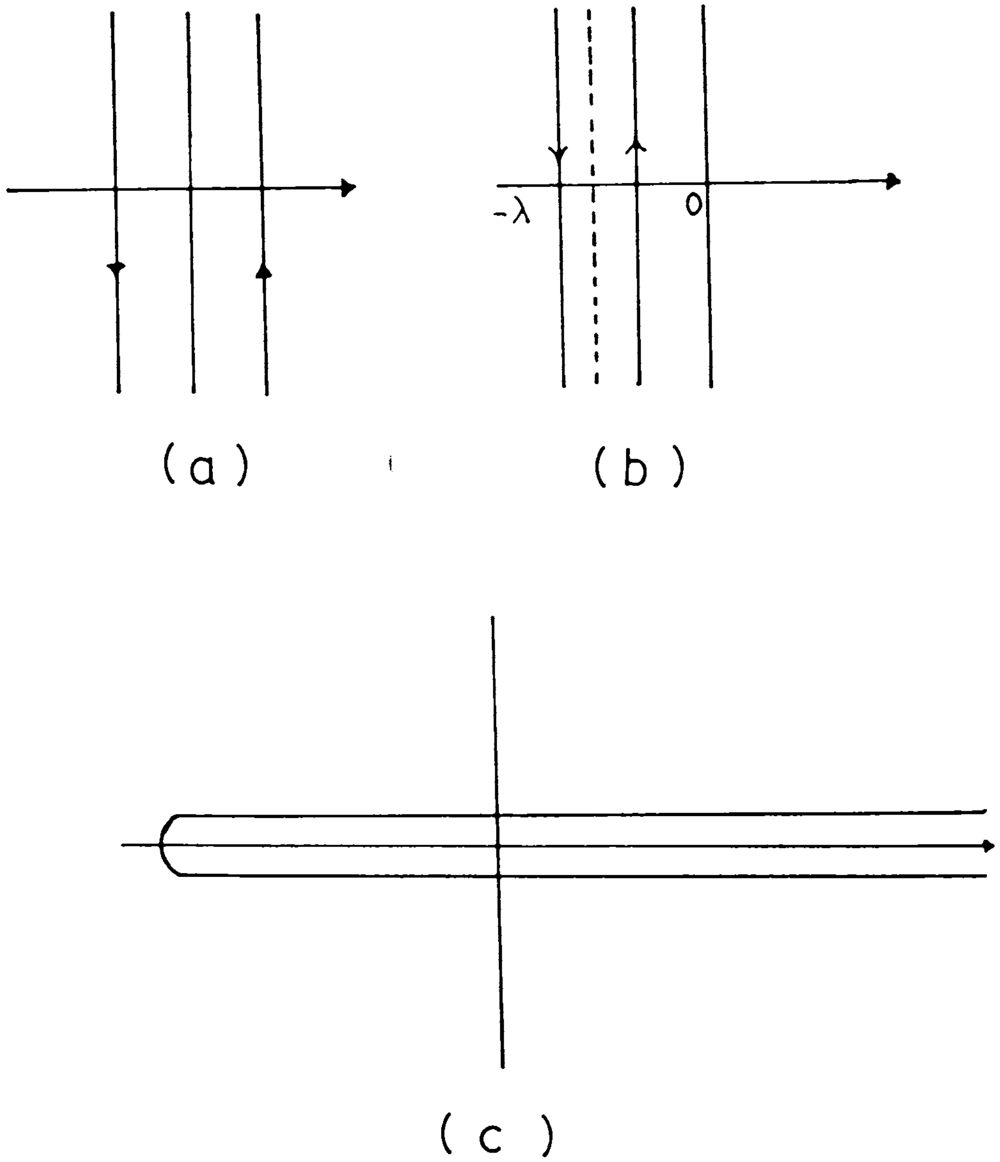
$$\sum_m \ln[1-D_0^\lambda(i\nu_m)\Pi^\lambda(i\nu_m)]$$

can be found by considering a contour integral.

$$\beta\int\frac{dz}{2\pi i}b(z)\ln(1-D_0^\lambda(z)\Pi^\lambda(z)) \tag{2.239}$$

According to Cauchy's residue theorem this integral should be equal to $2\pi i$ times the sum of the residues at the poles of the Bose function $b(z)$. This contour should not enclose the poles or branch cuts of the function $\ln[1-D_0^\lambda(z)\pi^\lambda(z)]$. The quantity which is $2\pi i$ times the sum of the residues will be giving the frequency sum. One should do this contour integration carefully. As λ is a real variable, the principal branch of the logarithm has a cut along the line $\mathrm{Im}(z)=\lambda$ with branch point at $E_0+i\lambda$, and $E_0<0$. The contour of integration Γ_1 must not cross this cut. The technical difficulty is overcome by shifting λ integration to the complex plane $\lambda\rightarrow\lambda-i\lambda_0$ with constant λ_0. With the shift in λ, the branch point in the logarithm is displaced to $(E_0+\lambda_0)+i\lambda$. By choosing $E_0+\lambda_0>0$, the cut may be located entirely to the right half plane. Then the step in equation 2.239 is allowed.

We change the integration variable by transforming to $z\rightarrow z+i\lambda$.



(a) (b)

(c)

fig(2.8.2)

a. Contour of integration Γ_1 for performing the Bose frequence sums in equation 2.239

b. Contour of integration Γ_2 after the variable shift has been made. $z \longrightarrow z+i\lambda$ with $\lambda_0 = \mathrm{Im}(\lambda)$. The quantity λ_0 may be choosen sufficiently negative to ensure that Γ_2 lies entirely to the left of the singularities of equation 2.240 .

c. Contour of integration encircling the singularities of the logarithm in a counter clockwise fashion.

Thus equation 2.239 becomes

$$\sum_m \ln[1 - D_0^\lambda(i\nu_m)\Pi^\lambda(i\nu_m)] = \beta\int_{\Gamma_2}\frac{dz}{2\pi i}b(z+i\lambda)\ln[1-\frac{\bar{\Pi}^\lambda(z)}{z}] \tag{2.240}$$

where

$$\bar{\Pi}^\lambda(z) \equiv NV^2\sum_k\frac{f(\epsilon_k)-f(\epsilon_f+i\lambda)}{z+\epsilon_k-\epsilon_f} \tag{2.241}$$

and Γ_2 as in figure (2.8.2b)

The Bose and Fermi functions can be approximated as follows.

$$\begin{aligned} b(z+i\lambda) &= e^{-\beta(z+i\lambda)} + 0(e^{-2i\beta\lambda}) \\ f(\epsilon_f+i\lambda) &= e^{-\beta(\epsilon_f+i\lambda)} + 0(e^{-2i\beta\lambda}) \end{aligned} \tag{2.242}$$

The expansion of the Bose and Fermi functions within the λ integral may be simply justified. The expansion in equation 2.242 are uniformly convergent for $\mathrm{Re}\lambda \in [-\frac{\pi}{\beta}, \frac{\pi}{\beta}]$. Equation 2.240 can be written as

$$\sum_m \ln[1 - D_0^\lambda(i\nu_m)\Pi^\lambda(i\nu_m)] = \beta e^{-i\beta\lambda}\int_{\Gamma_1}\frac{dz}{2\pi i}e^{-\beta z}\ln[1-\frac{\Sigma_0^{(1)}(z)}{z}] + O(e^{-2i\beta\lambda}) \tag{2.243}$$

where

$$\Sigma_0^{(1)}(z) \equiv NV^2\frac{f_k}{z+\epsilon_k-\epsilon_f} \tag{2.244}$$

When the contour is distorted in figure(2.8.2c) the right hand side of equation 2.243 becomes

$$-\beta e^{-i\beta\lambda}\int_\Gamma\frac{dz}{2\pi i}e^{-\beta z}\ln[1-\frac{\Sigma_0^{(1)}(z)}{z}] + O(e^{-2i\beta\lambda}) \tag{2.245}$$

Using equation2.245 the $O(1)$ partition function becomes

$$\begin{aligned} Z^{(1)} &= \int_{-\frac{\pi}{\beta}}^{\frac{\pi}{\beta}}\frac{\beta d\lambda}{2\pi}e^{i\beta\lambda}(1+e^{-\beta(\epsilon_f+i\lambda)})^N\frac{1}{(1-e^{-i\beta\lambda})} \\ &\quad . \left(1+\beta e^{-i\beta\lambda}\int_\Gamma\frac{dz}{2\pi i}e^{-\beta z}\ln[1-\frac{\Sigma_0^{(1)}(z)}{z}] + O(e^{-2i\lambda\beta})\right) \end{aligned} \tag{2.246}$$

The first term in equation 2.246 becomes

$$e^{i\beta\lambda}\frac{[1+e^{-\beta(\epsilon_f+i\lambda)}]^N}{(1-e^{-i\beta\lambda})} \approx e^{i\beta\lambda}\frac{(1+Ne^{-\beta(\epsilon_f+i\lambda)}+O(e^{-2i\lambda\beta})}{(1-e^{-i\beta\lambda})} \tag{2.247}$$

$$= \frac{e^{i\beta\lambda}+Ne^{-\beta\epsilon_f}}{(1-e^{-i\beta\lambda})} \tag{2.248}$$

$$\approx (e^{i\beta\lambda}+Ne^{-\beta\epsilon_f})(1+e^{-i\beta\lambda}+e^{-2i\beta\lambda}+\ldots)$$

$$= (1+Ne^{-\beta\epsilon_f})+e^{i\beta\lambda}+e^{-i\beta\lambda}(1+Ne^{-\beta\epsilon_f})+O(e^{-2i\beta\lambda}) \tag{2.249}$$

On performing integration with respect to λ, the first term in equation 2.249 becomes $(1 + Ne^{-\beta\epsilon_f})$. On integration with respect to λ, the second and third terms vanishes. Thus equation 2.246 becomes

$$Z^{(1)} = (Ne^{-\beta\epsilon_f} + 1) + \beta \int_\Gamma \frac{dz}{2\pi i} e^{-\beta z} \ln[1 - \frac{\Sigma_0^{(1)}(z)}{z}] \tag{2.250}$$

Integrating by parts on z in equation 2.250,

$$Z^{(1)} = Ne^{-\beta\epsilon_f} + \int_\Gamma \frac{dz}{2\pi i} e^{-\beta z} \frac{(1 - \frac{\partial\Sigma_0^{(1)}(z)}{\partial z})}{(z - \Sigma_0^{(1)}(z))} \tag{2.251}$$

In a similar way but with more involved calculations we could obtain the $O(\frac{1}{N})$ correction to the partition function. The additional term appearing in the action at $O(\frac{1}{N})$ is the second order term in the expansion of the logarithm in equation 2.220

$$S^{(\frac{1}{N})} = \frac{1}{2}\frac{(NV^2)^2}{N} \sum_{k,k'} \mathrm{Tr} G(\epsilon_f + i\lambda) X G(\epsilon_k) X^\dagger G(\epsilon_f + i\lambda) X G(\epsilon_{k'}) X^\dagger \tag{2.252}$$

The partition function to $O(\frac{1}{N})$becomes

$$\begin{aligned} Z &= Z^{(1)} + Z^{(\frac{1}{N})} \\ &= Z^{(1)} + \int_{-\frac{\pi}{\beta}}^{\frac{\pi}{\beta}} \frac{\beta d\lambda}{2\pi} e^{i\beta\lambda} (1 + e^{-\beta(\epsilon_f + i\lambda)})^N \int_b (-S^{\frac{1}{N}}) e^{-S^1} \end{aligned} \tag{2.253}$$

By evaluating the functional integral over b and then performingλ integration the partition function can be evaluated to $O(\frac{1}{N})$.

2.10 General slave Boson techniques

In several problems in condensed matter physics, basic Hamiltonians which describes charge/spin dynamics contain very strong interaction terms so that they cannot be treated within the framework of conventional manybody techniques. The systems of this class are found to exhibit strongly correlated behaviour. For studying these systems slave boson techniques are used. The slave boson technique we have already discussed in section 2.8 has the disadvantage that the auxiliary bosons introduced to take care of the constraints do not carry spin. Spin correlations appear only as a second order process in this formulation. Another method which is used in spin models is called Schwinger boson[27] model. This has the disadvantage that the charge dynamics appear as a second order process. The disadvantage of the above two models can be avoided by adopting a new slave boson technique introduced by Kotliar and Ruckentein[28]. The following are the important features of this technique.

1) A strongly correlated site can be in any of the four states empty, singly occupied with spin up, singly occupied with spin down and doubly occupied. Each of these states is represented by four different slave bosons.

2) A spin doublet of fermion fields to the singly occupied sites.

The results of the calculation based on such a representation leads to results identical to the Gutzwiller approximation in meanfield theory for the Hubbard model [29,30]. It could also predict a metal insulator transition at half filling. One disadvantage of the Kotliar Ruckenstein scheme is that the representation is not manifestly spin rotation invariant. A spin rotation invariant reformulation has been performed by Li et al. [31].

In this section we will discuss the spin rotation invariant representation of the Hubbard model. In the original idea put forward by Kotliar and Ruckenstein, two pseudofermions $f_\uparrow, f_\downarrow$ and two slave bosons e and d for empty and doubly occupied sites and two bosons $p_\uparrow$ and $p_\downarrow$ for the two singly occupied sites are introduced to describe the system.

$$\begin{aligned} \mid 0 > &= e^\dagger \mid \text{vacuum} > \\ \mid \sigma > &= P^\dagger_\sigma f^\dagger_\sigma \mid \text{vacuum} > \\ \mid\uparrow\downarrow> &= d^\dagger f^\dagger_\uparrow f^\dagger_\downarrow \mid \text{vacuum} > \end{aligned} \tag{2.254}$$

The representation of the state $\mid \sigma >$ is not spin rotation invariant, but depends on the choice of the spin quantization axis in the spin space. In order to recover the two degrees of freedom associated with the spin quantization axis in $\mid \sigma >$ the operator product $P^\dagger_\sigma f^\dagger_\sigma$ in equation2.254 is considered as creating a composite particle, whose spin is 1/2. This is the restriction on the spin of the composite particle. The spin of the pseudofermion (f), the two component spinor field should be $\frac{1}{2}$. Therefore the only possible spin values for the p-bosons are $S = 0$ and $S = 1$. Therefore we define a scalar field ($S = 0$) represented by p_0 and a vector ($S = 1$) field $p = (p_x, p_y, p_z)$, where p_x, p_y and p_z are cartesian components.

We may define angular momentum eigen states

$$p_{1,1} = -\frac{1}{\sqrt{2}}(p_x + ip_y), p_{1,-1} = \frac{1}{\sqrt{2}}(p_x - ip_y), p_{1,0} = p_z \tag{2.255}$$

Both p_0, p_x, p_y, p_z and $p_{1,m}$ satisfy canonical Bose commutation relations.

The coupling of bosons with spin $S = 1$ and pseudofermions with $S = \frac{1}{2}$ giving a total spin $\frac{1}{2}$ is given by

$$\mid \sigma >_{S=1} = \sum_{\sigma' = \pm} C(j_1 = 1, j_2 = \frac{1}{2}; m_1 = \sigma - \sigma', m_2 = \sigma' \mid j = \frac{1}{2}; \sigma) p^{\dagger}_{1m_1} f^{\dagger}_{\sigma'} \mid \text{vac} > \tag{2.256}$$

with the Clebsch Gordon coefficient

$$C(1, \frac{1}{2}; m \pm \frac{1}{2}, \pm \frac{1}{2} \mid \frac{1}{2}, m) = \mp \sqrt{\frac{3 \mp 2m}{6}} \tag{2.257}$$

When the component in which bosons with $S = 0$ and pseudofermion having spin $\frac{1}{2}$ is also included, the state $\mid \sigma >$ can be represented as

$$\mid \sigma > = \sum_{\sigma'} p^{\dagger}_{\sigma,\sigma'} f^{\dagger}_{\sigma'} \mid \text{vac.} > \tag{2.258}$$

where

$$p^{\dagger}_{\sigma,\sigma'} = \begin{pmatrix} ap^{\dagger}_0 + bp^{\dagger}_z & b(p^{\dagger}_x - ip^{\dagger}_y) \\ b(p^{\dagger}_x + ip^{\dagger}_y) & ap^{\dagger}_o - bp^{\dagger}_z \end{pmatrix} \tag{2.259}$$

Orthonormalization of the states $\mid \sigma >$ yields

$$a^2 + 3b^2 = 1 \tag{2.260}$$

The ratio $\frac{a}{b}$ is not determined and may be considered as a free parameter. Choosing $a = b$

$$p^{\dagger}_{\sigma,\sigma'} = \frac{1}{2} \sum_{\mu=0}^{3} p^{\dagger}_{\mu} \tau_{\mu\sigma\sigma'} \tag{2.261}$$

Where τ_μ are the Pauli matrices, including the unit matrix τ_0. The Hermitian conjugate operator is

$$p_{\sigma\sigma'} = \frac{1}{2} \sum_{\mu=0}^{3} p_{\mu} \tau_{\mu,\sigma,\sigma'} \tag{2.262}$$

The matrix elements of the two matrix operators satisfy the commutation relation

$$[p_{\sigma_1\sigma_2}, p^\dagger_{\sigma_3\sigma_4}] = \frac{1}{2}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3} \tag{2.263}$$

In terms of $p_{\sigma\sigma'}, e, d$ and f_σ the electron operators may be expressed as

$$\begin{aligned} C^\dagger_\sigma &= \sum_{\sigma'}(p^\dagger_{\sigma\sigma'} f^\dagger_{\sigma'} e + \sigma\sigma' d^\dagger f^\dagger_{\sigma'} p_{-\sigma',-\sigma}) \\ C_\sigma &= \sum_{\sigma'}(e^\dagger f_{\sigma'} p_{\sigma'\sigma} + \sigma\sigma' p^\dagger_{-\sigma,-\sigma'} f_{\sigma'} d) \end{aligned} \tag{2.264}$$

The terms involving the operator d may be expressed using the transformation properties of the Bose operators under time reversal operation $\hat{T}$.

$$\tilde{p}_0 \equiv \hat{T} p_0 \hat{T}^{-1} = p_0 \tag{2.265}$$

$$\tilde{p} \equiv \hat{T} p \hat{T}^{-1} = -p \tag{2.266}$$

These simply

$$\tilde{p}_{\sigma\sigma'} = (\hat{T} p \hat{T}^{-1}_{\sigma\sigma'} = \sigma\sigma' p_{-\sigma',-\sigma} \tag{2.267}$$

It follows that

$$C^\dagger_\sigma = \sum_{\sigma'} Z^\dagger_{\sigma\sigma'} f^\dagger_{\sigma'} \tag{2.268}$$

$$C_\sigma = \sum_{\sigma'} f_{\sigma'} Z_{\sigma'\sigma} \tag{2.269}$$

with

$$Z_{\sigma'\sigma} = e^\dagger p_{\sigma'\sigma} + \tilde{p}^\dagger_{\sigma'\sigma} d \tag{2.270}$$

When the commutation relations for p operators in equation 2.263 and the canonical anticommutation relation for pseudofermion operators are used we get the correct anticommutation relations for the original fermi operators $(C, C^\dagger)$, provided the following constraints are satisfied.

$$e^\dagger e + d^\dagger d + \sum_\mu p^\dagger_\mu p_\mu = 1 \tag{2.271}$$

A second set of constraints follow from the fact that the matrix elements of $f^\dagger_{\sigma'} f_\sigma$ are related to those of $p^\dagger p$ and $d^\dagger d$ in the physical subspace.

$$f^\dagger_{\sigma'} f_\sigma = 2\sum_{\sigma_1} p^\dagger_{\sigma_1\sigma} p_{\sigma',\sigma_1} + \delta_{\sigma\sigma'} d^\dagger d \tag{2.272}$$

In terms of the p_μ's the constraints in equation 2.272 can be written as

$$\sum_\sigma f_\sigma^\dagger f_\sigma = \sum_{\mu=0}^{3} p_\mu^\dagger p_\mu + 2d^\dagger d. \tag{2.273}$$

$$\sum_{\sigma\sigma'} \vec{\tau}_{\sigma\sigma'} f_{\sigma'}^\dagger f_\sigma = p_0^\dagger \wp + \wp^\dagger p_0 - i\wp^\dagger \times \wp \tag{2.274}$$

The above discussion summarizes the strategy of the manifestly spin rotation invariant slave boson treatment. More details regarding this can be had in the references[32,33].

