SUPERCONDUCTIVITY : PENETRATION DEPTH AND PHYSICAL PROPERTIES

A THESIS
SUBMITTED TO THE
UNIVERSITY OF HYDERABAD

FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

BY
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FEBRUARY, 1997.

to my father...

DECLARATION

I hereby declare that the work embodied in this thesis has been carried out by me under the supervision of Prof. K. N. Shrivastava, in the School of Physics, and the same has not been submitted at any other University.

Place: Hyderabad

Date: 24 Feb '97

(Murali Krishna Nandigama)

CERTIFICATE

Certified that the work embodied in this thesis entitled SUPERCONDUCTIVITY: PENETRATION DEPTH AND PHYSICAL PROPERTIES has been carried out by **Mr.Murali Krishna Nandigama** for the full period prescribed under Ph. D. Ordinances of the University, under my supervision and the same has not been submitted for the award of research degree of any other University.

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Synopsis

Thesis by	:	***Murali Krishna Nandigama.***
For the degree of	:	Doctor of Philosophy.
Title of the thesis	:	Superconductivity: Penetration depth and physical properties.
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The introductory chapter,I, of the thesis contains an overview of various properties that are related to the superconductors. A general review of superconductors is given in this chapter. Specific heat, London penetration depth and physical properties of high-T_c superconductors have been reviewed. There are a total of five chapters in the thesis including the introductory chapter.

In chapter II, we have calculated the penetration depth in a mixed wave superconductor. At low temperatures the ground state has $d_{x^2-y^2}$ symmetry which at elevated temperatures becomes of the type of $ wave. We have used the experimental measurements of the surface resistance of $Bi_2Sr_2CaCu_2O_{8+\delta}$ crystals of $T_c \sim S2K$ at microwave frequencies to extract the London penetration depth as a function of temperature. It is found that the experimental data is consistent with the interpretation of $d_{x^2-y^2}$ wave at low temperatures becoming s wave at high temperatures. The $d_{x^2-y^2}$ + *is* wave is estimated to start changing over to s at a temperature of $\sim 40K$. The theoretically calculated values of the penetration depth as a function of temperature are

in reasonable agreement with those extracted from the experimental measurements.

In chapter III, we have reexamined the electron-phonon interaction from the view point of its dependence on the crystal structure, particularly on the position of atoms in the unit cell. It is found that the strength of the interaction depends on the number of Cu-0 layers per unit cell only when there are defects. Accordingly the transition temperature depends on the variable number n of Cu-0 layers per unit cell. The larger the number of layers, the larger is the transition temperature. We find that the lattice waves can be treated by spherical Bessel functions so that the electron-phonon interaction oscillates as a function of number of layers of Cu-0 planes. The transition temperature of the superconductor then oscillates as a function of n having a large value at $n = 3$ and smaller value at $n = 4$. We predict that the next maximum value of T_c occurs at $n = 7$. The predicted variation of T_c as a function of n is in reasonable agreement with the experimental values.

In chapter IV, we described about two new processes that occur in a superconducting film when it is used as a detector of x-rays. One of these processes is the scattering of the x-ray by a single electron which gives rise to the broadening of the x-ray line. Another process describes the breaking of a Cooper pair by the x-ray which also contributes to the width of the x-ray. The line width arising from the single electron process depends on T^4 whereas that arising from the pair breaking process varies almost as T^6 at low temperatures. Lines occur at $\hbar\omega_q \pm 2\Delta$, and at $\hbar\omega_q$ where $\hbar\omega_q$ is the energy of the x-ray and 2A is the gap of the superconductor.

In chapter V, the orbit-lattice interaction which gives rise to a Berry's phase factor in the wave function is described. This phase depends on the symmetry of the potential and on the band gap of the system. Thus in the case of a lattice distortion the exponent of the phase factor vanishes above a transition temperature.

The thesis on the whole discussess the physical properties of superconductors from various view points and the related theory that explains the experimental observations that are made in the literature. The work described in the chapters II - IV is new and projects our own efforts in search for interpretation of physical phenomena.

The various parts of this thesis are published as follows: Chapter-II in "Penetration depth in a mixed wave superconductor"; N.Murali Krishna and K.N.Shrivastava, Physica B **230,** 939 (1997). Chapter-Ill in "Transition temperature of a superconductor with defects in crystal structure: Application to Cu-O layers and $K_xRb_{3-x}C_{60}$ type systems"; N.Murali Krishna and K.N.Shrivastava, Superconductor Science and Technol.(1997).(in press). Chapter-IV in "Detection of x-rays by pair breaking in superconductors"; N.Murali Krishna and K.N.Shrivastava, Indian J.Cryog. 19, 19(1994). Chapter-V in "Berry's phase factor accompanying orbit-lattice interaction"; N.Murali Krishna, Lydia S.Lingam, P.K.Ghosh and K.N.Shrivastava (Communicated).

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Chapter 1

Introduction

The d.c. resistivity of some of the metals becomes zero below a certain temperature. Kamerlingh Onnes, as early as in 1911, described this approach of resistance to zero as follows "The value of the mercury resistance used was 172.7 Ω in the liquid condition at 0 °C, extrapolation from the melting point to 0 °C by means of the temperature coefficient of solid mercury gives a resistance corresponding to this of 39.7 Ω in the solid state. At 4.3 K this had sunk to 0.084 ohms that is to 0.0021 times the resistance which the solid mercury would have at 0 °C. At 3 K the resistance was found to have fallen below 3 x $10^{-6}\Omega$, that is to one ten-millionth of the value which it would have at 0 °C. As the temperature sunk further to 1.5 K, this value remained the upper limit of the resistance[1]" and he called this phenomena as **superconductivity.** At present we know that even in superconducting state, there is a finite a.c. resistivity which can be used to measure the London Penetration depth. Superconductivity is now well understood and it is a field with many practical and theoretical aspects. The fact that so far about 10 Nobel prizes have been awarded to people who are closely associated with this field is self explanatory and makes a strong case to pursue further studies in this area.

A general review of superconductors is given in this chapter. Specific heat, London penetration depth and physical properties of high-T_c superconductors have been reviewed.

Special features of the superconducting state

The most common methods for identifying superconductivity of a material are naturally based on the two outstanding features of superconductivity, the zero electrical resistance and the expulsion of magnetic flux or ideal diamagnetism which has negative susceptibility, below a critical temperature T_c. Measurements of the temperature dependence of the electrical resistivity and magnetization are made employing both a.c. and d.c. techniques. Magnetization experiments are usually performed in a small alternating or steady external magnetic fields. Since these methods are not sufficient to ensure the bulk nature of superconductivity, an important aspect, especially when new materials are studied, corresponding investigations of chemically complicated substances often include experimental techniques that are suited to be decisive in this respect. To mention are measurements of magnetization loops M(H) in external fields, the specific heat $C_p(T)$,the thermal conductivity $\kappa(T)$or the absorption of ultrasound $\alpha(T)$. While all these properties are only influenced by the onset of superconductivity, it should also be remembered that the occurrence of certain features is only possible in the superconducting state. These are the London penetration depth of magnetic fields $\lambda_L(T)$ and the features of the Josephson effects. We shall see below a brief discussion of some characteristic features of classical superconductors before proceeding to other types like organic, high-T_c etc.

It should also be mentioned here that in the literature there are quite a few number of experimental observations that deviate from the behaviors that we discuss below.

Magnetization M(H)

Magnetization curves are one of the best indicators of the type of the superconducting material although the exact form of the M(H) curve depends on the geometrical form of the investigated sample. In principle the M(H) curves are also best suited for the determination

of the values of critical fields,viz., the thermodynamic critical field H_c in the case of type -I superconductors or H_{c1} and H_{c2}, the lower and upper critical field ,respectively, in the case of type -II superconductors. Most of the recently discovered materials these days belong to the type -II category. M(H) curves also provide information which is of interest in the possible technical applications like values of critical current J_c and the degree of flux trapping or pinning.

Specific Heat

In zero external magnetic field, the transition from the normal to the superconducting state is a second order phase transition and therefore it manifests itself by an anomaly in the temperature dependence of the specific heat C_p. This anomaly and the electronic part of $C_p(T)$ in the superconducting state as compared to that in the normal state is shown schematically in Fig. 1.

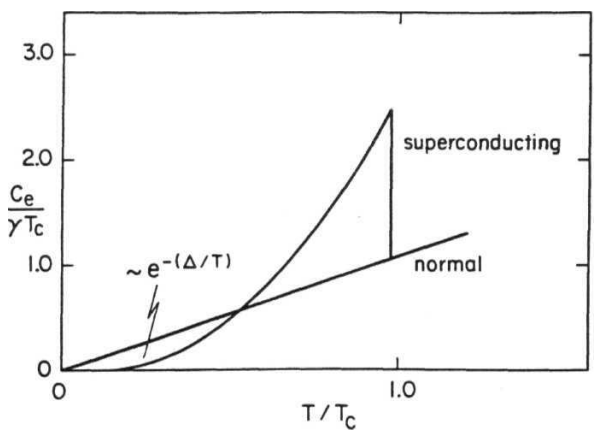

Fig.1: Comparison of the electronic specific heats of a metal in the normal and the superconducting state. The discontinuity at T_c is fixed by the BCS theory[2] (eq.1).

The relevant part of $C_p(T)$ is dictated by the energy excitation spectrum of the electrons.

Since the onset of superconductivity is, usually, accompanied by the opening of a gap in this excitation spectrum at the Fermi energy E_F, $C_p(T)$ has characteristic features that are treated in the BCS theory. At T_c the discontinuity is implicitly a measure of the electronic specific heat parameter 7 through

$$|C_s - C_n|_{T_c} = 1.43\gamma T_c \tag{1}$$

and at low temperatures far below T_c, $C_s(T)$ varies exponentially with temperature as

$$C_s(T) \simeq e^{-\Delta/k_B T} \tag{2}$$

where 2A is the energy gap of the superconductor.

For some of the superconductors discussed in recent literature, it appears that this simple description may not be valid, and modifications for lattice distortions, hopping due to Hubbard model or band mixing as in the Anderson lattice may be needed.

The electronic contribution to the complete $C_p(T)$ curve below T_c can also be used to evaluate the thermodynamical critical filed $H_c(T)$, which is defined by the difference of the free-energy densities in the superconducting and normal state respectively

$$f_n - f_s = \frac{1}{8\pi} H_c^2. \tag{3}$$

For high-T_c superconductors, the difficulty in evaluating the electronic part of $C_p(T)$ arise from the uncertainties connected with other contributions to the specific heat because the lattice contributions from the phonon excitations dominate $C_p(T)$ in the region of T_c completely.

Energy gap & Critical current density

For many years, even before the development of the BCS theory, the idea of an energy gap separating the superconducting ground state from excited state has been considered.

Exponential fall of the electronic specific heat below $T < T_c$, instead of the approximate T^3 law in the superconducting state was a pointer towards this. We also know that direct infra-red absorption and tunneling spectroscopy have experimentally established the existence of the energy gap in a superconductor. For a superconductor, single-particle excited states (quasi-particles) can be defined in one-to-one correspondence with the excitations of the normal metal. If, for example, the single-particle excitation energy measured from the Fermi-surface(chemical potential) in the normal state for the Bloch state k is given by $\epsilon_{\vec{k}}$, the excitation energy in the superconducting state is given by

$$E_{\vec{k}} = (\epsilon_k^2 + \Delta_k^2)^{\frac{1}{2}}. \tag{4}$$

In the one parameter BCS model, Δ_k = A= constant, for energies less than the range $\hbar\omega_D$ of the attractive interaction giving rise to pairing, and zero for energies above it. In contrast to the normal system one requires a minimum finite energy to create single-particle excitations from the ground superconducting state. The existence of this energy gap inhibits single-particle processes and is responsible for the superconducting behavior of the electronic system. It may also be noted that the density of quasi-particle excited states with E > A diverges at E = A as $(E^2 - \Delta^2)^{-1/2}$. In the presence of magnetic impurities, magnetic scattering can reduce the gap to zero, and one can have the so-called gapless superconductivity. In such a case, the finite value of the superconducting order-parameter $\psi(\vec{r})$ or $\Delta(\vec{r})$, rather than the energy gap, is responsible for the superconductivity. In an ideal superconductor(with energy gap), in the ground state of the superconductor all the electrons are in singlet pair-correlated BCS states of zero total momentum. In an excited state, excited electrons are in almost uncorrelated quasi-particle states, with a background of other correlated pair electrons as in the ground state. Thus at finite temperature one has almost two indepen-

dent fluids. The correlated portion of the wave function resists any change but each of the quasi-particles gives normal specific heat and resistance. When a steady current is applied to the system the condensed pair electrons short out the normal part and the net resistance is zero.