2.11 BCS Model studied using functional technique

In this section we derive the partition function and hence the energy gap for the BCS superconductor using functional integral technique.

The BCS reduced Hamiltonian has the form

$$H = \sum_{k,\sigma} \epsilon_{k\sigma} C_{k,\sigma}^\dagger C_{k\sigma} - \frac{1}{2} g \sum_{k,k',\sigma} C_{k',\sigma}^\dagger C_{-k',-\sigma}^\dagger C_{-k,-\sigma} C_{k,\sigma} \tag{2.275}$$

k stands for wave number. g is the electron (quasiparticle) - electron attractive interaction strength. This is assured to be positive.

The partition function can be set up as a functional integral over Grassmann variables.

$$\begin{aligned} Z &= \mathrm{Tr}[e^{-\beta H}] & (2.276)\\ &= \int_c e^{-S} & (2.277) \end{aligned}$$

where

$$\int_c \equiv \lim_{N\to\infty} \prod_{k,\sigma} (-1)^N \prod_{l=1}^{N} d\bar{c}_l^{k\sigma} dc_l^{k\sigma} \tag{2.278}$$

and

$$S = \bar{C}_l^{k\sigma}(C_{l+1}^{k\sigma} - C_l^{k\sigma}) + \Delta\tau(\epsilon_k \bar{c}_l^{k\sigma} C_l^{k\sigma} - g\bar{b}_l b_l) \tag{2.279}$$

where

$$\bar{b}_l = \bar{c}_l^{k\uparrow} \bar{c}_l^{-k\downarrow} \tag{2.280}$$

$$b_l = C_l^{-k\downarrow} C_l^{k\uparrow} \tag{2.281}$$

and

$$\Delta\tau = \frac{\beta}{N} \tag{2.282}$$

The two body interaction term can be written as two one body terms using the Stratanovich Hubbard transformation[1,2,3]. The idea is that when we have two arbitrary commuting variables $\bar{X}$ and Y we can write $e^{\alpha\bar{X}Y}$ as an integral.

$$e^{\alpha\bar{X}Y} = \int d\bar{\xi}d\xi \exp[-\beta \mid \xi \mid^2 - \sqrt{\alpha\beta}\xi\bar{X} - \sqrt{\alpha\beta}\bar{\xi}Y] \tag{2.283}$$

where

$$d\bar{\xi}d\xi = \frac{\beta}{\pi}d(\mathrm{Re}\xi)d(\mathrm{Im}\xi) \tag{2.284}$$

Applying this to equation 2.279 $\alpha = g\Delta\tau, \bar{X} = \bar{b}_l$ and $Y = b_l$, the partition function can be written as

$$Z = \int_{c\xi} e^{-S(c,\xi)} \tag{2.285}$$

with

$$\begin{aligned} S(c,\xi) &= \bar{c}_l^{k\sigma}(c_{l+1}^{k\sigma} - c_l^{k\sigma}) + \Delta\tau\epsilon_k\bar{c}_l^{k\sigma}c_l^{k\sigma} + \beta\bar{\xi}_l\xi_l \\ &+ \sqrt{g\beta\Delta\tau}(\xi_l\bar{b}_l + \bar{\xi}_l b_l) \end{aligned} \tag{2.286}$$

with

$$(D\bar{\xi}D\xi)^N = \prod_{l=1}^{N}\frac{\beta}{\pi}d(\mathrm{Re}\xi_l)d(\mathrm{lm}\xi_l) \tag{2.287}$$

Fourier transforming all variables in equation 2.286

$$Z = \int_{c\xi} e^{-S} \tag{2.288}$$

where

$$\begin{aligned} S &= -\Delta\tau\bar{c}_n^{k\sigma}G_{\Delta}^{-1}(i\omega_n, \epsilon_k)C_n^{k\sigma} + \beta\bar{\xi}_m\xi_m \\ &+ \Delta\tau\sqrt{g}(\xi_m\bar{c}_n^{k\uparrow}\bar{c}_{m-n}^{-k\downarrow} + \bar{\xi}_m C_n^{-k\downarrow}C_{m-n}^{k\uparrow} \end{aligned} \tag{2.289}$$

where

$$G_{\Delta}^{-1}(i\omega_n, \epsilon_k) = -\frac{(e^{-i\omega_n\Delta\tau} - 1)}{\Delta\tau} - \epsilon_k \tag{2.290}$$

The following variable transformations are made in the Grassmann variables.

$$\bar{f}_n^{k\uparrow} = \bar{c}_n^{k\uparrow} - G_{\Delta}(i\omega_n, \epsilon_k)\sqrt{g}\bar{\xi}_m C_{m-n}^{-k\downarrow} \tag{2.291}$$

$$f_n^{k\uparrow} = c_n^{k\uparrow} - G_\Delta(i\omega_n, \epsilon_k)\sqrt{g}\bar{\xi}_m \bar{c}_{m-n}^{-k\downarrow} \tag{2.292}$$

$$\bar{f}_n^{k\downarrow} = \bar{c}_n^{k\downarrow} \tag{2.293}$$

$$f_n^{k\downarrow} = c_n^{k\downarrow} \tag{2.294}$$

The Jacobian of this transformation is unity. Thus

$$Z = \int_{f,\xi} e^{-S} \tag{2.295}$$

where

$$\begin{aligned} S &= -\Delta\tau \bar{f}_n^{k\sigma} G_\Delta^{-1}(i\omega_n, \epsilon_k) f_n^{k\sigma} + \beta\bar{\xi}_m\xi_m \\ &+ g\Delta\tau G_\Delta(i\omega_n, \epsilon_k)\xi_m\bar{\xi}_{m'} f_{m'-n}^{-k\downarrow}\bar{f}_{m-n}^{-k\downarrow} \end{aligned} \tag{2.296}$$

After performing the $(\bar{f}^{k\uparrow}, f^{k\uparrow})$ integrals, one finds

$$Z = Z_0^{\uparrow}\int_{f^{\downarrow},\xi} e^{-S_{\downarrow}} \tag{2.297}$$

with

$$S^{\downarrow} = \beta\bar{\xi}_m\xi_m - \Delta\tau\bar{f}_n^{k\downarrow}[G_\Delta^{-1}(\epsilon_k)_{nn'} + M_\Delta(\epsilon_k)_{nn'}]f_{n'}^{k\downarrow} \tag{2.298}$$

and

$$\begin{aligned} Z_0^{\uparrow} &= \prod_k \lim_{N\to\infty}\prod_n [e^{-i\omega_n\Delta\tau} - 1 + \epsilon_k\Delta\tau] \\ &= \prod_k (1 + e^{-\beta\epsilon_k}) \end{aligned} \tag{2.299}$$

and

$$G_\Delta^{-1}(\epsilon_k)_{nn'} = G_\Delta^{-1}(i\omega_n, \epsilon_k)\delta_{nn'} \tag{2.300}$$

$$M_\Delta(\epsilon_k)_{nn'} = g\xi_{n-n''}G_\Delta(-i\omega_{n''}, \epsilon_k)\bar{\xi}_{n'-n''} \tag{2.301}$$

The fact that $\epsilon_k = \epsilon_{-k}$ has been used to simplify the expression for M.

For a more concise notation, we redefine the complex variables as matrices

$$X_{nn'} = \xi_{n-n'} \tag{2.302}$$

$$(X^\dagger)_{nn'} = \bar{\xi}_{n'-n} \tag{2.303}$$

so that

$$M_\Delta(\epsilon_k)_{nn'} = g[XG_\Delta^{\dagger}(\epsilon_k)X^\dagger]_{nn'} \tag{2.304}$$

On performing the $\bar{f}^{k\downarrow}, f^{k,\downarrow}$ integrals we get

$$\begin{aligned} Z &= Z_0 \int_\xi \prod_k \det[1 + G_\Delta(\epsilon_k, M_\Delta(\epsilon_k)] \exp[-\beta \bar{\xi}_m \xi_m] \\ &= Z_0 \int_\xi \exp\{-\beta \bar{\xi}_m \xi_m + \sum_k \mathrm{Tr} \ln[1 + G_\Delta(\epsilon_k) M_\Delta(\epsilon_k]]\} \end{aligned} \tag{2.305}$$

with

$$Z_0 = \prod_k (1 + e^{-\beta\epsilon_k})^2 \tag{2.306}$$

$\{G_\Delta(\epsilon_k) M_\Delta(\epsilon_k)\}$ is written as

$$G_\Delta(\epsilon_k) M_\Delta(\epsilon_k) = g G(\epsilon_k) X G^\dagger(\epsilon_k) X^\dagger \tag{2.307}$$

with the new frequency space matrix (the $\Delta\tau \to 0$ limit ofG_Δ)

$$\begin{aligned} \lim_{\Delta\tau \to 0} G_\Delta(i\omega_n, \epsilon_k) &= \lim_{\Delta\tau \to 0} - \frac{\Delta\tau}{e^{-i\omega_n \Delta\tau} - 1 + \epsilon_k \Delta\tau} \\ &= \frac{1}{i\omega_n - \epsilon_k} \end{aligned} \tag{2.308}$$

ie.,

$$G_\Delta(\epsilon_k)_{nn'} = \frac{1}{(i\omega_n - \epsilon_k)} \delta_{nn'} \tag{2.309}$$

The partition function for the BCS model becomes

$$\frac{Z}{Z_0} = \int \prod_{m=-\infty}^{\infty} d\bar{\xi}_m d\xi_m e^{-\beta \sum_m |\xi(\nu_m)|^2 + \sum_k \mathrm{Tr} \ln\{I + gG(\epsilon_k) X G^\dagger(\epsilon_k) X^\dagger\}} \tag{2.310}$$

In the static approximation, only contribution from the zero frequency component of the auxiliary field ξ is considered.

$$\frac{Z}{Z_0} = Z_{\mathrm{stat}} Z_F \tag{2.311}$$

where

$$Z_{\mathrm{stat}} = \int d\bar{\xi} d\xi e^{-\beta|\xi|^2 + \sum_{k,n} \ln(1 + \frac{g|\xi|^2}{\omega_n^2 + \epsilon_k^2})} \tag{2.312}$$

where Z_F is the fluctuation contribution.

The integral in equation 2.312 can be evaluated by a saddle point approximation. The saddle point value of this pairing field will give us an expression for the zero temperature energy gap. Taking derivative with respect to ξ in the quantity appearing in the exponent in equation 2.312, we get

$$-\beta\xi + \sum_{k,n} \frac{g\xi}{\omega_n^2 + \epsilon_k^2 + g \mid \xi \mid^2)} = 0 \tag{2.313}$$

Doing the Fermi frequency sum in the above equation using contour integral technique we arrive at the equation.

$$\frac{g}{2} \sum_k \frac{1}{\sqrt{\epsilon_k^2 + g\xi^2}} = 1 \tag{2.314}$$

Using the approach of[34] the summation over k is performed. We get

$$\sqrt{g}\xi = 2\hbar\omega_D e^{-\frac{1}{N_{(O)}g}} \tag{2.315}$$

Where $\sqrt{g}\xi$ is the energy gap, ω_D is the Debye frequency, g the coupling constant and $N_{(O)}$ the density of quasiparticle states at the Fermi level. Thus we have seen that the functional integral provides us a new technique for obtaining the energy gap equation from the BCS reduced Hamiltonian.

2.12 Variable transformations in functional integrals

The behaviour of partition function (defined as functional integral) under variable transformation is given by a theorem due to t'Hooft and Veltman(1974) [26,35].The theorem can be stated as follows.

Let Z be the partition function defined as a functional integral over ϕ fields.

$$Z = \int_\phi e^{-S(\phi)} \tag{2.316}$$

Under a variable transformation defined by

$$\phi = \chi + R(\chi) \tag{2.317}$$

It should be invertible in the vicinity of $\phi = 0$. All ϕ Green's functions defined by equation 2.316 will remain invariant when Z is written as

$$Z(\chi) = \int_\chi e^{-S'(\chi)} \tag{2.318}$$

with

$$S'(\chi) = S(\chi + R(\chi)) - \mathrm{Trace}\ln[1 + \frac{\delta R}{\delta \chi}] \qquad (2.319)$$

The logarithmic trace in equation 2.319 is the formal Jacobian of the variable transformation. $Z(\phi)$ is obtained by performing Gaussian integration over the full real line or complex plane. Similarly $Z(\chi)$ is also obtained by similar Gaussian integration over the same domain.

The functional integral provides a powerful tool for obtaining perturbation theory in the zero temperature limit. In this limit, the constraint integral in section 2.9 need not be performed exactly, but may be treated in a saddle point approximation.The formal perturbation series that arises from the fluctuations about the saddle point may be transformed to an equivalent series by applying the theorem of t'Hooft and Veltman.

2.13 References

1. R.L. Stratanovich, Dokl. Acad. Nauk, SSSR 115, 1097 (1957)
2. J. Hubbard, Phys. Rev. Lett. 3, 77 (1959)
3. J.W. Negalle and H. Orland, Quantum Many Particle Systems (page 333) (Addison-Wesley Publishing Company, 1988)
4. B. Muhlschlegal, J. Math. Phys. 3, 522 (1962)
5. B. Muhlschlegal and J. Zittartz, Z. Phys. 175, 553 (1963)
6. D.R. Hamann, Phys. Rev. Lett. 23, 95 (1969)
7. R.P. Feynman, Rev. Mod. Phys. 20, 367 (1948)
8. R.P. Feynman and A.R. Hibbs, Quantum Mechanics and Path integrals (McGraw Hill: New York, 1965)
9. J.J. Sakurai, Modern Quantum Mechanics (page 116- 123) (Addison - Wesley Publishing Company, Inc. 1985)
10. S.F. Edwards and R.E. Peierls, Proc. Roy. Soc. Lond. A224, 24 (1954)
11. I.M. Gelfand and R.A. Minlos, Dokl. Akad. Nauk, SSSR 97, 209 (1954)
12. P.T. Mathews and A. Salam, Nuovo Cimento 2, 120 (1955)
13. J.D. Bell in Lectures on the manybody Problems (Naples Spring School), Ed. E.R. Caianiello (Academic Press: New York, 1962)
14. S.F. Edwards, Analysis in function space, ed. W.T. Martin and I. Segel (M.I.T. Press, Cambridge, 1964)

15. L.S. Schulman, Techniques and Applications of Path Integration, (John Wiley and Sons 1981)

16. V.N. Popov, Functional Integrals in Quantum field theory and Statistical Physics (D. Reidel Publishing comp. Boston, 1983)

.pl64 17. F.A. Berezin, The Method of Second Quantization (Academic Press: New York, 1966)

18. C. Itzykson and J.B. Zuber, Quantum Field Theory (McGraw Hill, New York, 1980)

19. P. Ramond, Field theory: A Modern Primer (Benjamin/Cummings Publishing Co., 1981)

20. S.E. Barnes, J. Phys. F6, 1375 (1976)

21. P. Coleman, Phys. Rev. 29, 3035 (1984)

22. P.W. Anderson, Phys. Rev. 124, 41 (1961)

23. A.A. Abrikosov, Physics 2, 5 (1965)

24. P.W. Anderson, in valence fluctuations in Solids, ed. L.M., Falikov et al. (North Holland, Amsterdam 1981)

25. T.V. Ramakrishnan, in valence fluctuations in Solids, ed. L.M. Falikov et al. (North Holland, Amsterdam, 1981)

26. N.E. Bickers, Rev. Mod. Phys. 59, 4 (1987)

N.E. Bickers, Ph.D. thesis (Cornell University, 1987)

27. J. Schwinger, Atomic Energy Commission Report No.NYO- 3071 (1952)

28. G. Kotliar and A.E. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986)

29. M.C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963)

30. W.F. Brinkman and T.M. Rice, Phys. Rev. B2, 4302 (1970)

31. T. Li, P. Wolfle, and P.J. Hirchfeld, Phys. Rev. B40, 6817 (1989)

32. T. Li, Y.S. Sen, and P. Wolfle, Z. Physik, B82, 369 (1991)

33. P. Wolfle and T. Li, Z. Physik B78, 45 (1990)

34. G. Rickayzen, Theory of Superconductivity (Interscience 1965)

35. G. t'Hooft and M. Veltman, "Diagrammar", reprinted in Particle interaction at very high energies (Plenum Press: New York, 1974) p.177.

Chapter 3

ELECTRON-PHONON INTERACTION WITHIN THE FRAME WORK OF THE FLUCTUATING VALENCE OF COPPER ATOMS - A THEORETICAL MODEL FOR HIGH TEMPERATURE SUPERCONDUCTIVITY

3.1 Introduction

The discovery of superconducting transition at high temperature in ceramic oxides [1,2] necessitates reconsideration of the conventional theoretical frame work of superconductivity. The microscopic theory of BCS [3] with phonons playing the role of exchange particles cannot explain superconducting transition at temperatures as high as 40K or 90K [4,5]. In chapter 1 we have explained such issues at length. Experiments show nearly the absence of isotope effect in these ceramic oxides [6]. The $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-\delta}$ group of materials have Cu-O layers which are the conducting planes of the crystal [7,8]. There is a strong anisotropy in these materials [9,10]. By substituting Sr atoms with the La atom of the parent compound La_2CuO_4, we can introduce holes into the oxygen 2p bands of the Cu-O planes [11].