We know the energy gap parameter A is the most important microscopic quantity characterizing a superconductor and both its value and its temperature dependence may serve as indicators for special features of the superconducting state. The original BCS theory in its weak coupling limit fixes the ratio of the energy gap at T=0 K with respect to the critical temperature as

$$\frac{2\Delta(0)}{k_B T_c} = 3.56 \qquad \textbf{(5)}$$

where A is the gap-parameter which is dependent on the temperature. The distribution function for the quasi-particles with energy $E > A$ is given by the Fermi factor $f(E) = (e^{(E/k_B T+1)})^{-1}$. It is maximum at T=0 and goes to zero as $(T_c - T)^{1/2}$ as $T \rightarrow T_c$. Also for an ideal BCS superconductor, $\gamma T_c^2 / H_c^2(0) = 0.170$ about which most experimental data seems to scatter.

Possibilities to evaluate A(T) from experiments are numerous. Some of the direct measurements of the energy gap as function of temperature include electron-tunneling experiments and absorption of the far-infra-red radiation.

Positive deviations from the above ratio (eq.5) are usually taken as evidence that strong coupling effects have to be considered. Smaller values of this ratio may occur, for example, if the superconducting state is characterized by an anisotropic gap, including the possibility of gap nodes of various symmetries on the Fermi surface. The latter would be indicative for unconventional pairing and most likely also for unconventional mechanisms inducing the superconducting state. In such cases this would have to go in parallel with observation-

s of non-exponential temperature dependencies of electronic, thermodynamic or transport properties well below T_c.

The London penetration depth & the coherence length

London has emphasized that the pure superconducting state is associated with a persistent shielding current in the presence of magnetic field. Since the Meissner effect is also a very well established phenomena and it specifies that B=0 inside the sample (of macroscopic dimension) in the superconducting state, due to perfect diamagnetism, this shielding current must be confined to a region very close to the surface. While expressing in terms of the field, we can say that B drops to a vanishingly small value over a characteristic penetration depth λ_L, whose magnitude is temperature dependent. Alternatively, we can say that the expulsion of magnetic flux from the superconductor may also be described as an exponential decay of external magnetic field at the surface of a superconductor and the characteristic length involved is the London penetration depth $\lambda_L(0)$ which is defined as

$$\lambda_L^2 = \frac{m^* c^2}{4\pi n_s e^2} \qquad \textbf{(6)}$$

where n_s is the density of itinerant charge carriers forming the superconducting state and m^* is their effective mass. Here the temperature dependence of λ_L is coming into the above equation through the temperature dependence of n_s. At average temperatures, $\backslash L\{T)$ may be approximated by

$$\lambda_L(T) = \lambda_L(0)(1 - t^4)^{-1/2} \qquad (7)$$

where $t = T/T_c$. This equation is a result of the two fluid model[3] and can also be considered as a valid approximation if strong coupling extensions of the BCS-theory have to be considered. Again at very low temperatures $T \ll T_c$, an exponential temperature dependence should result [3].

The second length that is important in the characterization of a superconductor is the coherence length ξ. There are various definitions for this factor and all these definitions coincide only at $T \ll T_c$ and in the clean limit only, i.e., if the electronic mean free path is very long. Since these lattice criteria are not always met, it is not easy to theoretise the coherence length $\xi(T)$. But, we can note that the difference between type-I and type-II superconductors can be characterized by noting that whether $\xi(T)$ is larger or smaller than λ_L at low temperatures.

High temperature superconductors

Prior to 1986, most experimentalists and theorists alike were convinced that the upper limit for the T_c of any superconducting material would be around 23 K. But, in that year itself Alex Muller and Georg Bednorz [4] have virtually started a new phase in the field of superconductivity by discovering a new class of materials whose parent materials themselves are no way connected with superconductivity individually. These materials are now called as cuprate superconductors or high-T_c superconductors. The great attention ascribed to these compounds is due to the fact that they have very good T_c values in the higher ranges. The maximum T_c value in these compounds is virtually raised up to 135 K in $HgBa_2Ca_2Cu_3O_{8+\delta}$ at atmospheric pressure in 1993[5] and in the same compound T_c can be increased up to 164 K at 30 G Pa pressure [6].This is more than five times the T_c in any conventional superconductor.

A list of some of the most prominent cuprate superconductors with their transition temperatures is given at the end of this sub-section.

The immediate question that can be asked about these high-T_c materials is that which new features are permited by these materials? The basic superconducting properties of these HTSCs are the same as in conventional superconductors e.g., zero resistance and per-

fect diamagnetism. The flux quantization in units of ϕ_o = — inside a superconducting ring [7] suggests the basic building blocks in these materials are the same paired quasi-particles of charge 2e. Even more astonishing is the fact that in an open ring that is bridged with a conventional superconductor, the same flux quantum is observed[8] so that we expect a coupling between high-T_c and low-T_c pairs if both are s-wave. If the nature of superconductivity is different in these two varieties, we would not expect the same. However a bit of caution is to be exercised in generalizing the above statement since boundary processes can potentially couple order parameters with different symmetries with suitable phase factors.

The superconducting materials are basically derived from those materials which are by themselves non-superconducting in nature. They are antiferromagnetic insulators and this can be verified by neutron scattering techniques[9].

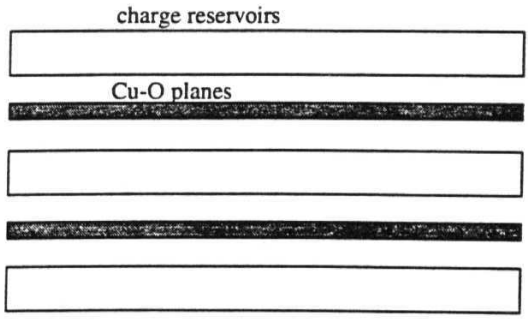

Fig.2: Schematic building blocks of the cuprate superconductors.

The typical structure of these HTSC materials consists of 2D layers of CuO_2 which are separated by charge reservoir layers of varying chemical content between the different cuprate

superconductors, as shown in Fig.2.

The strong antiferromagnetic correlations in the CuO_2 planes emerge **from** chemical bonds between the copper $3d_{x^2-y^2}$ orbitals and the neighboring oxygen $2p_x$ and $2p_y$ orbitals[10] as shown in the Fig.3.