In $YBa_2Cu_3O_{7-\delta}$ the introduction of oxygen vacancies affects the number of holes in oxygen 2p bands of the Cu-O planes [12]. It is found that T_c in these materials have a strong dependence on hole concentration [13].

The above features of the materials have been explained in chapter 1. In this chapter we consider a theoretical model where the rather strong electron lattice interaction and the on site repulsion at copper sites is taken into account.

3.2 The model

Various theoretical models have been suggested to explain superconductivity in these ceramic oxides. Some of these theories assume a model system where the role of 2p bands is not appropriately taken into account. Hubbard model Hamiltonian with the hopping term and the on site repulsive term are considered to contain the essential interaction to describe the superconducting transition. The Resonating Valence Bond (RVB) theory approaches the situation along these lines [14]. In this chapter We take the view that RVB description is correct in the insulating limit where antiferromagnetic correlation of the Cu spins is possible. When the material is doped it leads to the creation of holes in the Oxygen 2p bands unfavourably affecting superexchange interaction between Cu spins. The copper $3d^9$ electrons hybridises with the oxygen 2p bands when there are holes in the 2p bands. This strength of the hybridisation depends on the doping concentration. In this framework we are taking into account the interaction of the 2p band electrons with the lattice. Double occupancy of the Cu sites is energy wise made unfavourable by the Hubbard on site repulsive term [15] These requirements are satisfied by Anderson's Lattice Hamiltonian [16] with a few additional terms.

We assume that the electron - electron repulsive interaction is only of the on site Hubbard type and the effective electron phonon interaction can be replaced by a Frohlich type electron-electron interaction term [17].

Under the above conditions, the Hamiltonian for the system takes the form

$$\begin{aligned} H &= \sum_{k\sigma} C^{\dagger}_{k,\sigma} C_{k,\sigma} + E_0 \sum_{i,\sigma} a^{\dagger}_{i,\sigma} a_{i,\sigma} + \sum_{q} \hbar\omega_q b^{\dagger}_q b_q \\ &+ U/2 \sum_{i,\sigma,\sigma'}{}^{\prime} a^{\dagger}_{i,\sigma} a_{i,\sigma} a^{\dagger}_{i,\sigma'} a_{i,\sigma'} \end{aligned}$$

$$
\begin{aligned}
&+ \frac{V_1}{\sqrt{N}}\sum_{i,k,\sigma}(e^{-ikRi}a^{\dagger}_{i,\sigma}C_{k,\sigma} + e^{ikRi}C^{\dagger}_{k,\sigma}a_{i,\sigma}) \\
&+ \sum_{q,k.\sigma} V_2(q)(C^{\dagger}_{k+q,\sigma}C_{k,\sigma}b_q + b^{\dagger}_qC^{\dagger}_{k,\sigma}C_{k+q,\sigma}) \qquad (3.1)
\end{aligned}
$$

Where ϵ_k is the band energy with wave vector$k$. $C^{\dagger}_{k,\sigma}$ and $C_{k,\sigma}$ are the fermion creation and annihilation operators for electrons in Oxygen 2p bands. E_0 is the orbitally nondegenerate $3d^9$ energy level of Cu atom. $a^{\dagger}_{i,\sigma}$ and $a_{i,\sigma}$ are the fermi creation and annihilation operators for electrons at site i in Cu$3d^9$orbital. $b^{\dagger}_q$ and b_q are the phonon creation and annihilation operators. $\hbar\omega_q$ is the energy of the phonons in the q th mode. V_1 is the strength of the hybridisation between localised and band states. $V_2(q)$ is the strength of electron-phonon interaction.

The energy levels ϵ_k and E_0 are measured from the chemical potential and hence their values depend on the doping strength.

The Hamiltonian is transformed from the site representation to the wave vector representation by defining the following relations.

$$
\begin{aligned}
a^{\dagger}_{i,\sigma} &= 1/\sqrt{N}\sum_k a^{\dagger}_{k,\sigma}e^{-ikRi} \\
a_{i,\sigma} &= 1/\sqrt{N}\sum_{k'} a_{k',\sigma}e^{ik'Ri} \qquad (3.2)
\end{aligned}
$$

After substituting and replacing the electron phonon interaction terms with the Frohlich type electron-electron interaction term, the Hamiltonians becomes

$$
\begin{aligned}
H &= \sum_{k,\sigma}\epsilon_kC^{\dagger}_{k,\sigma}C_{k,\sigma} + E_0\sum_{k,\sigma}a^{\dagger}_{k,\sigma}a_{k,\sigma} \\
&+ U/2N \sum_{k_0,k_1,k_2,\sigma,\sigma',\sigma\neq\sigma'} a^{\dagger}_{k_2+k_0,\sigma}a^{\dagger}_{k_1-k_0,\sigma'}a_{k_1\sigma'}a_{k_2\sigma} \\
&+ V_1\sum_{k,\sigma}[a^{\dagger}_{k,\sigma}C_{k,\sigma} + C^{\dagger}_{k,\sigma}a_{k,\sigma}] + \sum_{k,k',q,\sigma,\sigma'} V_2(k,k',q)C^{\dagger}_{k+q,\sigma}C^{\dagger}_{k',\sigma'}C_{k'+q,\sigma'}C_{k,\sigma} \qquad (3.3)
\end{aligned}
$$

Let us consider the retarded Green's functions [18]defined by

$$G_1 \equiv << C^{\dagger}_{k,\sigma}(t); C_{k',\sigma'}(t') >>= \theta(t-t') < [C^{\dagger}_{k,\sigma}(t), C_{k',\sigma'}(t')] > \qquad (3.4)$$

$$G_2 \equiv << a^{\dagger}_{k,\sigma}(t); C_{k',\sigma'}(t') >>= \theta(t-t') < [a^{\dagger}_{k,\sigma}(t), C_{k',\sigma'}(t')] > \qquad (3.5)$$

the equation of motion for G_1 and G_2 will be

$$i\frac{d}{dt}G_1 = i\delta(t-t') < [c^{\dagger}_{k,\sigma}(t), C_{k,\sigma'}(t')] > + << [C^{\dagger}_{k,\sigma}, H]; C_{k,\sigma'}(t') >> \qquad (3.6)$$

$$i\frac{d}{dt}G_2 = i\delta(t-t') < [a^{\dagger}_{k,\sigma}(t), C_{k,\sigma'}(t')] > + << [a^{\dagger}_{k,\sigma}(t), H]; C_{k,\sigma'}(t') >> \tag{3.7}$$

When the commutators $[C^{\dagger}_{k,\sigma}, H]$ and $[a^{\dagger}_{k,\sigma}, H]$ are evaluated and substituted in equation 3.6 and equation 3.7, we find that they contain terms with higher order Green's function in addition to the terms with the lower order Green's functions G_1 and G_2. These higher order Green's functions are decoupled by writing them as the product of correlation function and a lower order Green's function G_1 or G_2. Thus equation 3.6 and equation 3.7 become

$$i\frac{\partial}{\partial t}G_1 = i\delta(t-t')\delta_{\sigma\sigma'}\delta_{k,k'} + P_2G_1 - V_1G_2, \tag{3.8}$$

$$i\frac{\partial}{\partial t}G_2 = P_1G_2 - V_1G_1 \tag{3.9}$$

Where

$$P_1 = -[E_0 + U/N + U/N\sum_{k1} < a^{\dagger}_{k1,\sigma'}a_{k1,\sigma'} >] \tag{3.10}$$

$$P_2 = -[\epsilon_k + 2\sum_{k',\sigma'} V_2(k'-k) < C^{\dagger}_{k',\sigma'}C_{k',\sigma'} >] \tag{3.11}$$

In obtaining the two equations of motion, standard decoupling and approximation methods are adopted at the higher stage. The Fourier transform of the two equation of motion are found. Solving them $G_1(E)$ and $G_2(E)$ are found.

$$G_1(E) = \frac{(-\frac{i}{2\pi})\delta_{k,k'}\delta_{\sigma,\sigma'}}{(E-P_2) - (V_1^2)/(E-P_1)} \tag{3.12}$$

and

$$G_2(E) = \frac{\frac{-i}{2\pi}\delta_{k,k'}\delta\sigma,\sigma' V_1/(E-P_1)}{(E-P_2) - V_1^2/(E-P_1)} \tag{3.13}$$

Diagonalising the set of coupled Fourier transform of equation of motion, we get

$$G_{\mp} = U_kG_2(k,k',E) \mp V_kG_1(k,k',E) \tag{3.14}$$

with energies

$$E_{\mp} = P_2 + P_1 \mp \sqrt{(P_1-P_2)^2 + 4V_1^2} \tag{3.15}$$

where V_k and V_k are given by

$$U_k = 1/\sqrt{2}\{1 + \frac{(P_2-P_1)}{\sqrt{(P_2-P_1)^2+4V_1^2}}\}^{1/2} \tag{3.16}$$

$$V_k = 1/\sqrt{2}\{1 - \frac{(P_2 - P_1)}{\sqrt{(P_2 - P_1)^2 + 4V_1^2}}\}^{1/2} \tag{3.17}$$

The system can be described as an assembly of noninteracting quasiparticles belonging to two different species, characterized by excitation energies $E_{\substack{+\\-}}$ and the corresponding creation operators are

$$a^\dagger_{\substack{+\\-},\sigma}(k) = U_k a^\dagger_{k,\sigma} \overset{+}{-} V_k C^\dagger_{k,\sigma} \tag{3.18}$$

Thus we are making a canonical transformation from the original set to a new set of operators. The various terms of the Hamiltonian are expressed in terms of the quasiparticle operators. By doing this, we intend to diagonalize the Hamiltonian. Expressing the original operators in terms of the new operators, we have substituted for various operators the combination of new operators. As expected, the Hamiltonian is not in the diagonal form. It contains off-diagonal terms of the form $a^\dagger_{+,\sigma}(k)a_{-,\sigma}(k)$ and $a^\dagger_{-,\sigma}(k)a_{+,\sigma}(k)$ .It also contains terms which involve four operators which do not satisfy the conservation of quasiparticle species. Such terms are neglected. Those fourth order terms which conserve quasiparticle species are combined and their coefficient is set equal to zero. On simplifying we get

$$V_2(k, k') = -(U/2N)\{\frac{V_k^2 V_{k'}^2}{U_k^2 U_{k'}^2}\} \tag{3.19}$$

At OK very few quasiparticles are excited and hence the number operators for quasiparticles $m_{+,\sigma}(k), m_{-,\sigma}(k)$ etc. have vanishingly small expectation values. Therefore off-diagonal terms and fourth order terms containing number operators are neglected.

Equating the coefficient of off-diagonal terms to zero, after simplification, we have

$$E_0\frac{V_k^2}{U_k^2} - \epsilon_k = -\sum_{k'} V_2(k, k') \tag{3.20}$$

By using equation 3.19 for $V_2(k, k')$, equation 3.20 leads to

$$\frac{E_0 V_k^2}{U_k^2} - \epsilon_k = \frac{U}{2N}\frac{V_k^2}{U_k^2}\sum_{k'}\frac{V_{k'}^2}{U_{k'}^2} \tag{3.21}$$

Putting $U_k = (1/2 + x_k)^{1/2}$ and $V_k = (1/2 - x_k)^{1/2}$.
By substituting U_k and V_k and then putting

$$\frac{U}{2N}\sum_{k'}\{\frac{(1/2 - x_{k'})}{(1/2 + x_{k'})}\} = \Delta_k(0) \tag{3.22}$$

we obtain

$$x_{k'} = \frac{1/2(E_0 - \Delta_{k'}) - \epsilon_{k'}/2}{E_0 + \epsilon_{k'} - \Delta_{k'})} \tag{3.23}$$

Substituting for $x_{k'}$ in the equation for Δ_k, the energy gap at $0k$ leads to

$$\Delta_k(0) = \frac{U}{2N}\sum_{k'} \frac{\epsilon_{k'}}{\{E_0 - \Delta_{k'}(0)\}} \tag{3.24}$$

Assuming Δ_k as slowly varying with k and introducing $D(\epsilon_k$ as the density of localized states per Cu atom, we get

$$\Delta_k(0) = \frac{U}{2(E_0 - \Delta_k(0))}\int_0^{\epsilon_{k_0}} D(\epsilon_{k'})\epsilon_{k'} d\epsilon_{k'}, \tag{3.25}$$

where ϵ_{k_0} is the upper bound of the hybridized $2p$ bands, and $D(\epsilon_k)$ is the localized states per Cu atoms. For each value of ϵ_k there are two values of ω and hence we have to sum the two density of states corresponding to E_+ and E_-. Linear relations are assumed to hold between the doping strength x and the parameters $E_0, \epsilon_{k_0}$and, V_1.

Since the Fermi level decreases linearly with doping, the relationship between E_0 and the doping strength x will be$E_0 = R_1 x + 0.5$. In the undoped case $x = 0$, the localized Cu state and the narrow $2p$ band of the oxygen atoms are of nearly equal energy. This justifies the introduction of the small energy difference 0.5 between the upper bound of the 2p band and the cu$3d^9$ level. ϵ_{k_0} is the topmost level of the 2p band as measured from the Fermi level and hence the relation $\epsilon_{k_0} = R_2 x$ holds . The hybridisation parameter V_1 should change with the overlapping integral which in turn has a linear dependence on the concentration of the dopants in the out of the plane sites. Therefore we choose $V_1 = V_{10} + R_3 x$, where v_{10} stands for the residual mixing parameter .

We have assigned the following numerical values $R_1, R_2,$ and$R_3$are given the values 2.0,2.0,and 0.2, respectively. $V_{10} = 0.05$, $V_2 = -0.056$ eV, $U = 6.0$ eV and the density of band states per Cu atom = 1.0.

The set of equations for the Green's functions are solved and the correlation function in P_1 and P_2 are found by iterative computation. For $x = 0.19$, the computed values are

$$2\sum_k V_2 < C^{\dagger}_{k,\sigma} C_{k,\sigma} >= -0.8867X10^{-5}$$

and

$$\frac{1}{N}\sum_{k'} < a^{\dagger}_{k',\sigma'} a_{k',\sigma'} >= 0.7841X10^{-4}$$

The density of localized states is calculated using Green's function technique with the help of a digital computer. Substituting for the density of states the integration is performed and hence $\Delta_k(0)$ is calculated [19]. Corresponding to $x = 0.19$, $\Delta_k(0)$ has the value $6.4326X10^{-3}$ eV and $\frac{2\Delta(0)}{k_B T_c} = 3.739$ for a $T_c = 40K$.

The mixing parameter is determined by the overlap integral of the band states with the localized states of Cu atom. This integral is determined by the ordering of the out of the plane dopants, which have a quasi periodic character.

3.3 conclusions

The work was undertaken at a time, when the relevant parameter regime was highly disputed and hence the parameter regime assumed in this chapter do not agree with currently held parameter values. Another defect of the analysis is the treatment of the strong correlations in the double time Green's function technique. The large on site repulsion is not amenable to conventional perturbation treatments and hence the results are inadequate in several respects. In the next chapter we analyse a more realistic Anderson lattice model, where strong local correlation are properly taken into account. In the strong coupling analysis of this chapter the nature of the paired state is not clear. This is an important deficiency of this type of analysis.

See appendix B

3.4 References

1. J.G. Bednorz and K.A. Muller, Z.Phys. B64(1986)188.
2. P.H. Hor, L. Gao, R.L. Merg, Z.J. Huang, Y.Q. Wang, K. Forster, J. Vassilions, C.W. Chu, M.K. Wu, J.R. Ashburn, and C.J. Torng, Phys. Rev. Lett. 58(1987)911.
3. J.Bardeen, N.Cooper and J.R. Schrieffer, Phys. Rev.108(1957)1175
4. C.R.Leavens, Solid State Commun. 17(1975)1499
5. W.L.McMillan, Phys. Rev. 167(1968)331.
6. B.R. Batlogg, R.J. Cava, A.Jayaraman, R.B. Van Dovor, G.A. Kononklin, S. Sunshine, D.W. Murphy, L.W. Rupp, H.S. Chen, A.White, K.T. Short, A.M. Mujsce, and E.A. Rietman, Phys. Rev. Lett.58(1987)2333.

7. J.D. Jorgensen, H.B. Schuttler, D.G. Hinko, B.W. Copone, K.Zang, M.B. Brodsky, and D.J. Scalapino, Phys. Lett. 58(1987)1024.

8. J.Yu, A.J. Freeman, and J.H. Xu, Phys. Rev. Lett. 58(1987)1035.

9. Y.Hidaka, V.Enomoto, M.Suzuki, M.Oda, and T. Murakami, Jpn. J. Appl. Phys. 26 (1987) L377.

10.T.R. Dinger, T.K. Worthington, W.J.Gallangher, and R.L. Sandstorm, Phys. Rev. Lett. 58(1987)2687.

11.M.Nucker, J.Fink, J.C. Fuggle, P.J. Durham, and W.M. Temmerman, Phys. Rev. B37(1988)5158.

12.P.Steiner, S.Hufner, V.Kinsinger, I.Sander, B.Siegwart, H.Schmitt, R.Schulz, S.Junk, G.Schwitzgebel, A.Gold, C.Politis, H.P. Muller, R.Hoppe, S.Kemmler Sack, and C.Kunz, Z.Phys.B69(1988)449.

13.M.W. Shafer, T.Penny, and B.L.Olson, Phys. Rev. B36(1987)4047 .

14.P.W. Anderson, Science 235(1987)1196.

15.J.Hubbard, Phys. Rev. B17(1978)494.

16.P.W. Anderson Phys. Rev.124(1961)41.

17.H.Frohlich, Proc. Roy.Soc.London A215(1952)291.

18.S.V. Tyablikov, in Methods in the Quantum Theory of magnetism (Plenum, 1967).

19.Suresh V Vettoor and V.M. Nandakumaran Mod.Phys.Lett.B,4(1990)325-331.

Chapter 4

DENSITY OF STATES IN HIGH-Tc SUPERCONDUCTORS

4.1 Introduction

High temperature superconductivity in ceramic oxides raises serious questions regarding the mechanism of normal and superconducting state properties of these systems. A detailed investigation of such issues have been carried out in chapter 1 of this thesis .Ever since the discovery [1] , various theoretical models have been suggested and different mechanisms ranging from conventional weak coupling BCS like to novel strong coupling formulations have been proposed [2-4].

It is believed that the essential physics of normal and superconducting state reside in the Cu-O planar subsystem which is common to the copper oxide superconductors. Many theoretical models begin with a two-dimensional extended Hubbard model or Anderson lattice model with a strong on-site repulsive interaction [5-7]. The introduction of nearest neighbour repulsion in the extended Hubbard model [8] emphasizes the relevance of charge degrees of freedom. In the $t-J$ models and *RVB* theories the low energy sector of the problem is dominated by the spin degrees of freedom [9-10]. In this chapter we analyze the extended model without nearest neighbour repulsion, but with a direct oxygen-oxygen hopping between the P_σ orbitals which brings to the scene, in addition to the spin degrees of freedom, the charge degrees of freedom. These models have been previously studied using a mean field scheme [11,12]. We have studied this strongly correlated problem using a slave boson [13] functional integral formalism [14] adopting a uniform saddle point approximation in the complex variables.