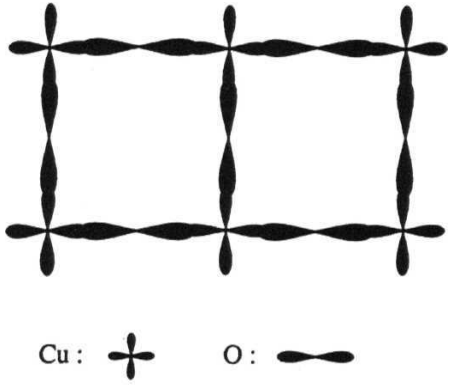

Fig.3: The strong bondage between Cu and 0 that cause the planar antiferromagnetic correlations.

When the charge removal by (hole)doping is done in CuO_2 planes, they become increasingly conducting and at sufficient doped levels, we can observe a transition from the conducting state to a superconducting state below T_c. A typical phase diagram representing the phase transition in $YBa_2Cu_3O_{6+x}$ is shown in Fig.4.

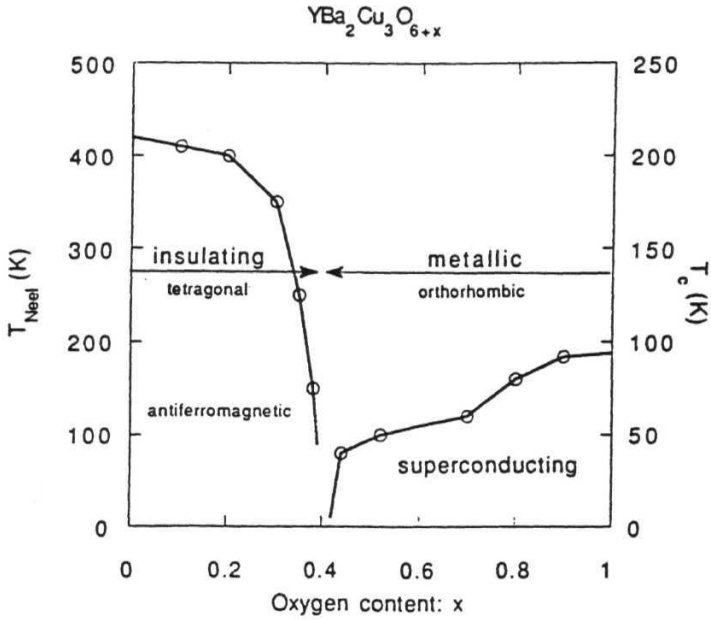

Fig.4: The phase diagram of $YBa_2Cu_3O_{6+x}$ showing insulating, antiferromagnetic, metallic and superconducting phases.

Also, the electronic structure of the undoped and the doped CuO_2 plane is given in Fig.5.

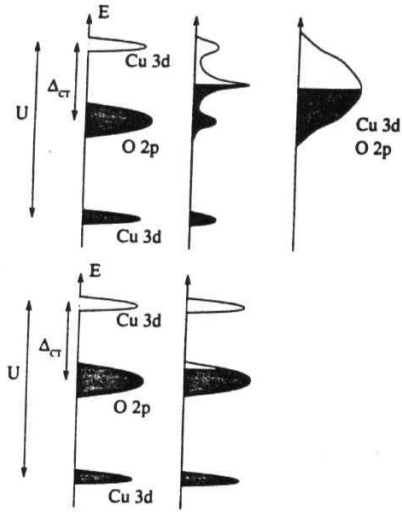

Fig.5: Two different scenarios for the evolving electronic structure in the doped CuO_2plane. On the left is the undoped insulating parent compound, in the middle is the moderately doped and on the right is the strongly doped cuprate. The upper row shows the presence of mid-gap states and the lower row shows the scenario without mid-gap states.

The undoped plane has two Cu 3d bonds which correspond to singly occupied states on Cu which is completely filled and a band which corresponds to doubly occupied Cu which is completely empty. The splitting of these two bands is governed by strong Coulomb repulsion energy U on Cu. The 0 2p band falls within these two bands and is also completely filled.

The gap between the 0 2p and the unoccupied Cu 3d band is the charge transfer gap which is in the range of 1.5-2 eV[11]. The chemical potential lies in the charge transfer gap. Upon doping one possibility is that the chemical potential does not shift. However doping induces states in the mid-gap region which are formed by rearrangement of both conduction and valence band states of the insulators and in the overdoped region a single band of mixed character remains[11]. Another possibility is that the chemical potential drops immediately into the 0 2p band removing the states progressively from those bands and at the same time the electronic structure of this band changes rapidly creating a large Fermi surface and extended saddle points in the vicinity of the Fermi energy[12].

While the undoped compound is a correlation induced insulator, it is possible to create a non-zero carrier density by doping. The carrier density is correlated approximately linearly with the hole concentration in the CuO_2 plane[11]. The resistivity shows a pronounced anisotropy $\rho_c/\rho_{ab} \sim 40 — 100$ of the value perpendicular to the planes divided by the in-plane resistivity. This anisotropy increases with the lowering of the temperature which is indicative of the strongly two dimensional character of the electronic states at low temperatures. If the hole doping is less than a few percent, the antiferromagnetic properties set in at T_N, the Neel temperature. For roughly 5% to 25% hole doping, no antiferromagnetic long range order is present. This is the doping range where the cuprates have a superconducting phase transition at T_c and the resistivity falls to zero together with a perfect diamagnetic behavior at sufficiently small fields.

Let us look at what is special about these cuprates. A comparison with other layered transition metal oxides reveal the following unique properties[11]:

- a large superexchange coupling $J \sim 0.1eV \propto t_{pd}^3/[\Delta_{CT}(\Delta_{CT}+ U)]$,
- a large on-site Coulomb energy U,
- two-dimensionality.

The large J comes from the small Δ_{CT} and the large overlap of Cu 3d and O 2p states. The combination of these four factors is somewhat complementary because they combine to a high antiferromagnetic ordering temperature T_N for the undoped compound but the last two lead to strong quantum and thermal fluctuations of the magnetic correlations. Therefore a small percentage of doping can destroy long range magnetic order and this ease of "metalization" is quite exceptional.

During the past few years it has become evident that not only the normal state of these cuprate superconductors is peculiar but also the superconducting state. The main observations came from photoemission measurements. The angular resolved photoemission experiments[13] showed a strongly anisotropic superconducting gap in $Bi_2Sr_2CaCu_2O_{8+\delta}$ with a large gap along the Cu-0 bond direction of about 20 meV and a nearly vanishing gap in the Cu-Cu directions. This variation of the magnitude of the gap function is consistent with a $d_{x^2-y^2}$ wave gap model.

The transition temperatures and chemical formulae of some of the important high temperature superconductors is given here.