The slave boson scheme [13] has been discussed in detail in chapter 2 within the framework of functional integration. Photoemission studies show that the copper on site repulsion is the largest energy scale in the problem. At half filling, the materials are antiferromagnetically spin ordered insulators. The proximity to being a magnetic insulator makes strong correlation relevant to the doped case.

Here we consider a model, in which the on site repulsion imposes a double occupancy constraint on the copper

$3d_{x^2-y^2}$ orbital. We study this using a large N expansion technique which is nonperturbative in the coupling constants. The essential features of large N techniques is discussed in chapter 2.The study is restricted to the meanfield theory ($N = \infty$).The partition function and the free energy are derived in section 2. The expression for the specific heat and the density of states have been derived in section 3. The numerical computations are presented in section 4. The conclusion regarding the renormalized energy bands and the comparison with experiments are also discussed in section 4.

4.2 The model

The model we consider in this chapter has three essential bands . As a consequence of the oxygen ligand environment the copper 3d degeneracy is lifted and the orbital which is closer to the Fermi energy is the copper $3d_{x^2-y^2}$ orbital. The relevant oxygen orbital are the p_σ orbitals of x and y symmetry. The Hamiltonian for the system can be written as

$$\begin{aligned} H &= \epsilon_d \sum_{i,\sigma} d^\dagger_{i\sigma} d_{i\sigma} + \epsilon_p/2 \sum_{i.\eta 1,\sigma} P^\dagger_{i+\eta 1,\sigma}(x) P_{i+\eta 1,\sigma}(x) \\ &+ \epsilon_p/2 \sum_{i,\eta 2,\sigma} P^\dagger_{i+\eta 2,\sigma}(y) P_{i+\eta 2,\sigma}(y) + t_{pd} \sum_{i,\eta 1,\sigma} d^\dagger_{i\sigma} P_{i+\eta 1,\sigma}(x) \\ &+ t_{pd} \sum_{i,\eta 2,\sigma} d^\dagger_{i\sigma} P_{i+\eta 2,\sigma}(y) + h.c. + U/2 \sum_{i,\sigma,\sigma',(\sigma\neq\sigma')} d^\dagger_{i,\sigma} d_{i\sigma} d^\dagger_{i\sigma'} d_{i\sigma'} \\ &+ t_p \sum_{\eta 1,\eta 2,i,\sigma} P^\dagger_{i+\eta 1,\sigma}(x) P_{i+\eta 2,\sigma}(y) \\ &+ t_p \sum_{\eta 1,\eta 2,i,\sigma} P^\dagger_{i+\eta 2,\sigma}(y) P_{i+\eta 1,\sigma}(x) \end{aligned} \tag{4.1}$$

where $\eta 1$ takes values a_x and $-a_x$ and $\eta 2$ takes values a_y and $-a_y$. The scale is so chosen that their magnitudes are 1, ϵ_p and ϵ_d are the unrenormalized energy levels. They include the chemical potential $d^\dagger_{i,\sigma}$ and $d_{i,\sigma}$ are the Fermi creation and annihilation operators for holes in the filled copper $3d_{x^2-y^2}$ orbital. $P^\dagger_{i+\eta 1,\sigma}(x)$ and $P_{i+\eta 1,\sigma}(x)$ are the creation and annihilation operators for holes in a P_σ orbital next to the i th planar copper atom. Similarly the other p operators corresponds to the oxygen P_σ orbital with y symmetry. In the low energy sector which is relevant at low temperatures, the large U limit imposes constraints on hole dynamics.

Using a large N slave boson technique with $b^\dagger_i$ and b_i as the slave boson operators, the Hamiltonian take the form

$$\begin{aligned} H &= \epsilon_d \sum_{i,\sigma} d^\dagger_{i,\sigma} d_{i\sigma} + \epsilon_p/2 \sum_{i,\eta 1,\sigma} P^\dagger_{i+\eta 1,\sigma}(x) P_{i+\eta 1,\sigma}(x) \\ &+ \epsilon_p/2 \sum_{i,\eta 2,\sigma} P^\dagger_{i+\eta 2,\sigma}(y) P_{i+\eta 2,\sigma}(y) + (t_{pd}/\sqrt{N}) \sum_{i,\eta 1,\sigma} b_i d^\dagger_{i\sigma} P_{i+\eta 1,\sigma}(x) \\ &+ t_{pd}/\sqrt{N} \sum_{i,\sigma,\eta 2} b_i d^\dagger_{i\sigma} P_{i+\eta 2,\sigma}(y) + (h.c.) \\ &+ t_p/\sqrt{N} \sum_{i,\sigma,\eta 1,\eta 2} P^\dagger_{i+\eta 1,\sigma}(x) P_{i+\eta 2,\sigma}(y) \\ &+ t_P/\sqrt{N} \sum_{i,\sigma,\eta 1,\eta 2} P^\dagger_{i+\eta 2,\sigma}(y) P_{i+\eta 1,\sigma}(x) \\ &+ i \sum_i \lambda_i (b^\dagger_i b_i + \sum_\sigma d^\dagger_{i\sigma} d_{i\sigma} - q_0 N) \end{aligned} \tag{4.2}$$

The partition function for the model in the functional integral formalism takes the form

$$Z = \int D[d] D[p] D[b] d[\lambda_i] e^{-S} \tag{4.3}$$

where

$$S = \int_0^\beta L d\tau \tag{4.4}$$

$$\begin{aligned} L &= \sum_i \{ \sum_\sigma \bar{d}_{i\sigma} \frac{\partial}{\partial \tau} d_{i\sigma} + \sum_{\sigma,\eta 1} \bar{P}_{i+\eta 1,\sigma}(x) \frac{\partial}{\partial \tau} P_{i+\eta 1,\sigma}(x) \\ &+ \sum_{\sigma,\eta 2} \bar{P}_{i+\eta 2,\sigma}(y) \frac{\partial}{\partial \tau} P_{i+\eta 2,\sigma}(y) \} \\ &+ i \sum_i \lambda_i (\bar{b}_j b_i - q_0 N) + \bar{H} \end{aligned} \tag{4.5}$$

where

$$\bar{H} = \sum_{i,\sigma} \bar{d}_{i\sigma} d_{i\sigma} (\epsilon_d + i\lambda_i) + \sum_{i,\sigma,\eta 1} \bar{P}_{i+\eta 1,\sigma}(x) P_{i+\eta 1,\sigma}(x) \epsilon_P$$

$$\begin{aligned}
&+ \sum_{i,\sigma,\eta 2} \bar{P}_{i+\eta 2,\sigma}(y) P_{i+\eta 2,\sigma}(y)\epsilon_P + (t_{pd}/\sqrt{N}) \sum_{i,\sigma,\eta 1} \bar{d}_{i\sigma} P_{i+\eta 1,\sigma}(x) b_i \\
&+ (t_{pd}/\sqrt{N}) \sum_{i,\eta 2,\sigma} \bar{d}_{i\sigma} P_{i+\eta 2,\sigma}(y) b_i + (h.c) \\
&+ (t_P/\sqrt{N}) \sum_{i,\sigma,\eta 1,\eta 2} (\bar{P}_{i+\eta 1,\sigma}(x) P_{i+\eta 2,\sigma}(y) \\
&+ \bar{P}_{i+\eta 2,\sigma}(y) P_{i+\eta 1,\sigma}(x))
\end{aligned} \tag{4.6}$$

where $\bar{d}_{i\sigma}, d_{i\sigma}, \bar{P}_{i+\eta 1,\sigma}(x), P_{i+\eta 1,\sigma}(x), \bar{P}_{i+\eta 2,\sigma}(y)$,and $P_{i+\eta 2,\sigma}(y)$ are Grassmann variables corresponding to Fermi creation and annihilation operators.

We make a uniform saddle point approximation in the slave boson variables and Lagrange multiplier variables. We denote them as λ and b. The functional integrals over the Grassmann variables are performed after converting the Grassmann variables from real space to momentum space and from imaginary time to imaginary frequency representation.

The conversion of functional integrals over Grassmann variables from one set to another and how Grassmann functional integrations are carried out is discussed in chapter 2. The partition function then becomes

$$Z = e^{-\beta F}, \tag{4.7}$$

where the free energy is given for real degeneracy of σ which is 2

$$\begin{aligned}
F &= -(1/\beta) \sum_{k,\sigma} \{\ln(1 + e^{-\beta\bar{\epsilon}_d}) + 2\ln(1 + e^{-\beta\epsilon_p})\} \\
&- (1/\beta) \sum_{n,k,\sigma} \{2\ln(G(\epsilon_p, i\omega_n)) \ln(A(x)A(y) - B)\} \\
&+ N_s \lambda b^2 - N_s \lambda
\end{aligned} \tag{4.8}$$

where N_s is the number of copper sites in the planar subsystem,

$$G(\epsilon_p, i\omega_n) = (\epsilon_p - i\omega_n)^{-1}, \tag{4.9}$$

$i\omega_n$ are the Matsubara frequencies

$$i\omega_n = (2n + 1)(i\pi/\beta), \tag{4.10}$$

and n varies from $-\infty$ to ∞, and we have

$$\bar{\epsilon}_d = \epsilon_d + \lambda, \tag{4.11}$$

$$A(x) = \frac{(\epsilon_p - i\omega_n)(\bar{\epsilon}_d - i\omega_n) - 4t_{pd}^2 \sin^2(k_x/2)}{(\bar{\epsilon}_d - i\omega_n)}, \tag{4.12}$$

$$A(y) = \frac{(\epsilon_p - i\omega_n)(\bar{\epsilon}_d - i\omega_n) - 4t_{pd}^2 \sin^2(k_y/2)}{(\bar{\epsilon}_d - i\omega_n)}, \tag{4.13}$$

and

$$B = 16\{t_p - t_{pd}^2 b^2 (\bar{\epsilon}_d - i\omega_n)^{-1}\}^2 \sin^2(k_x/2) \sin^2(k_y/2) \tag{4.14}$$

The saddle point values are determined by

$$\begin{aligned} \frac{\partial F}{\partial \lambda} &= 0 \\ \frac{\partial F}{\partial b^2} &= 0 \end{aligned} \tag{4.15}$$

We can write

$$A(x)A(y) - B = \frac{P(i\omega_n)}{(\bar{\epsilon}_d - i\omega_n)^2}, \tag{4.16}$$

where

$$P(i\omega_n) = a_0(i\omega_n)^4 - 2a_1(i\omega_n)^3 + a_2(i\omega_n)^2 + a_3(i\omega_n) + a_4, \tag{4.17}$$

and a_0, a_1, a_2, a_3, a_4 stand for

$$a_0 = 1 \tag{4.18}$$

$$a_1 = \bar{\epsilon}_d + \epsilon_p \tag{4.19}$$

$$a_2 = a_1^2 + \epsilon_p \bar{\epsilon}_d - 4t_{pd}^2 b^2 \gamma_1 - 16t_p^2 \gamma_2, \tag{4.20}$$

$$a_3 = (4t_{pd}^2 b^2 \gamma_1 - 2\bar{\epsilon}_d \epsilon_P) a_1 + 32(t_p^2 \bar{\epsilon}_d - t_{pd}^2 t_p b^2)\gamma_2, \tag{4.21}$$

and

$$a_4 = \bar{\epsilon}_d \epsilon_p - 4t_{pd}^2 \bar{\epsilon}_d \epsilon_p b^2 \gamma_1 + 16(2t_{pd}^2 b^2 - t_p \bar{\epsilon}_d) t_p \bar{\epsilon}_d \gamma_2, \tag{4.22}$$

where $\gamma_1$andγ_2 are

$$\gamma_1 = \sin^2(k_x/2) + \sin^2(k_y/2), \tag{4.23}$$

$$\gamma_2 = \sin^2(k_x/2) \sin^2(k_y/2) \tag{4.24}$$

$P(i\omega_n)$ can be written as

$$P(i\omega_n) = \prod_{j=1}^{4} (E(j) - i\omega_n) \tag{4.25}$$

where Ej are the roots of the polynomial $P(i\omega_n)$. When frequency sums are performed after simplification the expression for the free energy becomes

$$F = \sum_{k,\sigma} (\frac{1}{\beta}) \{\ln(1 + e^{-\beta\bar{\epsilon}_d}) - \sum_{j=1}^{4} \ln(1 + e^{-\beta E(j)})\} + N_s \lambda b^2 - N_s \lambda \tag{4.26}$$

4.3 The electronic specific heat capacity and density of states

The electronic specific heat capacity is given by the expression

$$C_v = -T\frac{\partial^2 F}{\partial T^2}, \tag{4.27}$$

where T is the temperature . At the low temperatures of interest to us, we can set $\beta \to \infty$. The limit is applied after taking the derivatives. We can write

$$\frac{\partial^2 F}{\partial T^2} = \sum_{k,\sigma} \bar{\epsilon}^2{}_d k_B^2 \beta^3 \frac{e^{\beta\bar{\epsilon}_d}}{(e^{\beta\bar{\epsilon}_d}+1)^2} - \sum_{k,j,\sigma} k_B^2 \beta^3 \frac{E^2(j)e^{\beta E(j)}}{(e^{\beta E(j)}+1)^2} \tag{4.28}$$

The summation over k can be replaced by integration. when this is done the contribution of the first term vanishes in the $\beta \to \infty$ limit since the integrand is independent of the integration variables. The second term is simplified and on substitution in equation 4.27 yields the specific heat capacity per copper site in the planar structures as

$$C_v = \frac{2\pi k_B^2 T}{3}\{\frac{2}{\pi}\int_0 dk_y \sum_{j=1}^{4}\{\frac{\partial E(j)}{\partial k_y}\ |_{E(j)=0}\}^{-1}\}, \tag{4.29}$$

where the quantity appearing as the multiplicative factor of $\frac{2\pi k_B^2 T}{3}$ can be identified as the density of states at the Fermi surface.

4.4 Numerical results and conclusions

The saddle point values λ and b^2 are determined numerically using equation 4.15 for β in the ∞ limit. When the numerical integrations over k_x and k_y are performed, at each integration step, equation 4.17 is numerically solved to determine the energy values $E(j)$. Using the saddle point values, the density of states calculation is carried out. The variation of density of states with doping is plotted. The chemical potentials are so chosen that the average number of particles is given by

$$N_s(1+\delta) = -\frac{\partial F}{\partial \mu} \tag{4.30}$$

where δ is the doping concentration and μ is the chemical potential. The computation are carried out for two sets of parameter values

(1) $t_p = -0.5\text{eV}$ $t_{pd} = -1.5\text{eV}$ $\epsilon_p = -4.0t_p\text{eV}$ $\epsilon_d = (\epsilon_p - 1.8)\text{eV}$
(2) $t_p = -0.1\text{eV}$ $t_{pd} = -1.5\text{eV}$ $\epsilon_p = -4.0t_p\text{eV}$ $\epsilon_d = (\epsilon_p - 1.8)\text{eV}$

The variation of the density of states with δ is shown in figure (4.1). For very small values of δ (close to the half filled case) the saddle point values show large deviations. The corresponding density of states also show an increase. When δ is very small the saddle point values become a poor approximation for the functional integral in view of the constraint in the problem. Therefore we are not including the limiting half filled case in the discussion. In the other domain the pattern of the variation of the density of states is similar to that of reference[11]. The renormalized energy bands are shown in figures (4.2) and (4.3). The two dimensional analogue of the Fermi surface is shown in figure (4.4). The calculated values are in good agreement with the values deduced by Grilli etal[11] from susceptibility measurements [15]. The renormalized energy bands in figure(4.2) and (4.3) show that in the low energy domain the physics is governed by a single band as has been advocated by Anderson [16].

We have shown [17] that even for moderately large t_p values and for the parameter regime considered in this paper the effective one band description holds. The calculated values of the density of states are in good agreement with estimations from experiments.

4.5 References

1. G.Bednorz and A.Muller, Z.Phys. B 64 (1986) 189
2. P.W.Anderson, Science 235(1987) 1196
3. V.J.Emery, Phys.Rev.Lett. 58(1987)2794
4. R.B.Laughlin, Science 242(1988)525
5. C.M.Varma, P.B.Littlewood, S.Schmitt-Rink and E.Abrahams, Solid State Commun. 62 (1987) 681.
6. G.Kotliar, P.A.Lee and N.Reed, Physica C 153-155 (1988) 538
7. D.M.Newns, M.Rasolt, and P.C.Pattnaik, Phys.Rev. B38 (1988) 6513
8. S.Schmitt-Rink, C.M.Varma and A.E.Runkenstein, Phys. Rev. Lett. 60 (1988) 2793
9. F.C.Shang and T.M.Rice, Phys.Rev.B 37(1988)3759
10. G.Baskaran, Z.Zou and P.W.Anderson, Solid State Commun. 63 (1987) 973

11. M.Grilli, B.G.Kotliar and A.J.Millis, Phys.Rev. B42 (1990) 329

12. C.A.Balaseiro, M.Avignon, A.G.Rojo and B.Alascio, Phys. Rev. Lett. 62 (1989) 2624.

13. S.E.Barnes, J.Phys.F6(1976)1375

14. J.W.Negele and H.Orland, Quantum Many Particle Systems (Addison- Wesley, Reading, MA, 1988)

15. L.F Schneemeyer, J.V.Wasziczak, E.A.Reitman, and R.J.Cava, Phys. Rev. B35 (1987) 8421

16. P.W.Anderson, Int.J.Mod. Phys.B4 (1990)181.

17. Suresh V. Vettoor and V.M. Nandakumaran, Physica C 191 (1992) 277

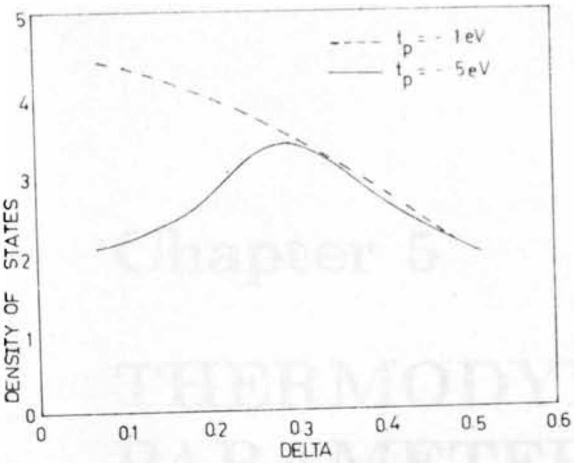


Fig 4.1. Density of states vs. doping for $t_p = -0.5$ eV and $t_p = -0.1$ eV.

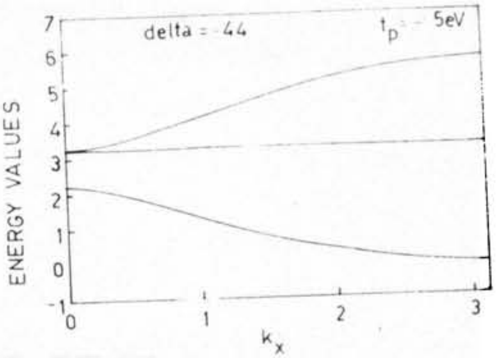


Fig 4.2. Energy values vs. k_x in the range 0 to π for $k_y = 0$.

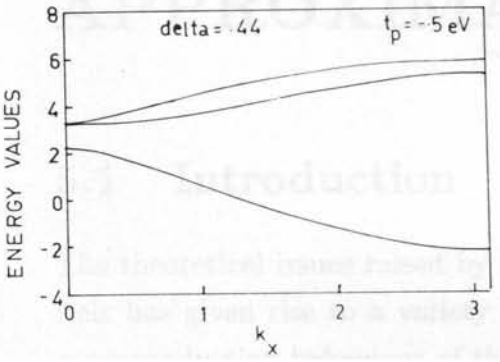


Fig 4.3. Energy values vs. k_x in the range 0 to π for $k_y = k_x$.

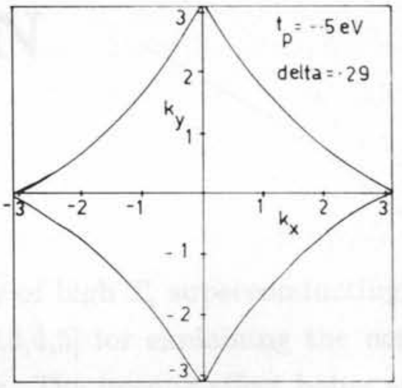


Fig 4.4. Contour in the two-dimensional k space where the energy value crosses zero.

Chapter 5

THERMODYNAMIC PARAMETERS OF HIGH Tc SUPERCONDUCTORS IN A FUNCTIONAL INTEGRAL CALCULATION USING A NON UNIFORM SADDLE POINT APPROXIMATION

5.1 Introduction

The theoretical issues raised by the discovery of high T_c superconducting[1] materials has given rise to a variety of theories[2,3,4,5] for explaining the normal and superconducting behaviour of these materials. The isotope effect being at a much a reduced level, a BCS mechanism[6] is a remote possibility. These materials show in their normal state several anomalous behaviour (This is discussed in the first chapter), and their normal state can not be explained along the conventional fermi liquid theory of weakly interacting quasiparticles.

The structural details of these materials show that the superconducting materials exist in the proximity of insulators with antiferromagnetic spin ordering in their sublattices[7]. Doping these materials either removes oxygen from the chain like structures in $YBa_2Cu_3O_7$ materials or substitutes some of the metallic ions in the valence state +3 by those elements which exist in the +2 valence state. The dopants which destroys the translational invariance of the lattice have their positions outside the planar structures of Cu-O. The holes doped either way exist in the planar subsystem and their dynamics has to be treated taking into account the dominant interactions in the system.

When the Cu-O planar subsystems are considered, the symmetry of the configuration shows that the ligand environment has its influence on the copper 3d orbitals. Copper atom has its outer electron configuration $3d^{10}4s^{1}$. When copper is existing in the +1 valence state the outer orbitals will be $3d^{10}$. There are 5 d orbitals and this degenerate orbitals will be split up into nondegenerate levels by the electrostatic fields of the oxygen ions, which exist in the -2 valence state. The copper d orbital which is most affected by this ligand environment is the $3d_{x^2-y^2}$ orbital. When a second electron is removed from the copper ion, it is taken from the copper $3d_{x^2-y^2}$ orbital. In the superconducting compounds and nonsuperconducting parent compounds, the copper atoms of the planar subsystem exist in the +2 valence state. When these parent compounds are doped, the electrons are removed from the planar subsystem. These electrons are taken from the oxygen P_σ orbitals. In a hole scheme of description, there is only a single hole in a $3d$ orbital of planar copper atom. It is possible to reduce the extended model, which includes both the copper and oxygen orbitals to a model in which Cu-O can have a single label. In this model electrons hops from site to site but there is no double occupancy of electrons on a single site. This is the Hubbard model[8]. In the large but not infinite U, a strong coupling perturbation treatment with certain approximations, this model Hamiltonian can be replaced by the $t-J$ model Hamiltonian[9]. In the $t-J$ model Hamiltonian, the essential interactions are the hopping term and the exchange interaction term. This one body hopping term is essentially not a one body term. It allows only those hoppings which will not lead to a double occupancy of electrons at a site. The $t-J$ model in the non doubly occupied case can be studied using the slave boson technique[10]. Grilli and Kotliar[11] has studied the $t-J$ model using a functional integral technique[12]. They make a uniform saddle point approximation in the Bose variables and Lagrange multiplier variables and then the functional integral over the Grassmann variables are performed. They have derived the expression for the free energy in a uniform saddle point approximation. In the next section of this chapter we derive the expression for the partition function by using a saddle point approximation in which we divide the $2D$ lattice of Cu into two sublattices in which the complex Bose variables are assumed to be phase shifted by π. The Lagrange multipliers are assumed to have a uniform saddle point value. Under this assumption the functional integral over the Grassmann variables are performed and the expression for the free energy is obtained. From this expression for the free energy the ground state energy and the density of states are obtained.

In section 3 the expression for the free energy, the ground state energy and the density of states are obtained in a uniform saddle point approximation in the evaluation of the functional integral for the partition function.

In section 4 the numerical computations are done on the analytic results of section 2 and 3 and the results are plotted in various figures for easy comparison. The important conclusion of the analysis is that the system prefer to behave in a periodic saddle point order as the ground state energy in this approximation is much smaller than that in the other approximation.

5.2 The model

In this section we consider the $t - J$ model Hamiltonian of reference[12]. The Hamiltonian can be written as

$$\begin{aligned} H &= \sum_{j,\sigma} C^\dagger_{j,\sigma} C_{j,\sigma} - \frac{t}{N} \sum_{<i,j>,\sigma} C^\dagger_{i\sigma} C_{j\sigma} \\ &+ \frac{J}{N} \sum_{<ij>,\sigma,\sigma'} C^\dagger_{i,\sigma} C_{i\sigma'} C^\dagger_{j\sigma'} C_{j\sigma} \end{aligned} \tag{5.1}$$

where $C^\dagger_{j\sigma}$ and $C_{j\sigma}$ are fermi creation and annihilation operators at site j. ϵ_d is the energy level of $3d_{x^2-y^2}$ symmetry. t is the hopping matrix element and J is the exchange integral given by $J = \frac{t^2}{U}$.

The Hamiltonian of equation 5.1 is subject to a nonholonomic constraint

$$\sum_{\sigma} C^\dagger_{j\sigma} C_{j\sigma} \leq q_0 N \tag{5.2}$$

Where $q_0 = \frac{1}{N}$ and N stands for the spin degeneracy. The nonholonomic constraint in equation 5.2 can be imposed via a slave boson technique[10]. How this is carried out is discussed in detail in Chapter 2.

The partition function for the system in a functional integral formalism will be written as

$$Z = \int D[f]\, D[b]\, D[\Delta]\, d[\lambda]\, e^{-S} \tag{5.3}$$

where

$$\begin{aligned} S &= \bar{f}_l^{j\sigma}(f_l^{j\sigma} - f_{l-1}^{j\sigma}) + \bar{b}_l^j(b_l^j - b_{l-1}^j) \\ &+ \Delta\tau\Big\{\epsilon_d \bar{f}_l^{j\sigma} f_{l-1}^{j\sigma} + i\lambda_j \bar{b}_l^j b_{l-1}^j + i\lambda_j \bar{f}_l^{j\sigma} f_{l-1}^{j\sigma} \\ &- i\lambda_j q_0 N - \bar{f}_l^{j\sigma} f_{l-1}^{j+\eta,\sigma}\left[\Delta_{l-1}^{j,j+\eta} + \frac{t_0}{N}\bar{b}_l^{j+\eta} b_{l-1}^j\right] + \text{h.c.} + \frac{N}{J}\sum_{j,\eta}\bar{\Delta}_l^{j,j+\eta}\Delta_{l-1}^{j,j+\eta}\Big\} \end{aligned} \quad (5.4)$$

$\bar{f}_l^{j\sigma}$ and $f_l^{j\sigma}$ are the Grassmann variables corresponding to the pseudofermion operators for the creation and annihilation of particles when we adopt the slave boson technique. $\bar{b}_l^j$ and b_{l-1}^j are the complex variables corresponding to the slave bosons j is a site index and l the imaginary time label.

In equation 5.4 a summation over repeated indices is implied. $\bar{\Delta}$ and Δ are the complex variables (Stratanovich-Hubbard variables12,13 introduced to write the two body Fermi term as two one body fermion terms. We make the assumption that two neighbouring sites have maximum phase shift, and hence make a periodic saddle point approximation in the complex Bose fields with period $\frac{\pi}{a}$ where a is the lattice parameter which is set equal to 1.

Any lattice vector $\vec{R}_j$ can be realized as

$$\vec{R}_j = n_1\vec{i} + n_2\vec{j} \quad (5.5)$$

Where $\vec{i}$ and $\vec{j}$ are unit vectors and n_1 and n_2 are integers.

The vectors which takes saddle point values to their original value with a sign change are of the form

$$\vec{i}\pi + \vec{j}\pi = \vec{q} \quad (5.6)$$

We make a periodic saddle point approximation in the boson variables Δ_j and b_j and a uniform saddle point approximation in λ_j.

The approximation are indicated as follows.

$$\begin{aligned} i\lambda_j &= \lambda & (5.7) \\ \bar{\Delta}_l^{j,j+\eta} &= \bar{\Delta}\, e^{i\vec{q}\vec{R}_j} & (5.8) \\ \bar{b}_l^{j+\eta} &= \bar{b}\, e^{i\vec{q}\cdot(R_j + \vec{\eta})} & (5.9) \end{aligned}$$

After making the above substitution in equation 5.4 we make a transformation of the action in equation 5.4 from the imaginary time label to the imaginary frequency label and from real space to momentum space. After these transformations the action becomes

$$
\begin{aligned}
S &= \sum_{n,k,\sigma} \{ \; \Delta\tau[\tilde{\epsilon_d} - \frac{4t_0}{N}\bar{b}b\,(\cos(k_x-\pi)+\cos(k_y-\pi)-i\omega_n)]\bar{f}_n^{k\sigma} f_n^{k\sigma} \\
&- \Delta\tau 2\Delta_0(\cos k_x + \cos k_y)\bar{f}_n^{k\sigma} f_n^{k-\pi,\sigma} \\
&- \Delta\tau 2.\bar{\Delta}_0(\cos k_x + \cos k_y)\bar{f}_n^{k-\pi,\sigma} f_n^{k\sigma} \; \} + S_0
\end{aligned} \tag{5.10}
$$

where

$$
\begin{aligned}
\tilde{\epsilon_d} &= \epsilon_d + \lambda - \mu \\
S_0 &= \beta\lambda\bar{b}bN_s - \beta\lambda q_0 N N_s + \beta\frac{N}{J}\bar{\Delta}_0\Delta_0 N_s
\end{aligned} \tag{5.11}
$$

N_s is the number of lattice sites, μ is the chemical potential. But

$$\cos(k_x - \pi) = -\cos k_x \tag{5.12}$$

Equation 5.12 is substituted in equation 5.10 and functional integration over the Grassmann variables are performed. The frequency summations are carried out as described in Chapter 2. The partition function takes the form

$$Z = e^{-\beta F} \tag{5.13}$$

where

$$F = \sum_{k,j,\sigma} \ln(1 + e^{-\beta E_j}) + S_0 \tag{5.14}$$

and

$$E_j = \tilde{\epsilon_d} + (-1)^j 2.\sqrt{(\frac{4t_0^2 b^4}{N^2} + \bar{\Delta}_0\Delta_0)(\cos k_x + \cos k_y)} \tag{5.15}$$

The saddle point values are fixed by

$$\frac{\partial F}{\partial \lambda} = 0 \tag{5.16}$$

$$\frac{\partial F}{\partial \Delta_0^2} = 0 \tag{5.17}$$

$$\frac{\partial F}{\partial b^2} = 0 \tag{5.18}$$

We do the calculation for the degeneracy value $N = 2$. Equation 5.16 on simplification becomes

$$b^2 = \delta \tag{5.19}$$

where δ is the doping concentration. Equation 5.17 becomes

$$\frac{\sqrt{\frac{4t_0^2\delta^2}{N^2}+\Delta_0^2}}{J} = -\frac{1}{N_s}\sum_{j,k}\frac{(\cos k_x+\cos k_y)(-1)^j}{(e^{\beta E_j}+1)} \tag{5.20}$$

Setting $\epsilon_d = 0$, we get

$$E_1 = \lambda - \mu - 2(\cos k_x + \cos k_y)\sqrt{t_0^2\delta^2+\Delta^2} \tag{5.21}$$

This will be less than zero for lower values of k and the other band will not be occupied.

Setting equation 5.21 as equal to zero, we solve for $k_x(1)$, the k_x value at which the energy crosses zero for a particular k_y value. This is given by

$$k_x(1) = \cos^{-1}\left\{\frac{\lambda-\mu}{2\sqrt{t_0^2\delta^2+\Delta^2}} - \cos(k_y)\right\} \tag{5.22}$$

We fix another parameter by setting $k_y = 0$ in equation 5.22. We get

$$k\phi = \cos^{-1}\left\{\frac{\lambda-\mu}{2\sqrt{t_0^2\delta^2+\Delta^2}} - 1\right\} \tag{5.23}$$

From the symmetry of the situation we find that k_y values lies between $-k\phi \leq k_y \leq k\phi$. Solving the saddle point equation we find

$$\lambda = \frac{4t_0^2\delta}{J} \tag{5.24}$$

The energy values can be rewritten as

$$E_j = \frac{4t_0^2\delta}{J} - \mu + (-1)^j 2(\cos k_x + \cos k_y)\sqrt{t_0^2\delta^2+\Delta^2} \tag{5.25}$$

The particles enclosed within the fermi surface will be

$$8\frac{N_s}{4\pi^2}\int_{k_y=0}^{k\phi} dk_y \int_{k_x=0}^{k_x(1)} dk_x = N_s(1-\delta) \tag{5.26}$$

where $k_x(1)$ is given by equation 5.22 and $k\phi$ by equation 5.23. On simplification equation 5.26 becomes

$$\frac{2}{\pi^2}\int_0^{k\phi} dk_y \cos^{-1}\{1+\cos(k\phi)-\cos(k_y)\} = 1-\delta \tag{5.27}$$

The ground state energy per site can be obtained from equation 5.25

$$\begin{aligned} E &= \frac{2}{\pi^2}(\frac{4t_0^2\,\delta}{J} - \mu)\int_0^{k\phi} dk_y \cos^{-1}\{1 + \cos k\phi - \cos k_y\} \\ &- \frac{4}{\pi^2}(t_0^2\,\delta^2 + \Delta^2)^{\frac{1}{2}}\int_0^{k\phi} dk_y \sin\left\{\cos^{-1}(1 + \cos k\phi - \cos k_y)\right\} \\ &- \frac{4}{\pi^2}(t_0^2\,\delta^2 + \Delta^2)^{\frac{1}{2}}\int_0^{k\phi} dk_y \cos k_y \cos^{-1}\{1 + \cos k\phi - \cos k_y\} \qquad (5.28) \end{aligned}$$

The density of states at the fermi surface is given by

$$D(\epsilon_F) = \frac{2}{4\pi^2}\int_{-\pi}^{\pi} dk_y \int_{-\pi}^{\pi} dk_x\, 2\pi\,\delta(E) \qquad (5.29)$$

where E is a function of k_x and k_y and $\delta(E(\vec{k}))$ is given by

$$\delta(\,E(\vec{k})) = \frac{\delta(\vec{k} - \vec{k_0})}{\mid \frac{dE}{dk} \mid_{\vec{k}} = \vec{k_0}} \qquad (5.30)$$

But

$$\mid \frac{dE}{dk} \mid = \sqrt{(\frac{\partial E}{\partial K_x})^2 + (\frac{\partial E}{\partial k_y})^2} \qquad (5.31)$$

and

$$\delta(\vec{k} - \vec{k_0}) = \delta(k_y - k_y(0))\delta(k_x - k_x(0) \qquad (5.32)$$

$$\text{But}\frac{\partial E}{\partial k_x} = 2\sin k_x\sqrt{t_0^2\,\delta^2 + \Delta^2} \qquad (5.33)$$

The k_x corresponding to $E = O$ is given by

$$\cos k_x = \frac{\lambda - \mu}{2\sqrt{t_0^2\,\delta^2 + \Delta^2}} - \cos k_y \qquad (5.34)$$

$$\frac{\partial E}{\partial k_y} = 2\sin k_y\sqrt{t_0^2\,\delta^2 + \Delta^2} \qquad (5.35)$$

Making these substitutions in equation 5.29, the expression for the density of states at the fermi surface becomes

$$D(\epsilon_f) = 4\int_0^{k\phi} \frac{d\theta}{\sqrt{p + q\cos\theta}} \qquad (5.36)$$

where

$$\begin{aligned} P &= 8(t_0^2\,\delta^2 + \Delta^2) - (\lambda - \mu)^2 \qquad (5.37) \\ q &= 4\sqrt{t_0^2\,\delta^2 + \Delta^2(\lambda - \mu)} \qquad (5.38) \end{aligned}$$

5.3 Expression for the Ground state energy and Density of states in a uniform saddle point approximation

The calculation of the partition function in a functional integral formalism using a uniform saddle point approximation is carried out as in reference[11]. The saddle point equation are simplified.

They become

$$\lambda = -\frac{4t_0}{N_s}\sum_k f(E_k)(\cos k_x + \cos k_y) \tag{5.39}$$

$$\Delta = \frac{J}{N_s}\sum_k f(E_k)(\cos k_x + \cos k_y) \tag{5.40}$$

and

$$b^2 = Nq_0\delta \tag{5.41}$$

In the situation of interest

$$Nq_0 = 1 \tag{5.42}$$

$$\text{and}E_k = \mu - \lambda + 2(\cos k_x + \cos k_y)(\Delta + \frac{t_0 b^2}{N}) \tag{5.43}$$

On simplification we get the result

$$\frac{\lambda}{4t_0} = \frac{\Delta}{J} \tag{5.44}$$

The ground state energy is given by

$$U = -\sum_k E_k + \frac{2NN_s\Delta^2}{J} + \lambda N_s b^2 - \lambda N_s \tag{5.45}$$

where E_k is given by equation 5.43.