Chemical formula	Short name	T_c
$La_{1.85}Sr_{0.15}CuO_4$	214	38 K
$Bi_2Sr_2CaCu_2O_{8+\delta}$	2212, BSCCO	80-91 K
$YBa_2Cu_3O_7$	123, YBCO	92 K
$Tl_2Ba_2Ca_2Cu_3O_{10}$	2223, TlBCCO	120-125 K
$HgBa_2Ca_2Cu_3O_{8+\delta}$	1223, HgBCCO	135 (164 K at 30 G Pa)

Table: Some well known HTSC materials with their T_c values.

Raman Scattering

Over the years Raman scattering has proved to be a valuable tool for probing the normal as well as the superconducting states of high temperature superconductors. It has been observed in Raman scattering studies that one of the phonon modes is found to become soft which is characteristic of structural distortions. Amplitude modes are also found in high temperature superconductors. Recently non-Fermi liquid models have been applied to understand the normal state[14].

Microwave absorption and magnetization

At small magnetic fields microwaves are found to be absorbed by the high temperature superconductors. Such an absorption can be understood to arise from the weak link Josephson junctions in real materials[15]. At low fields the magnetization is found to change sign from the negative (diamagnetic) to positive values. This change is explained by π-junctions[16].

In this thesis, we have made efforts to understand the changes in the London penetration depth in going from the s-wave to d-wave symmetries, the changes in the T_c due to defects in the lattices, detection of x-rays using a superconducting film and the Berry's phase.

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Chapter 2

Penetration depth in a mixed wave superconductor

We have calculated the penetration depth in a mixed wave superconductor. At low temperatures the ground state has $d_{x^2-y^2}$ symmetry which at elevated temperatures becomes of the type of s wave. We have used the experimental measurements of the surface resistance of $Bi_2Sr_2CaCu_2O_{8+\delta}$ crystals of $T_c \sim 82K$ at microwave frequencies to extract the London penetration depth as a function of temperature. It is found that the experimental data is consistent with the interpretation of $d_{x^2-y^2}$ wave at low temperatures becoming s wave at high temperatures. The $d_{x^2-y^2} + is$ wave is estimated to start changing over to s at a temperature of $\sim 40K$. The theoretically calculated values of the penetration depth as a function of temperature are in reasonable agreement with those extracted from the experimental measurements.

In this chapter, we calculate the penetration depth for a system of mixed wave symmetry, $d_{x^2-y^2} + is$ ground state. The calculation is performed for a system which has $d_{x^2-y^2}$ at low temperatures and s wave symmetry at high temperatures. The experimentally deduced values from the surface resistivity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ crystals agree with the mixed wave interpretation.

The diamagnetic current is given by

$$j_D = -(e^2/mc) \sum_{k,q,\sigma} c^{\dagger}_{k+q,\sigma} c_{k,\sigma} e^{-iq.x} A(x) \tag{1}$$

so that the problem of determining the London penetration depth [1-3] is reduced to that of the conversion of summation into integration by the use of appropriate density of states [3] and multiplying the gap A by the factor /, where

$$\begin{aligned} f &= 1 && (s \text{ wave}) \\ &= cos2\phi && (d_{x^2-y^2} \text{ wave}) \\ &= sin2\phi && (d_{xy} \text{ wave}) \end{aligned} \tag{2}$$

The density of states can be described in terms of the complete elliptic integral so that the London penetration depth [4] is found to be,

$$\begin{aligned} |\frac{\lambda_{x^2-y^2}(0)}{\lambda_{x^2-y^2}(T)}|^2 &= 1 - \frac{4}{\pi k_B T}[\int_o^{\Delta_{x^2-y^2}} dE f_E(1-f_E)(E/\Delta_{x^2-y^2})K(E/\Delta_{x^2-y^2}) \\ &+ \int_{\Delta_{x^2-y^2}}^{\infty} dE f_E(1-f_E)K(\Delta_{x^2-y^2}/E)] \end{aligned} \tag{3}$$

which relates the temperature dependence of the penetration depth with that of the gap A 2(T). The temperature dependence of the gap is determined by [3],

$$\gamma^{-1} = 2\pi k_B T < |f|^2 >^{-1} \sum_n < \frac{|f|^2}{\sqrt{\omega_n^2 + \Delta^2 |f|^2}} > \tag{4}$$

where f is given by (2) and 7 is the dimensionless coupling constant, ω_n is the Matsubara frequency and the sum is cutoff at $\omega_n = \epsilon_c$. Due to the crystal field in metals the Fermi surface becomes anisotropic so that at low temperatures the ground state is of $d_{x^2 - 2}$ symmetry. However, in such a case upon warming from low temperatures, the ground state may change from $d_{x^2 - 2}$ to *s*. The London penetration depth for d_{xy} may be written from (3) by replacing $\Delta_{x^2 - 2}$ by Δ_{xy}. However this symmetry occurs only near the surface of the sample[5]. In the Landau model, the higher temperature phase is more symmetric than the lower temperature phase. Therefore, we predict that at higher temperatures, the superconductor will become the *s*-wave type. Therefore, the $d_{x^2 - 2}$ state should change to *s* state. This is possible only when the order parameter is complex, $d_{x^2 - 2} + is$. This result is in conformity with the calculations of the minimization of free energy[1]. For the complex order parameter, the penetration depth is given by

$$\left|\frac{\lambda_{x^2-y^2,s}(0)}{\lambda_{x^2-y^2,s}(T)}\right|^2 = 1 - \frac{4}{\pi k_B T}\Big[\int_{\Delta_{x^2-y^2}}^{\Delta_{x^2-y^2,s}} dE f_E(1-f_E)\frac{E}{\Delta_s} K\left(\frac{(E^2-\Delta^2_{x^2-y^2}-y^2 f^2)^{1/2}}{\Delta_s}\right) + \int_{\Delta_{x^2-y^2,s}}^{\infty} dE f_E(1-f_E)\frac{E}{(E^2-\Delta^2_{x^2-y^2}-y^2 f^2)^{1/2}} \times K\left(\frac{\Delta_s}{(E^2-\Delta^2_{x^2-y^2}-y^2 f^2)^{1/2}}\right)\Big] \quad (5)$$

where

$$\Delta_{x^2-y^2,s} = (\Delta^2_{x^2-y^2} + \Delta_s^2)^{1/2}$$
$$f_E = (e^{E/k_B T} + 1)^{-1} \quad (6)$$

The surface microwave resistivity is proportional to $\mu_o \omega \lambda_{ab}(0)$ where the permeability μ_o and the microwave frequency ω are known so that the penetration depth can be determined. The experimental measurements have been performed by Jacobs et al[6] using a single crystal

of $Bi_2Sr_2CaCu_2O_{8+\delta}$ from which the penetration depth has been deduced as a function of temperature. We have taken a few experimental points from their work and shown in Fig.1. The experimental values are linear upto a temperature of $T_{x^2-y^2s} \sim 40K$.