Those states outside the fermisurface will not be occupied at the zero of temperature and hence we have to solve for the k values for which the energy goes to zero.

For any k_y value inside an interval which will soon be defined, the corresponding maximum/minimum value of k_x will be denoted by $k_x(1)$ and is given by

$$k_x(1) = \cos^{-1}\left\{\frac{\mu - \lambda}{2(\Delta + \frac{t_0 b^2}{2})} - \cos k_y\right\} \tag{5.46}$$

when $k_y = 0$, we define another important quantity

$$k\phi = \cos^{-1}\left\{\frac{\mu - \lambda}{2(\Delta + \frac{t_0 b^2}{2}} - 1\right\} \tag{5.47}$$

Therefore $k_x(1)$ can be written as

$$k_x(1) = \cos^{-1}\left\{1 + \cos(k\phi) - \cos(k_y)\right\} \tag{5.48}$$

The saddle point value of Δ is given by

$$\begin{aligned} \Delta &= \frac{J}{\pi^2}\int_0^{k\phi} dk_y \int_0^{k_x(1)} dk_x\,(\cos k_x + \cos k_y) & (5.49) \\ &= \frac{J}{\pi^2}\int_0^{k\phi} dk_y\,\{\,\sin[\cos^{-1}(1 + \cos k\phi - \cos k_y)] \\ &\quad + \cos k_y \cos^{-1}(1 + \cos k\phi - \cos k_y)\,\} & (5.50) \end{aligned}$$

We do the calculation by using $k\phi$ as a free parameter in terms of which others are defined. For each value of $k\phi$, Δ is calculated and using the Δ value λ is calculated using equation 5.44. On simplification the expression for the ground state energy becomes

$$\begin{aligned} E &= (\frac{4t_0\Delta}{J} - \mu)(\frac{1}{\pi})^2 \int_0^{k\phi} dk_y \cos^{-1}(1 + \cos(k\phi) - \cos k_y) \\ &- 2(\Delta + \frac{\delta t_0}{2})(\frac{1}{\pi})^2 \int_0^{k\phi} dk_y \cos k_y \cos^{-1}(1 + \cos k\phi - \cos k_y) \\ &- 2(\Delta + \frac{\delta t_0}{2})(\frac{1}{\pi})^2 \int_0^{k\phi} dk_y \sin\left\{\cos^{-1}(1 + \cos k\phi - \cos k_y)\right\} & (5.51) \end{aligned}$$

From equation 5.50 we find that Δ is depending on $k\phi$ and J and not on any other parameters. For a particular value of $J, k\phi$ pair, Δ is calculated. Using this value of $k\phi$, J, and, Δ the chemical potential is calculated. We find that the chemical potential depends in addition to the above quantities the doping concentration δ,

$$\mu = t_0\delta(1 + \cos k\phi) + 2\Delta(\frac{2t_0}{J} + 1 + \cos k\phi) \tag{5.52}$$

The density of states at the fermi surface is obtained as in the previous section.

$$D(\epsilon_F) = 4\int_0^{k\phi} \frac{A\,dk_y}{\sqrt{2 - (\lambda - \mu)^2 A^2 - 2(\lambda - \mu)A\cos k_y}} \tag{5.53}$$

where

$$A = .5(\Delta + .5b^2 t_0)^{-\cancel{2}\,1} \tag{5.54}$$

5.4 Numerical calculations and conclusions

Numerical calculations have been carried out for various parameter values both in the periodic saddle point version and the uniform saddle point version for the ground state energy and the density of states at the fermi surface. The results of these computations are given in figures. In periodic saddle point calculation the relation between δ and $k\phi$ is plotted in figure (5.1). It shows a linear relation to hold between the above two quantities. In figure (5.2) μ is plotted against $k\phi$ in a uniform saddle point analysis. Figure(5.3) shows the variation of the ground state energy with doping concentration obtained in a periodic saddle point calculation and figure (5.4) shows that in a uniform saddle point calculation. From these figures it is clear that for the same parameter regime, the periodic saddle point has a lower ground state energy than the uniform saddle point results. Hence the system should obey the periodic saddle point behaviour. The relationship between chemical potential and $k\phi$ in a uniform saddle point calculation which is related to the fermi momentum is plotted in figure (5.5). In figure(5.6) the density of states per Cu is plotted against doping concentration in a periodic saddle point calculation and in figure(5.7) This is done for the uniform saddle point case.

The results presented in figures(5.6) and (5.7) shows that the density of states per Cu atom evaluated in a periodic saddle point agrees better with experimental results[14] and previous calculations[15,16]. In this technique the fluctuation correction have to be performed for the Bose variables and Lagrange multiplier variables about the saddle point. Unlike the uniform case a straight forward technique is hard to come by and hence the treatment is postponed for a future work.

5.5 References

1. J.G. Bednorz and K.A. Muller, Z. Phys. B64, 188 (1986)
2. P.W. Anderson, Science 235, 1196 (1987)
3. C.M Varma, S. Schmitt - Rink and E. Abraham, Solid State Commun. 62, 681 (1987)
4. V.Z. Kresin, Phys. Rev. B 35, 8716 (1987)
5. R. Jagadish and K.P. Sinha, Current Science 56, 291 (1987)
6. J. Bardeen, L.N. Cooper and J.R. Schrieffer, Phys. Rev. 106, 162 (1957)

7. D. Vaknin, S.K. Sinha, D.E. Moncton, D.C. Johnston, J.M. Newsam, C.R. Safinya and H.E. King Jr., Phys. Rev. Lett. 58, 2802 (1987)

8. J. Hubbard, Proc. Roy. Soc. (London) A 276, 238 (1963); 277, 238 (1964)

9. A.B. Harris and R.V. Lange, Phys. Rev. 157, 279 (1967)

10. S.E. Barnes, J. Phys. F6, 1375 (1976)

11. M. Grilli and G. Kotliar, Phys. Rev. Lett. 64, 1170 (1990)

12. J.W. Negele and H. Orland, Quantum Many Particle Systems (Addison - Wesley, Reading, M.A. 1988)

13. R.L. Stratanovich, Dokl. Akad. Nauk. S.S.S.R. 115, 1957 (1958, Sov. Phys. Dokl. 2, 416)

14. M. Grilli, B.G. Kotliar and A.J. Millis, Phys. Rev. B 42, 329 (1990)

15. D.M. Newns, M. Rasolt and P.C. Pattnaik, Phys. Rev. B38, 6513 (1988)

16. Suresh V. Vettoor and V.M. Nandakumaran, Physica C 191, 277 (1992)

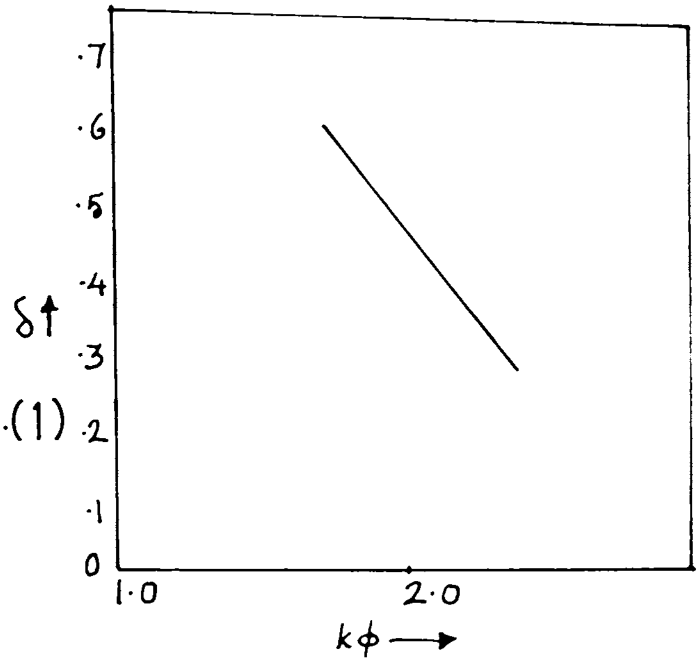
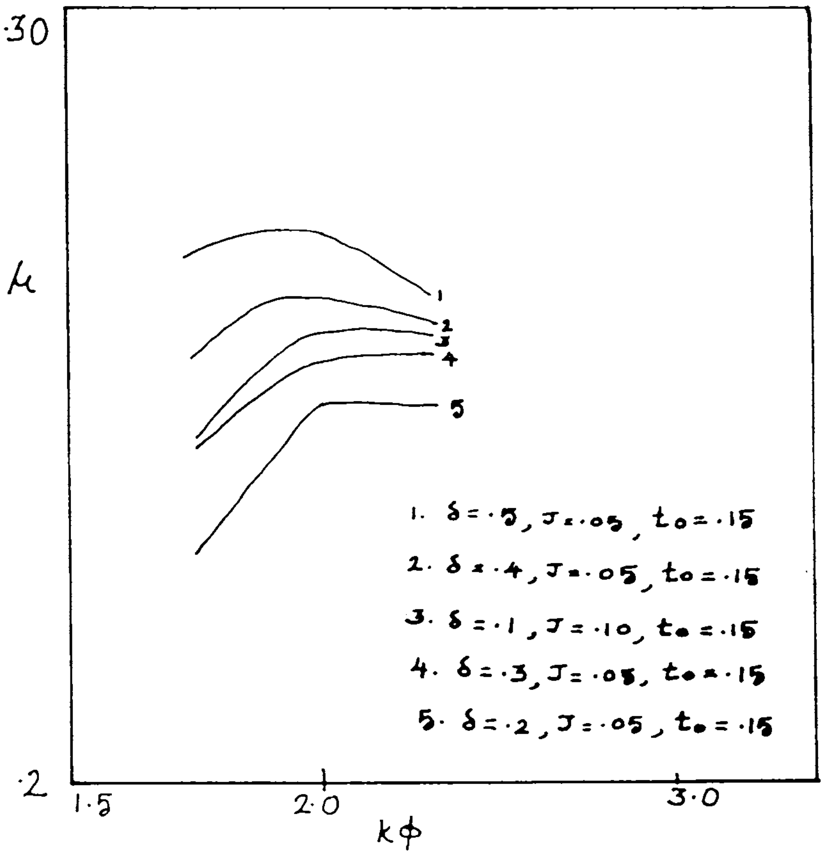
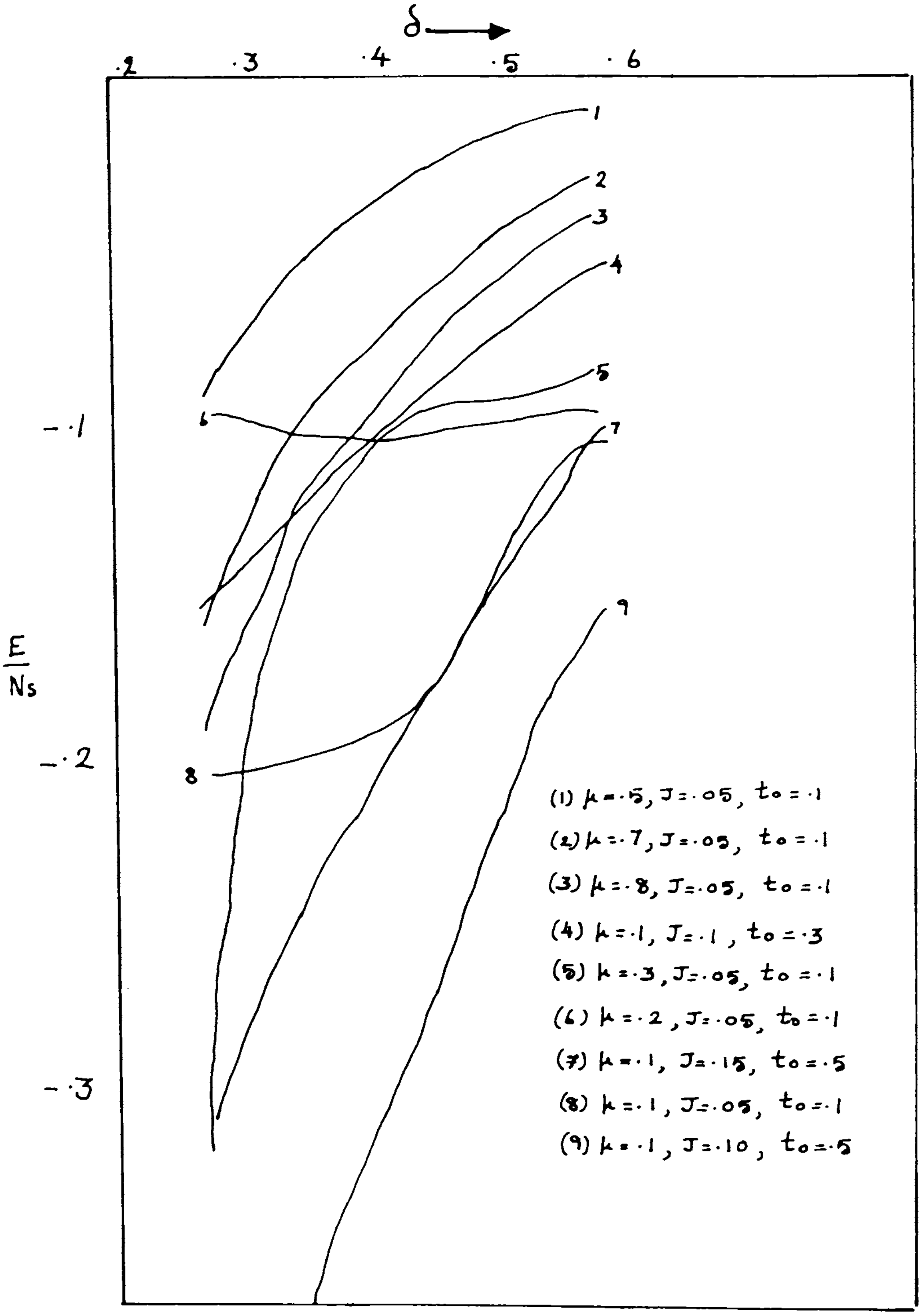

·7
·6
·5
·4
·3
·2
·1
0
δ↑
1·0
2·0
kφ ⟶

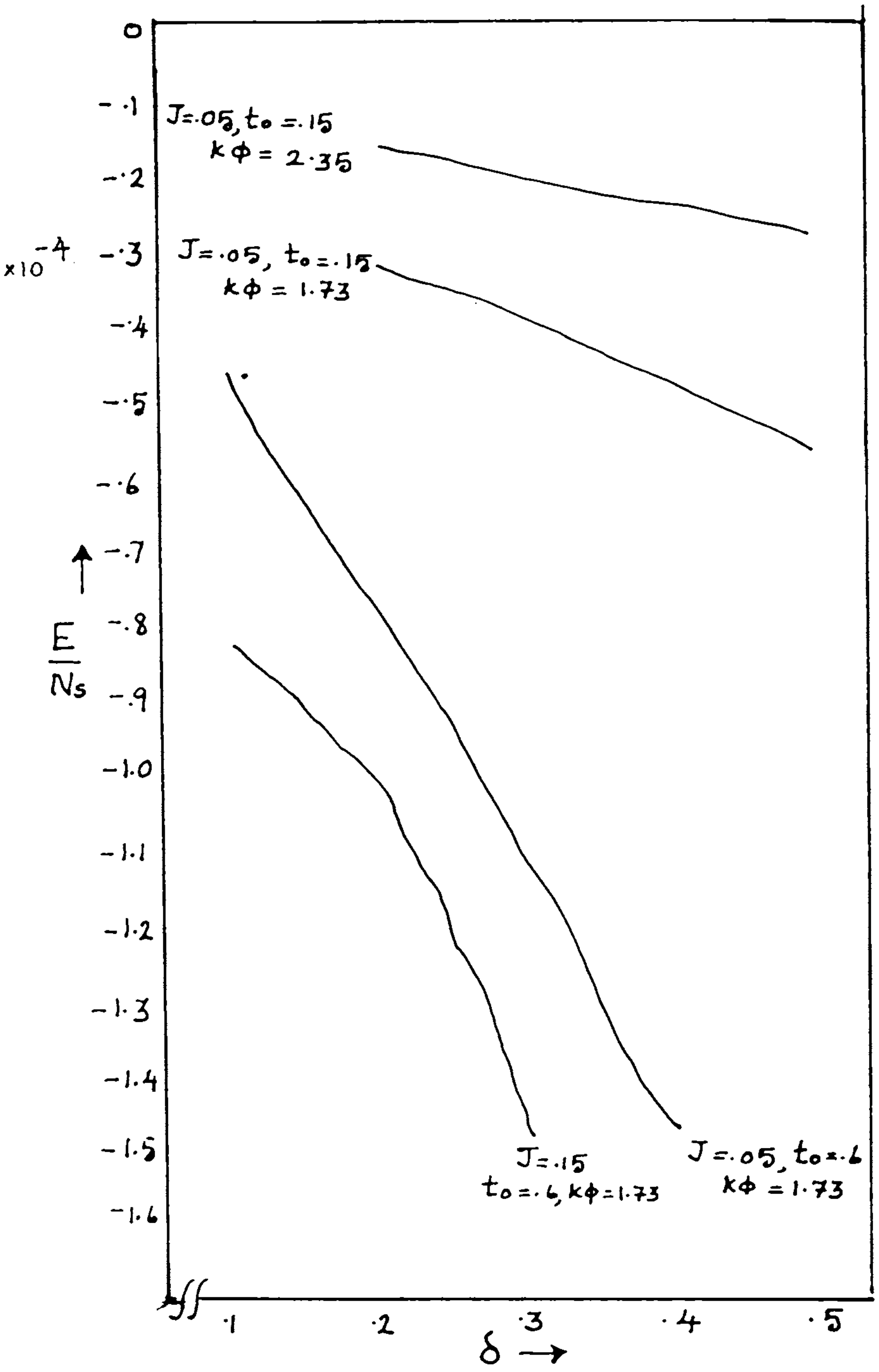
fig.(1)


·30
μ
·2
1·5
2·0
3·0
kφ
1
2
3
4
5
1. δ = ·5, J = ·05, t₀ = ·15
2. δ = ·4, J = ·05, to = ·15
3. δ = ·1, J = ·10, t₀ = ·15
4. δ = ·3, J = ·05, t₀ = ·15
5. δ = ·2, J = ·05, t₀ = ·15