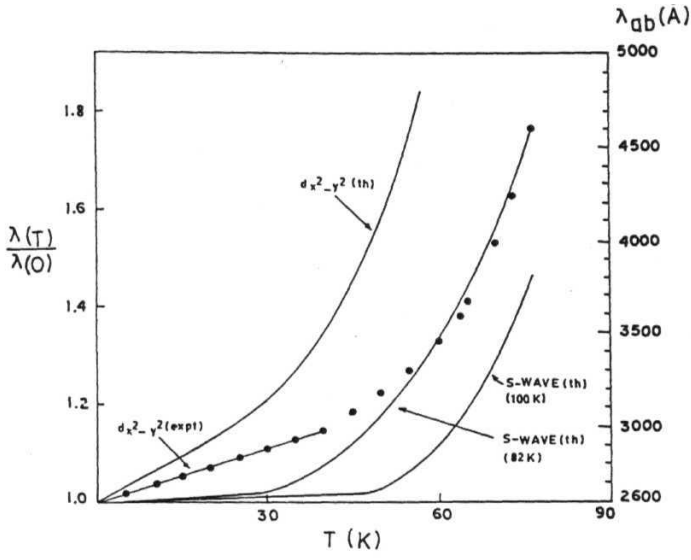

Figure.1: Temperature dependence of the London penetration depth $\lambda_{ab}(T)$ showing linear slopes corresponding to $d_{x^2-y^2}$ which agrees with the experimentally measured values. The curves marked as $d_{x^2-y^2}$(th), *s*-wave (th 100K) and *s*-wave (th 82K) are all theoretically calculated. The dots are deduced from some of the the experimental measurements of the microwave surface resistivity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals. The theoretically calculated penetration depth for the *s* wave is in reasonable agreement with the experimentally measured values for $T > 60K$.

It is found that the theoretical expression (3) for $d_{x^2-y^2}$ state is also linear[4],

$$\frac{\lambda_{x^2-y^2}(T)}{\lambda_{x^2-y^2}(0)} \simeq 1 + 0.69 k_B T/\Delta_{x^2-y^2}(0) \qquad \textbf{(7)}$$

Therefore, it is identified that the low temperature behaviour is caused by a $d_{x^2-y^2}$ type state. The experimentally measured slope for $d_{x^2-y^2}$ is $\frac{d}{dT}\delta\lambda_{x^2-y^2} = 10\mathring{A}/K$. The theoretical value of the slope $\frac{d}{dT}[\lambda(T)/\lambda(0)] \sim 15.3K^{-1}$ is larger than the experimental value. The theoretically calculated value of $A_{x^2-y^2}(T)/\lambda_{x^2-y^2}(0)$ for T_c=82K and A(0) = $2600\mathring{A}$, is also shown in Fig.1. This value depends on temperature a bit more strongly than the experimentally deduced values. Using $\Delta_s = 1.77 k_B T_c(1- T/T_c)^{1/2}$ we find $\lambda_s(T)/\lambda_s(0)$ for two different values of T_c=82K and 100K which are also shown in Fig.1. These calculated values of $\lambda_s(T)/\lambda_s(0)$ are less than the experimentally measured values. But for $T > 60K$ only *s* wave agrees with the experimental data. Thus we see that for T<40K the order parameter has $d_{x^2-y^2}$ symmetry becoming *s* wave for $60 < T < 82K$. The occurrance of multiple symmetries in the gap is permitted[7] by the group theory. According to the expression (5) both the *s* wave and the $d_{x^2-y^2}$ wave type gaps occur at all temperatures with the average value given by the first of the expressions in (6) for a given value of the ratio $\Delta_{d_{x^2-y^2}}$/A, so that the calculated $\lambda(T)$ for the mixed wave occurs in between the two curves, $\lambda_{d_{x^2-y^2}}(T)$ and $\lambda_s(T)$. It may be noted that in the case of ^3He the $|0>$ and $|\pm 1>$ states are phase separated. Therefore it is possible to construct the theory in such a way that at low temperatures only the $d_{x^2-y^2}$ phase occurs and at elevated temperatures only the *s* phase occurs with a phase boundary seperating the two phases. However evidence for such a phase boundary has not yet been reported in high T_c superconductors.

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Chapter 3

Transition temperature of a superconductor with defects in the crystal structure: Application to Cu- O layers and $K_xRb_{3-x}C_{60}$ type systems

We have reexamined the electron-phonon interaction from the view point of its dependence on the crystal structure, particularly on the position of atoms in the unit cell. It is found that the strength of the interaction depends on the number of Cu-0 layers per unit cell only when there are defects. Accordingly the transition temperature depends on the variable number *n* of Cu-0 layers per unit cell. The larger the number of layers, the larger is the transition temperature. We find that the lattice waves can be treated by spherical Bessel functions so that the electron-phonon interaction oscillates as a function of number of layers of Cu-0 planes. The transition temperature of the superconductor then oscillates as a function of *n* having a large value at $n = 3$ and smaller value at $n = 4$. We predict that the next maximum value of T_c occurs at $n = 7$. The predicted variation of T_c as a function of *n* is in reasonable agreement with the experimental values.

Introduction

It was found that compounds of the formula $RBa_2Cu_3O_{7-}$ (R = *Y*, rare earth) have a superconducting phase with transition temperature, $T_c \sim 90K$. The compounds containing *Bi* and Tl have even higher transition temperatures, $\sim$ 100 - $110K$. $Tl_2CaBa_2Cu_2O_{8+\delta}$ has a $T_c \sim 105K$ while $Tl_2Ca_2Ba_2Cu_3O_{10}$ has a T_c of 125K. The compounds of the general formula $(Bi/Tl)_2Ca_{n-1}(Sr/Ba)_2Cu_nO_{2n+4}$, ($n$ = 1,2,3, • - •) have a superconducting transition temperature which seems to increase with increasing number of layers of *Cu* atoms but the combination of other atoms is also important [1]. It has been noted that in $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$ the transition temperature may increase monotonically with n upto a saturation value as $T_c \sim 90, 110$ and $125K$ for n = 1,2 and 3, respectively [2,3]. However the value of T_c reduced for n = 4 down to the value of $110K$ as for n = 2. Therefore, there is an optimum value of n that maximizes T_c for a given class of compounds. Similar phenomenon of rise in T_c with increasing n is found in $TlBa_2Ca_{n-1}Cu_nO_{2n+3}$ also. It is possible to substitute *Bi* in place of *Tl* without changing $T_c(n)$ characteristics. The larger is the number of O ions per unit cell, the larger is the transition temperature as long as one builds larger cells. For n > 3 the charge distribution is highly nonhomogeneous in analogy with the graphite intercalation compounds. Such, an effect is not contained in the BCS theory according to which the transition temperature is independent of the structure within the unit cell. Phillips [4] has explained the chemical trends in three multilayer cuprate superconductive families, $Bi_2Sr_2Ca_{n-1}Cu_nO_{4+2n+\delta}$, $Tl_2Ba_2Ca_{n-1}Cu_nO_{4+2n+\delta}$ and

$HgBa_2Ca_{n-1}Cu_nO_{2+2n+\delta}$ by using the ideas of resonant pinning, anti-Jahn-**Teller** effect, oxygen ordering and phenomenology as minimal modifications of the BCS theory.

The charge distribution in the case of $F^- - Cu^{2+} - F^-$ has been calculated in detail [5]. Since the electronic configuration of F^- ion is the same as that of O^{2-} $(1s^2, 2s^2p^6)$ except for the nuclear charge, the charge distribution in Cu^{2+}- O^{2-} - Cu^{2+} follows exactly from that of Cu^{2+}- F^- - Cu^{2+}. The layering is caused by the extra oxide of $Tl_2Ca_2Ba_2$ combination of ions keeping the lattice electrically neutral. It is clear that layering is an advantage for increased interaction between electrons and phonons and pairing is induced within the layers. On the basis of earlier results [5] it may be concluded that the charge as a function of distance shows a shallow minimum at a certain distance R between Cu^{2+} and O^{2-} ions and there is a flat region at larger distances. The shallow minima may provide the regions where the binding occurs but the attractive interaction which leads to pairing is more extended. However, the shallow minima indicate the possibility of hopping from site to site so that intersite interactions are expected to be important.

According to the BCS theory [6], the superconductivity is caused by the pairs of electrons formed by the electron-phonon interaction which in second order leads to an effective attraction between electrons. The larger the electron-phonon interaction the larger is the transition temperature. This theory explains the zero resistivity and hence the Meissner effect. The isotopic shift of the transition temperature arises as a natural consequence of the dependence of the T_c on the phonon frequency. Because of the binding

energy between pairs of electrons, there is a gap in the dispersion relation which explains the infrared absorption. The region of energy in which the electrons are attractive starts near the Fermi energy, ϵ_F and extends upto about $\epsilon_F + \hbar\omega_D$ where $\hbar\omega_D$ is the Debye cutoff single phonon energy. Therefore, the density of states near the Fermi energy occurs in the bound state equation and hence in the expression for the transition temperature. The larger the density of states, the larger is the transition temperature.

Phillips [7] has suggested that for isovalent ionic compounds, the electron-phonon deformation potential coupling should depend on the ionic charge and polarizability of the ions. Therefore, the T_c should depend linearly on the strength of the electron phonon interaction. The T_c as a function of n, the number of layers of Cu - O atoms in the series $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$ for small values of n is a linear function of n but for larger values of n, there are oscillations. Thus linearization of the T_c with the electron-phonon interaction, as suggested by Phillips is justified for small values of n.

In this work, we calculate the electron-phonon interaction to determine the dependence of the attractive interaction on the unit cell size and from that on the number of layers of Cu — O atoms. The transition temperature is found to increase with increasing number of layers of Cu — O atoms. We calculate the electron-phonon interaction in a defect lattice without the approximation of infinite wave length for lattice phonons so that the matrix element depends on the number of layers, n of Cu — O atoms. The larger the value of n, the larger is the matrix element and hence larger is the transition temperature. Because of the occurrance of the spherical Bessel functions, the

matrix element oscillates with T_c peaked at n = 3 and next peak is predicted at n = 7 but its value is less than at n = 3. At $n = 4$, the T_c is smaller than at n = 3. The predicted dependence of T_c is in accord with the experimental findings. The main result of this work is that the transition temperature in a crystal with defects is a function of the size of the unit cell and in the case of a layered superconductor it is a periodic function of the number of elementary layers in the unit cell.

Electron-phonon interaction

The unperturbed Hamiltonian consists of electrons in the conduction band with ϵ_F as the Fermi energy and the phonon continuum as,

$$\mathcal{H}_o = \sum_{k\sigma}(\epsilon_{k\sigma} - \epsilon_{F\sigma})C^+_{k\sigma}C_{k\sigma} + \sum_q \hbar\omega_q a^\dagger_q a_q \qquad (1)$$

where $C^+_{k\sigma}(C_{k\sigma})$ are the creation (annihilation) operators for the electrons with wave vector k and spin cr. The single particle energy for phonons is $\hbar\omega_q$ and $a^\dagger_q(a_q)$ are the phonon creation (annihilation) operators. The repulsive interaction between electrons is $\sim 4\pi e^2/\kappa q^2$, where κ is the dielectric constant and q is the momentum transfer. However, there are positively charged nuclei which have a charge of $+Ze$ which attract electrons. The potential between the nuclei of charge Ze_i and the electrons is $V - \Sigma'_{ij} Ze_i e_j/|R_i - r_j|$ where R_i are the coordinates of the nuclei and r_j that of the electrons. The displacement of the nuclei δR_i modulate the electron-nuclear potential. The displacement is described by the absorption and emission of phonons and the nuclear motion separates out so that we obtain the electron-phonon interaction, $\mathcal{H}'_e = \sum_i (\partial V/\partial R_i)\delta R_i$. Because of the normal modes of oscillations,

we write the electron-phonon interaction as,

$$\mathcal{H}'_{ep} = \sum_q \left(\frac{\partial V}{\partial R}\right)_o \left(\frac{\hbar}{2M\omega_q}\right)^{1/2} \left(a_q - a^\dagger_{-q}\right) e^{iq.R} + h.c. \qquad \textbf{(2)}$$