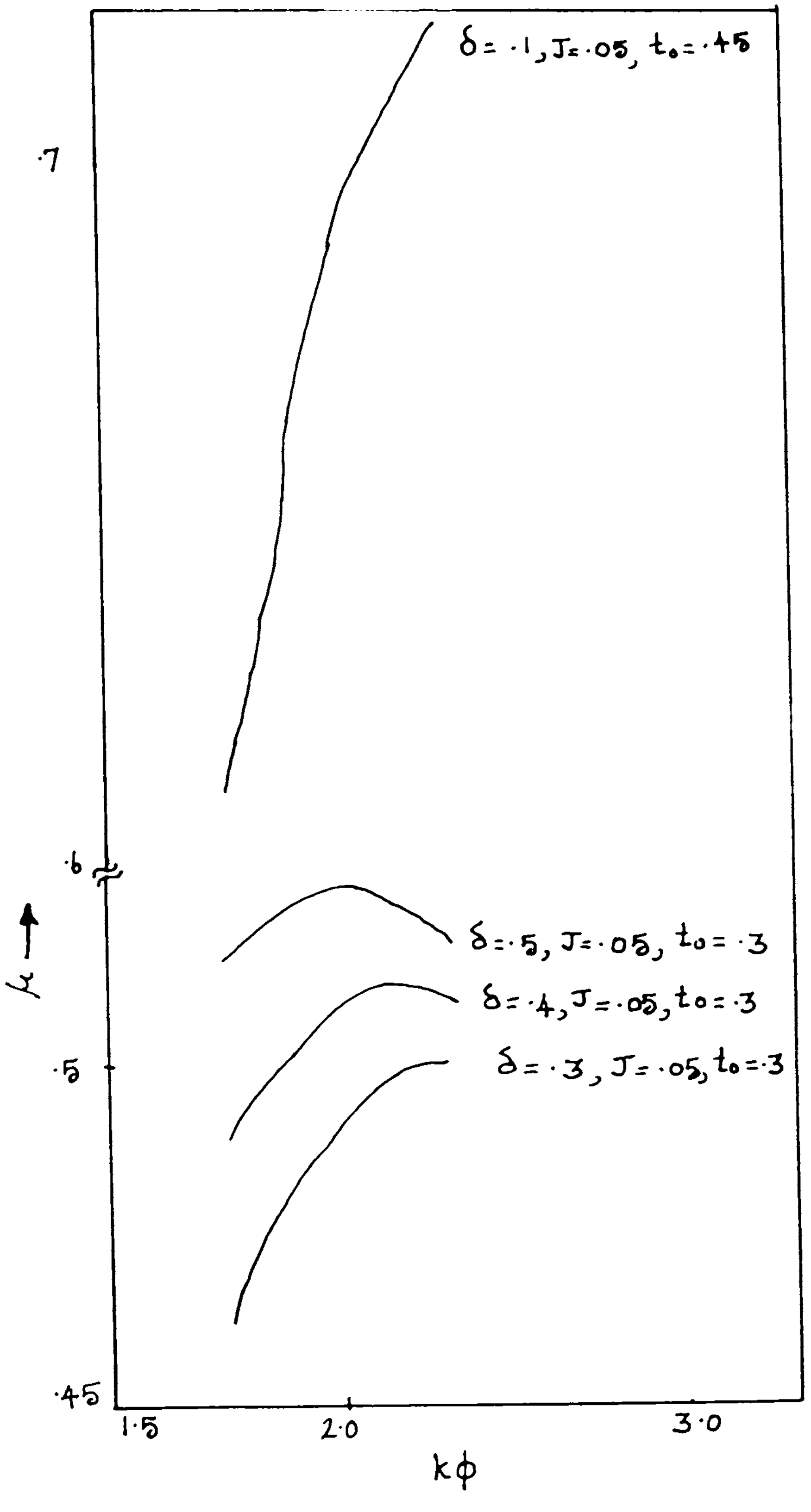
fig(2)


$\delta \rightarrow$
·2
·3
·4
·5
·6
$\frac{E}{N_s}$
−·1
−·2
−·3
1
2
3
4
5
6
7
8
9
(1) $\mu=\cdot5$, $J=\cdot05$, $t_o=\cdot1$
(2) $\mu=\cdot7$, $J=\cdot05$, $t_o=\cdot1$
(3) $\mu=\cdot8$, $J=\cdot05$, $t_o=\cdot1$
(4) $\mu=\cdot1$, $J=\cdot1$, $t_o=\cdot3$
(5) $\mu=\cdot3$, $J=\cdot05$, $t_o=\cdot1$
(6) $\mu=\cdot2$, $J=\cdot05$, $t_o=\cdot1$
(7) $\mu=\cdot1$, $J=\cdot15$, $t_o=\cdot5$
(8) $\mu=\cdot1$, $J=\cdot05$, $t_o=\cdot1$
(9) $\mu=\cdot1$, $J=\cdot10$, $t_o=\cdot5$

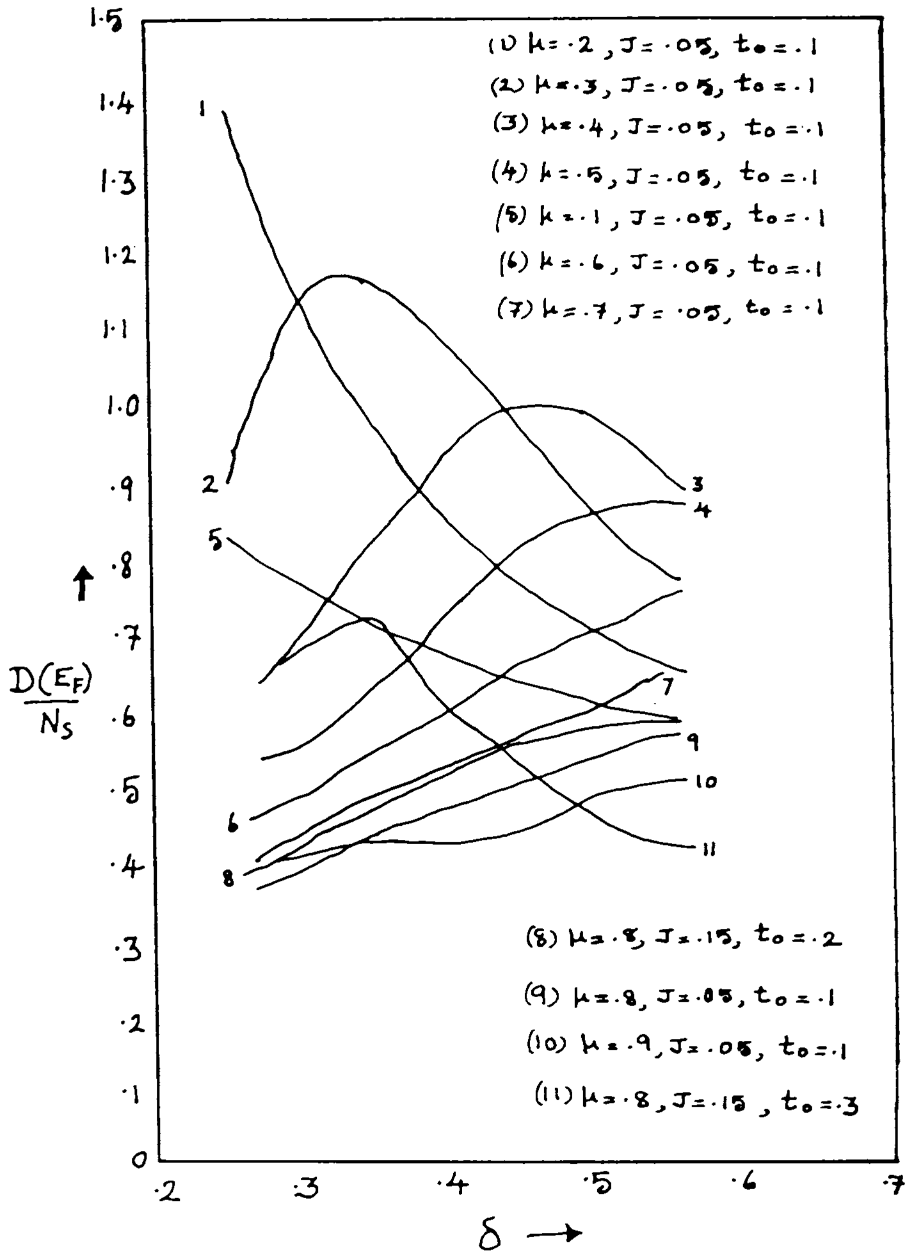
fig(3)


0
-·1
-·2
-·3
-·4
-·5
-·6
-·7
-·8
-·9
-1·0
-1·1
-1·2
-1·3
-1·4
-1·5
-1·6
$\times 10^{-4}$
$\frac{E}{N_s}$ ↑
·1
·2
·3
·4
·5
δ →
$J=\cdot 05, t_0=\cdot 15$
$k\phi = 2\cdot 35$
$J=\cdot 05, t_0=\cdot 15$
$k\phi = 1\cdot 73$
$J=\cdot 15$
$t_0=\cdot 6, k\phi=1\cdot 73$
$J=\cdot 05, t_0=\cdot 6$
$k\phi = 1\cdot 73$

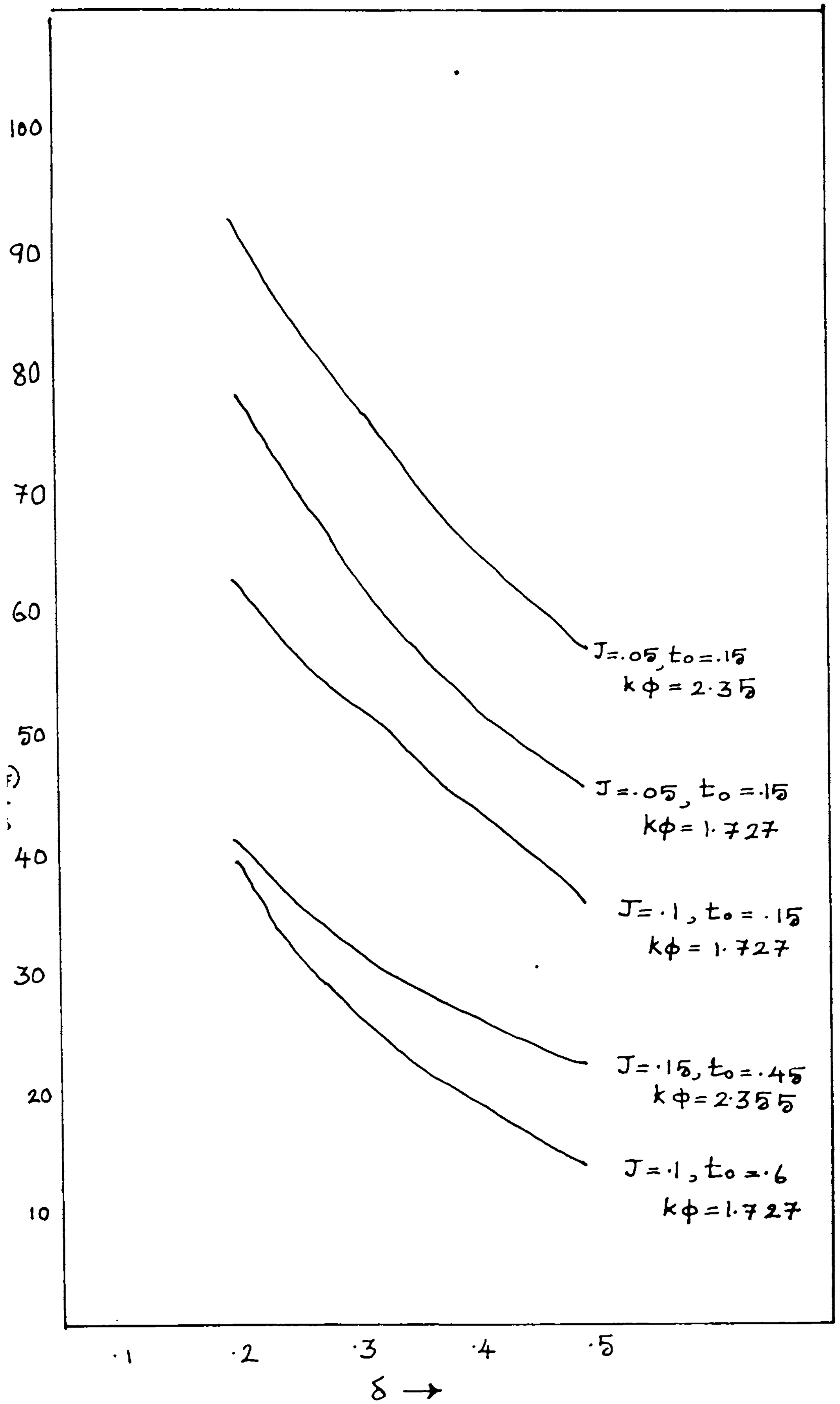
fig(4)



fig(5)


(1) μ= ·2 , J= ·05, t₀ = ·1
(2) μ=·3, J=·05, t₀ = ·1
(3) μ=·4, J=·05, t₀ =·1
(4) μ=·5, J=·05, t₀ =·1
(5) μ=·1 , J=·05, t₀=·1
(6) μ=·6, J=·05, t₀=·1
(7) μ=·7, J= ·05, t₀ = ·1
(8) μ=·8, J=·15, t₀ =·2
(9) μ=·8, J=·05, t₀ =·1
(10) μ=·9, J=·05, t₀=·1
(11) μ=·8, J=·15 , t₀=·3
1
2
3
4
5
6
7
8
9
10
11
D(E_F) / N_S
1·5
1·4
1·3
1·2
1·1
1·0
·9
·8
·7
·6
·5
·4
·3
·2
·1
0
·2
·3
·4
·5
·6
·7
δ →

fig(6)


100
90
80
70
60
50
40
30
20
10
·1
·2
·3
·4
·5
δ →
J=.05, t₀=.15
kφ = 2·35
J=·05, t₀ =·15
kφ= 1·727
J= ·1, t₀ = ·15
kφ = 1·727
J=·15, t₀=·45
kφ=2·355
J=·1, t₀ =·6
kφ=1·727

fig(7)

Chapter 6

CONCLUSIONS

We have discussed in the first chapter various experimental results which are peculiar to high Tc materials. These results imposes a variety of constraints on theory construction in this field. High superconducting transition temperature of these materials is only one of the puzzles to be unraveled. The various normal state properties of these materials are quite unlike that of conventional metallic superconductors.

The high Tc materials are generally believed to be strongly correlated and hence a rigorous theoretical formulation of the basic Physics can be achieved by adopting slave boson techniques of Barnes[1] and Coleman[2] or Kotliar and Ruckenstein[3]. With this end in view, the functional integral formalism is discussed at length in Chapter 2. In the same chapter the slave boson formalisms are briefly discussed within the framework of functional integration.

In Chapter 3 a strong coupling theory is suggested to explain superconductivity in high Tc materials in Anderson lattice model using double time Green's functions and equation of motion technique for the evaluation of Green's functions. In that analysis the large U limit is not appropriately taken into account.

In Chapter 4 the extended model is considered with direct hopping from oxygen to oxygen. Considering the large U limit of the model, the functional integral for the partition function is set up. A uniform saddle point approximation in the Bose variables and Lagrange multiplier variables are applied and the functional integration over the fermi variables are performed. From the expression for the free energy the density of states and specific heat capacity of the system is calculated and compared with experiments and previous calculations.

A reduction of the extended model with zero direct overlap between oxygen orbitals to a $t-J$ model became apparent[4,5,6,7]. It seemed plausible that some of the correlations in the system can be taken care of by adopting a periodic saddle point approximation in the Bose variables when the functional integral for the partition function of the system is performed.

The results so obtained are compared with the calculation based on a uniform saddle point approximation[8]. It is found from the estimation of the ground state energy that a periodic saddle point is a better description than a uniform saddle point approach. The density of states at the fermi surface is calculated for various parameter values. The numerical results are compared with experimental results.

The scenario of high temperature superconductivity theory research ranges from BCS like weak coupling to strong coupling theories where electron-electron attractive interaction has an essentially repulsive origin[9]. Quasi two dimensionality seems essential to any model of high Tc superconductivity. The basic Hamiltonian for the description of the normal state physics of the system is the extended Hubbard model[10]. But there is a dominant point of view that the extended model is an unnecessary tour de force of no value for the physics. According to P.W. Anderson[11], in the correct parameter regime, the extended model can be reduced to a Hubbard model with hopping term and an on site repulsion term. A standard strong coupling perturbation treatment of the single band Hubbard model will lead to the $t-J$ model Hamiltonian[7]. Studies on $1D$ Hubbard model has lead the RVB school of thought to propose the idea of spin-charge decoupling[12]. The idea is that the strongly correlated system sustains two types of excitations. The charge and spin excitations propagate with different velocities. The spin 1/2 chargeless excitations are called spinons and $\overset{+}{-}e$ charged spinless excitations called holons. In $1-D$ Hubbard model three powerful theoretical tools are employed - Jordan - Wigner[13] transformation (bosonization), conformal field theories[14] and the Bethe ansatz[15,16] techniques. Going to $2-D$, the exact solvability of the Hubbard model or $t-J$ model is yet to be achieved by any method not even the conformal field theory techniques or the Bethe ansatz technique. Yet another powerful method of study is the one using the manifestly spin rotation invariant generalization of Kotliar-Ruckenstein slave boson technique[17].

Another question debated in the context of high temperature superconductors is whether the systems are Luttinger liquids[18,19] or marginal fermi liquids[20]. Haldane has characterized the behaviour of a large variety of one dimensional quantum fluids by the term "Luttinger liquid" showing that they can all be solved by a common strategy. The strategy is bosonization in which the excitations close to the fermi surface are transformed in to phase and phase shift variables. The marginal fermi liquid phenomenology put forward by C.M. Varma and others is based on an analysis of several normal state properties of high Tc superconductors. The single hypothesis on which the results rests is that the low energy particle hole excitations have no energy scale other than the temperature.

Another candidate theoretical model is the spin bag model suggested by Schrieffer et al.[21]. Some of the weak coupling theories are based on various pairing mechanisms. These include interlayer pairing mechanisms[22], phonon mediated pairing with band structure effects[23], plasmon mediated pairing[24,25] models with various charge transfer excitations[26] playing the role exchange boson, and antiferromagnetic magnon[27] mediated pairing. It has been believed that most of these models are not appropriate for the ceramic oxide superconductors.

The phenomenological model of Varma et al.[20] bring together various anomalous features and hence any microscopic formulation should at some stage leads to these results. But this gives no clear idea about the pairing instabilities and also the pairing mechanisms.

In the extended Hubbard model suggested by Varma et al.[10], the essential two body terms are the on site repulsion at copper sites and the intersite repulsion between copper and oxygen holes. Here the nearest neighbour repulsion plays a crucial role in charge transfer and hence Varma et al. stresses the importance of including these terms. But with their inclusion, the problem becomes far more complicated to have a solution without adopting several approximations. This makes it difficult to compare experimental results with theoretical calculations. Notwithstanding these difficulties, it seems the only theory which contains the seeds of a pairing mechanism in the weak coupling limit.

The single band Hubbard model and its reduced version $t - J$ model contains fewer number of parameters and hence simpler for subjecting to a rigorous analysis. Studies on finite size versions of the above models in $2D$ using quantum Montecarlo techniques are abounding. They are providing us with valuable information about these models. But still the new concepts such as spin charge decoupling or Luttinger liquid still lacks a rigorous footing when we approach the 2-D version of the above models.

To conclude a brief look at the possible future work we plan to do, is given. In any analytical scheme for the many body problem an exact solution is impossible to obtain except in a limited number of simplified models. These simplified models may be of much practical value for the analysis of more complicated models.

The high temperature superconductors are doped materials. The doping can renormalize some of the small parameters to large values and large parameters to small values. We intend to do parameter rescaling in the extended Hubbard model with direct hopping between neighbouring oxygens included. To do this we intend to formulate the problem in a manifestly spin rotation invariant version of the Kotliar Ruckenstein slave boson technique[17]. A periodic saddle point is assumed to be favoured and such an evaluation is intended to be carried out. The correlation function on which the parameters have a dependence will be calculated and parameter rescaling will be done until self consistency is achieved. We hope that such an analysis will provide us with valuable information regarding the pairing instabilities of the system.

6.1 References

1. S.E. Barnes, J. Phys. F6, 1375 (1976)
2. P. Coleman, Phys. Rev. B29, 3035 (1984)
3. G. Kotliar and A.E. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986)
4. A.B. Harris and R.V. Lange, Phys. Rev. 157, 279 (1967)
5. J.E. Hirch, Phys. Rev. Lett. 54, 1317 (1985)
6. K. Huang and E. Manousakis, Phys. Rev. B36, 8302 (1987)
7. F.C. Shang and T.M. Rice, Phys. Rev. B37, 3759 (1988)
8. M. Grilli and G. Kotliar, Phys. Rev. Lett. 64 (1170) (1990)
9. P.W. Anderson, Science 235, 1196 (1987)
10. C.M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. 62, 681 (1987)
11. P.W. Anderson, Cargese lectures, June 1990
12. P.W. Anderson, Int. J. of Modern Physics B4, 181 (1990)
13. P. Jordan, E. Wigner, Z. Phys. 47, 631 (1928) 14. V. Dotsenko, Nucl. Phys. 235 B (FS11), 54 (1984)
15. H. Bethe, Z. Physik 71, 205 (1931)

16. M. Ogata and H. Shiba, Phys. Rev. B41, 2326 (1990)

17. T. Li, P. Wolfle and P.J. Hirschfeld, Phys. Rev B40, 6817 (1989)

18. F.D.M. Haldane, J. Phys. C. Solid State Phys. 14, 2585 (1981)

19. P.W. Anderson, Phys. Rev. Lett. 64, 1839 (1990)

20. C.M. Varma, P.B. Littlewood, S. Schmitt-Rink, E. Abrahams and A.E. Ruckenstein, Phys. Rev. Lett. 63, 1996 (1989)

21. J.R. Schrieffer, X.G. Wen, and S.C. Zhang, Phys. Rev. Lett. 60, 944 (1988); Phys. Rev. B39, 11663 (1989)

22. S.S. Jha, in Int. Conference on Superconductivity (ICSC) Jan. 10-14, Bangalore (1990) pages 372-384.

23. Y. Shuna and Y.O. Nakamura, Solid State Commun. 76, 1189 (1990)

24. V.Z. Kresin, Phys. Rev. B35, 8716 (1987)

25. V.M. Nandakumaran, Pramana J. Phys. 29, L113 (1987)

26. R. Jagadish and K.P. Sinha, Current Science, 56, 291 (1987)

27. A.E. Ruckenstein, P.J. Hirchfeld and J. Appel, Phys. Rev. B36, 2371 (1987)

Appendix A

Proof of the general relation between A^N and A

$$A(\bar{\eta},\eta) = e^{\bar{\eta}\eta} A^N(\bar{\eta},\eta)$$

Proof:

$$\hat{A} = \sum_{n,m} A_{nm} : (c^\dagger)^n e^{-c^\dagger c} c^m : \tag{.1}$$

$$\hat{A} = \sum_{n,m} A_{nm} \{ (c^\dagger)^n c^m - (c^\dagger)^{n+1} c^{m+1} \} \tag{.2}$$

The last expression is expressed in normal ordered form, so

$$A^N(\bar{\eta},\eta) = \sum_{n,m=0,1} A_{nm} (\bar{\eta}^n \eta^m - \bar{\eta}^{n+1} \eta^{m+1}) \tag{.3}$$

From equation 2.30

$$A(\bar{\eta},\eta) = \sum_{n,m=0,1} \bar{\eta}^n A_{nm} \eta^m \tag{.4}$$

Multiplying the righthand side of equation .3 with $e^{\bar{\eta}\eta} = 1 + \bar{\eta}\eta$ we get

$$e^{\bar{\eta}\eta} A^N(\bar{\eta},\eta) = \sum_{n,m} A_{nm} (\bar{\eta}^n \eta^m - \bar{\eta}^{n+1} \eta^{m+1} + \bar{\eta}\eta\bar{\eta}^n \eta^m - \bar{\eta}\eta\bar{\eta}^{n+1} \eta^{m+1}) \tag{.5}$$

On simplification we find that the righthand side is equal to $A(\bar{\eta},\eta)$ and hence the relation is proved.

Appendix B

We prove the following relation in this appendix.

$$(A_1 A_2)^N(\bar{\eta},\xi) = \int d\bar{\omega} d\omega e^{(\bar{\eta}-\bar{\omega})\omega} e^{(\bar{\omega}-\bar{\eta})\xi} A_1^N(\bar{\eta},\omega) A_2^N(\quad \bar{\omega} \quad ,\xi) \tag{.6}$$

Proof:

Repeatedly applying equation 2.29

$$\begin{aligned}
[A_1 A_2 f](\bar{\eta}) &= [A_1(A_2 f)](\bar{\eta}) && (.7)\\
\text{Put} A_2 f &= F && (.8)\\
[(A_1 A_2) f]\,(\bar{\eta}) &= [A_1 F](\bar{\eta}) && (.9)\\
&= \int d\bar{\omega} d\omega e^{-\bar{\omega}\omega} A_1(\bar{\eta},\omega) F(\bar{\omega}) && (.10)\\
&= \int d\bar{\omega} d\omega e^{-\bar{\omega}\omega} A_1(\bar{\eta},\omega) (A_2 f)(\bar{\omega}) && (.11)\\
&= \int d\bar{\xi} d\xi e^{-\bar{\xi}\xi} \int d\bar{\omega} d\omega e^{-\bar{\omega}\omega} A_1(\bar{\eta},\omega) A_2(\bar{\omega},\xi) f(\bar{\xi}) && (.12)
\end{aligned}$$

so that

$$(A_1A_2)(\bar\eta,\xi) = \int d\bar\omega d\omega e^{-\bar\omega\omega} A_1(\bar\eta,\omega)A_2(\bar\omega,\xi) \tag{.13}$$

Applying equation 2.41 separately to A_1A_2 and A_1 and A_2 leads to

$$\begin{aligned}
(A_1A_2)(\bar\eta,\xi) &= e^{\bar\eta\xi}(A_1A_2)^N(\bar\eta,\xi) && (.14)\\
A_1(\bar\eta,\omega) &= e^{\bar\eta\omega}A_1^N(\bar\eta,\omega) && (.15)\\
A_2(\bar\omega,\xi) &= e^{\bar\omega\xi}A_2^N(\bar\omega,\xi) && (.16)
\end{aligned}$$

substituting in equation .13, we get

$$\begin{aligned}
&e^{\bar\eta,\xi}(A_1A_2)^N(\bar\eta,\xi)\\
&\qquad = \int d\bar\omega d\omega e^{-\bar\omega\omega}e^{\bar\eta\omega}A_1^N(\bar\eta,\omega)e^{\bar\omega\xi}A_2^N(\bar\omega,\xi)\\
&\qquad = \int d\bar\omega d\omega e^{-\bar\omega\omega}e^{\bar\eta\omega}e^{\bar\omega\xi}A_1^N(\bar\eta,\omega)A_2^N(\bar\omega,\xi)
\end{aligned}$$

Multiplying both sides from the left with $e^{-\bar\eta\xi}$, we get

$$(A_1A_2)^N(\bar\eta,\xi) = \int d\bar\omega d\omega e^{-\bar\eta\xi}e^{-\bar\omega\omega}e^{\bar\eta\omega}e^{\bar\omega\xi}A_1^N(\bar\eta,\omega)A_2^N(\bar\omega,\xi) \tag{.17}$$

The R.H.S is equal to

$$\int d\bar\omega d\omega e^{-\bar\omega-\bar\eta)\xi}e^{(\bar\eta-\bar\omega)\omega}A_1^N(\bar\eta,\omega)A_2^N(\bar\omega,\xi) \tag{.18}$$

Thus equation 2.42 is proved.

Appendix C

Proof of the relation

$$\text{Trace}\hat{A} = \int d\eta d\bar\eta e^{2\bar\eta\eta}A^N(\bar\eta,\eta)$$

Proof:

$$A^N(\bar\eta,\eta) = A_{00} + A_{01}\eta + A_{10}\bar\eta + A_{11}\bar\eta\eta - A_{00}\bar\eta\eta \tag{.19}$$

Therefore

$$(1+2\bar\eta\eta)A^N(\bar\eta,\eta) = A_{00} + A_{01}\eta + A_{10}\bar\eta + A_{11}\bar\eta\eta - A_{00}\bar\eta\eta + 2A_{00}\bar\eta\eta \tag{.20}$$

Therefore

$$\int d\eta d\bar\eta e^{2\bar\eta\eta}A^N(\bar\eta,\eta) = A_{11} - A_{00} + 2A_{00} = A_{00} + A_{11} \tag{.21}$$

The righthand side is the sum of the diagonal terms.Hence

$$\int d\eta d\bar{\eta} e^{2\bar{\eta}\eta} A^N(\bar{\eta},\eta) = \mathrm{Trace}\hat{A} \tag{.22}$$

Appendix D

Functional representation of Fock space.Fock space for fermions(bosons) may be represented by a functional space based on Grassmann (complex) variables. The important relation between the Fock space for a single Fermion(Boson) level and the corresponding functional space are listed below. The ket $\mid n >$ represents an n particle state. Greek letters represents Grassmann variables and Roman letters represents complex numbers. Complex integration element is $d\bar{z}dz = \frac{d(\mathrm{Re}_z).d(\mathrm{Im}_z)}{\pi}$

Fock space		functional space
Fock space elements	F	$f(\bar{\eta}) = f_0 + f_1\bar{\eta}$
$\mid f >= \sum_n f_n \mid n >$	B	$f(\bar{z}) = \sum_{n=0}^{\infty} f_n \frac{\bar{z}^n}{\sqrt{n!}}$
Fock space operators	F	$A(\bar{\eta},\eta) = \sum_{n,m=0}^{1} A_{nm}\bar{\eta}^n\eta^m$
$\hat{A} = \sum_{n,m} A_{n,m} \mid n >< m \mid$	B	$A(\bar{z},z) = \sum_{n,m=0}^{\infty} A_{nm}\frac{\bar{z}^n}{\sqrt{n!}}\frac{z^m}{\sqrt{m!}}$
Normal ordered Fock space operators	F	$A^N(\bar{\eta},\eta) = \sum_{n,m=0}^{1} A_{nm}^N\bar{\eta}^n\eta^m$ $= e^{-\bar{\eta}\eta}A(\bar{\eta},\eta)$
$\hat{A} = \sum_{n,m} A_{nm}^N (a^\dagger)^n a^m$	B	$A^N(\bar{z},z) = \sum_{n,m=0}^{\infty} A_{nm}^N \frac{\bar{z}^n}{\sqrt{n!}}\frac{z^m}{\sqrt{m!}}$ $= e^{-\bar{z}z}A(\bar{z},z)$
Action of an operator on a Fock space element	F	$(Af)(\bar{\eta}) = \int d\bar{\xi}d\xi e^{(\bar{\eta}-\bar{\xi})\xi}A^N(\bar{\eta},\xi)f(\bar{\xi})$
$\hat{A} \mid f >$	B	same form with$\eta,\xi \rightarrow z,v$

Appendix E

Functional representation of Fock space. Greek letters represents Grassmann variables and Roman letters represents complex variables. Bose integration element is $d\bar{z}dz = \frac{d(\mathrm{Re}_z)d(\mathrm{Im}_z)}{\pi}$

Fock space		functional space
Operator product	F	$(A_1A_2)^N(\bar{\eta}\xi) = \int d\bar{\omega}d\omega e^{(\bar{\eta}-\bar{\omega})\omega}e^{(\bar{\omega}-\bar{\eta})\xi}A_1^N(\bar{\eta},\omega)A_2^N(\bar{\omega},\xi)$
$\hat{A}_1\hat{A}2$	B	same form with$\eta,\xi,\omega \rightarrow z,v,w$
Operator Trace	F	$\mathrm{Trace}\hat{A} = \int d\eta d\bar{\eta}e^{2\bar{\eta}\eta}A^N(\bar{\eta},\eta)$
$\mathrm{Tr}\hat{A}$	B	$\mathrm{Trace}\hat{A} = \int d\bar{z}dzA^N(\bar{z},z)$
Gaussian integrals	F	$\int_\eta e^{-\bar{\eta}A\eta+\bar{\omega}\eta+\bar{\eta}\xi} = \det Ae^{\bar{\omega}A^{-1}\xi}$
	B	$\int_z e^{-\bar{z}Az+\bar{u}z+\bar{z}v} = (\det A)^{-1}e^{\bar{u}A^{-1}v}$

Appendix F

In chapter 3 of the thesis , a study of electron-phonon interaction in an Anderson lattice model is done.There we identified erroneously the hybridization gap as an order parameter for superconductivity.In this appendix we carry out the energy gap calculation for the true superconducting gap. The lattice Anderson model in the large U limit can be analyzed by adopting a functional slave boson technique. For details of the method see chapter 2

The partition function for the model is set up as a functional integral over Grassmann variables (corresponding to fermi degrees of freedom) and complex variables (for Bose variables).It is elaborately given in chapter 2 that the slave boson technique necessitates another integration to enforce the constraint.These are the integration over Lagrange multiplier variables.The functional integral is approximated by the uniform saddle point values in the Lagrange multiplier variables and the slave boson variables.The two body term can be decoupled by adopting Stratanovich -Hubbard transformation.Here ,as we are investigating the superconducting instability, a pairing meanfield decomposition is done.How this is done is given in chapter 2.First the integration over Grassmann variables corresponding to localized states is done.Then the action is written in the form of equation (2.310) with $G(E)$ taking the new form

$$G(E) = \frac{i\omega_n - E}{(i\omega_n - \epsilon_k)(i\omega_n - E) - V_1^2 b^2} \tag{1}$$

where $E = E_0 + \lambda$ and b^2 is the saddle point value of slave boson fields. Then the arguments of an analysis given in chapter 2 follows.Thus the functional integral can be evaluated.We write the partition function as a product of a static part and a dynamic part.The static part is evaluated by making a saddle point analysis for the pairing mean field .This saddle point equation leads to

$$1 = -\frac{1}{\beta}\sum_{k,n}\frac{g}{\{(i\omega_n)^2 - \epsilon_k^2 - g \mid \xi \mid^2\}\{1 - A\}} \tag{2}$$

where g is the coupling constant and A is given by

$$A = \frac{V_1^2 b^2 A_1}{A_2} \tag{3}$$

$$A_1 = (i\omega_n + \epsilon_k)(i\omega_n + E) + (i\omega_n - \epsilon_k)(i\omega_n - E) \tag{4}$$

$$A_2 = \{(i\omega_n)^2 - \epsilon_k^2\}\{(i\omega_n)^2 - E^2\} - g \mid \xi \mid^2 \{(i\omega_n)^2 - E^2\} \tag{5}$$

assuming $V_1 <\mid E \mid$ equation 2 becomes

$$1 = -\frac{1}{\beta}\sum_{k,n}\{\frac{g}{\{(i\omega_n)^2 - \epsilon_k^2 - g \mid \xi \mid^2\}} + \frac{gA}{(i\omega_n)^2 - \epsilon_k^2 - g \mid \xi \mid^2}\} + O(V_1^4) \tag{6}$$

When the frequency summations are done along standard lines,we get the equation containing the order parameter.

$$1 = Ng\ln\{\frac{\hbar\omega_D + \sqrt{(\hbar\omega_D)^2 + g \mid \xi \mid^2}}{\sqrt{g \mid \xi \mid^2}}\} - 3gV_1^2 b^2 N\{I_1 + I_2\} \tag{7}$$

Where N is the density of states at the fermi level and I_1 and I_2 are the integrals to be evaluated.In the limit $V_1 \rightarrow 0$,this reduces to the BCS gap equation.The gap equation is solved approximately by discarding the term containing V_1^2. This expression for the gap (order parameter) is substituted in the term containing V_1^2.Then the gap equation takes the new form

$$\sqrt{g \mid \xi \mid^2} \approx 2\hbar\omega_D e^{-\frac{1}{Ng'}} \tag{8}$$

where g' is given by

$$g' = \frac{g}{1 + 3NgV_1^2 b^2 \{I_1 + I_2\}} \tag{9}$$

where I_1 and I_2 are given by

$$I_1 = \int_0^{\hbar\omega_D} \frac{d\epsilon_k}{p\sqrt{p + E^2}} \tag{10}$$

$$I_2 = (E/2) \int_0^{\hbar\omega_D} \frac{d\epsilon_k}{p^2} \tag{11}$$

where

$$p = \epsilon_k^2 + 4(\hbar\omega_D)^2 e^{-\frac{2}{Ng}} - E^2 \tag{12}$$

What we find in this analysis is that the role of hybridization is to renormalize the coupling constant.The second term in the denominator is called the coupling constant renormalization term.This term has a dependence on the density of states.Thus the density of states appears both in the coupling constant renormalization term and in the exponent .If the renormalization term is negative,an increase in density of states can enhance the gap and thereby T_c considerably. If the renormalization term is positive an enhancement in density of states will not decrease T_c to the same extent.The value of the other saddle points can be determined by discarding the electron -electron pairing term at an earlier stage in the calculation.When calculated it is found that b^2 is a small positive number,which can vary with doping and hybridization.The λ values are small negative numbers which will not appreciably affect the bare value of E_0.For large -ve values of E the integrals have a net -ve contrbution to the renormalization term and T_c enhancement with hybridization and density of states is expected.

The large U though excludes double occupancy, it allows virtual processes at second order in the hybridization term. Due to this some kind of exchange coupling between conduction electrons mediated by localized electrons is taking place.This may be the reason for the renormalization of the coupling constant to large values.