where M is the mass of the crystal, ω_q the phonon frequency and the derivative of the crystal potential is evaluated at the equilibrium. Usually the site summation with every site at ft occupied,gives the momentum conservation condition. However in the case of random vacancies at ft, the exponential factor is not removed. The potential now depends linearly on the concentration of defects.The BCS have evaluated the matrix elements of the electron-phonon interaction within an intrasite one independent atom model so that the site summation gives rise to a momentum conservation condition, so that the factor of *exp(iq.R)* disappears. However, in the case of lattice defects with many atom positions vacant, the lattice sum, has a factor of 1 — $\exp(iq.R)$ of which we can evaluate the real and imaginary parts separately [8,9]. For infinite wave length $\cos q.R \sim 1$ and $\sin q.R \sim 0$ so that only cosine term survives. Upon further expansion the interaction is seen to depend on the wave vectors. The symmetry considerations [10,11] lead to selection of sine or cosine terms. For even symmetry vibrations we take $\sin q.R$ while for old symmetry we take $\cos q.R$. If there is a centre of symmetry, sine term dominates and cosine term drops out. We therefore consider only the sine term so that

$$\mathcal{H}'_{ep} = \sum_{kk'q} v_{kk'q} (\hbar/2M\omega_q)^{1/2} C^\dagger_{k\sigma} C_{k'\sigma} (a_q + a^\dagger_{-q}) \sin q.R\delta(k - k' - q) + h.c. \quad (3)$$

where $h.c.$ means that the hermitian conjugate of the previous terms is to be taken. Here $v_{kk'q}$ is the matrix element of the distance derivative of the

electron-nuclear Coulomb potential which becomes $v_{k,q}$ when δ-function is evaluated. In the case of $q.R < 1$, $\sin q.R \sim q.R = q_x a + q_y b + q_z c$ where a, *b* and c are crystallographic unit cell dimensions along *x,y* and *z* axes, q_x, q_y and q_z are the components of the phonon wave vector so that the interaction becomes,

$$\mathcal{H}'_{ep} = \sum_{kq\sigma} v_{kq}(\hbar/2M\omega_q)^{1/2} C^{\dagger}_{k\sigma} C_{k-q,\sigma}(a_q + a^{\dagger}_{-q})(q_x a + q_y b + q_z c) + h.c., \quad (4)$$

The second-order effective interaction from the above is found to be

$$\mathcal{H}^{(2)}_{ep} = \sum_{kk'q\sigma\sigma'} \frac{\hbar\omega_q |M_q|^2 C^{\dagger}_{k'-q,\sigma'} C_{k'\sigma'} C^{\dagger}_{k+q,\sigma} C_{k\sigma}}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2} \quad (5)$$

where the square of the matrix element is given by

$$|M_q|^2 = |v_{kq}|^2 \left(\frac{\hbar}{2M\omega_q}\right)(q_x a + q_y b + q_z c)^2 \quad (6)$$

which depends on the unit cell dimensionsso that the larger unit cells have stronger interaction. Converting the summation over *a* in (5) to a three dimensional integral, $\sum_q = \int 4\pi \mathbf{V}/(2\pi)^3 q^2 dq$, where V is the volume of the sample, we see that the mass in the denominator of (6) MN becomes $MN/\mathbf{V} = \rho$, the mass density of the solid where TV is the total number of atoms in the crystal. When the attractive term dominates the repulsive term,

$$-V = \langle -\frac{|M_q|^2}{\hbar\omega_q} + \frac{4\pi e^2}{\kappa q^2} \rangle < 0 \quad (7)$$

the electrons form pairs.This interaction in the defect lattice depends on the unit cell dimensions, a, *b* and c. Although we have considered the wave vector dependence of the electron phonon interaction through the phonon

factor we have not considered the momentum and frequency dependence of the dielectric function. Thus only that part of the Coulomb interaction has been considered which can be linearly substracted from the matrix element of the second-order electron-phonon interaction. Since the effective electron-phonon interaction depends on the cell dimensions, the critical temperature will also depend on the same. In the first instance we predict that larger cells have larger transition temperatures. We use two elastic constants, $C_{11} = \rho v_l^2$ and $C44 = \rho v_t^2$. This is equivalent to using two sound velocities the transverse, v_t and the longitudinal, v_l. We also write (6) using $q_x = q_y = \omega/v_t$ and $q_z - \omega/v_l$. Therefore,

$$|M_q|^2 = |v_{kq}|^2 (\hbar\omega_q/2M) \left[\frac{1}{v_t}(a+b) + \frac{1}{v_l}c\right]^2 \qquad \textbf{(8)}$$

The coupling constant of the attractive interaction between electrons is then of the form,

$$-V = -\frac{|v_{kq}|^2}{2M}\left[v_t^{-1}(a+b) + v_l^{-1}c\right] \qquad (9)$$

whereas in the original BCS theory, the factor $\sin q.R$ does not exist and there is no defect concentration dependence so that the coupling constant of the electron phonon interaction, v_{kq}^{BCS} in second order gives the attractive potential determined by,

$$-V_{BCS} = -|v_{kq}^{BCS}|^2 (2M\omega_q^2)^{-1} \qquad \textbf{(10)}$$

which means that the frequency dependence of the effective electron-phonon interaction is changed by introducing sine waves in (3). We compare our interaction (9) with (10) to find that,

$$-V = -V_{BCS}\left[|v_{kq}|^2/|v_{kq}^{BCS}|^2\right]\omega^2 v_l^{-2}\left\{(v_l v_t^{-1})(a+b) + c\right\}^2 \qquad (11)$$

which shows that the attractive interaction depends on the sound velocities and on the unit cell constants, in addition to what is considered in the BCS theory. The binding energy of the pair with respect to the Fermi level for the attractive potential is then given by

$$\Delta = \frac{2\hbar\omega_D}{\exp\left[\rho_F^{-1} V_{BCS}^{-1} v_l^2 \omega_D^{-2} \left\{v_l v_t^{-1}(a+b)+c\right\}^{-2}\right] - 1} \tag{12}$$

where we assumed that the electrons are attrractive above the Fermi energy till $\epsilon_F + \hbar\omega_D$ with $\hbar\omega_D$ as the Debye cutoff energy for phonons. From (12) we find that the larger unit cell corresponds to larger gap in the dispersion relation but the sound velocities are also important. For large unit cells having loosely packed material, the longitudinal sound velocity is smaller for larger binding energy between electrons. The transition temperature of the BCS superconductor then becomes,

$$T_c \simeq 1.14(\hbar\omega_D/k_B)\exp\left[-\rho_F^{-1} V^{-1} v_l^2 \omega_D^{-2}\left\{\frac{v_l}{v_t}(a+b)+c\right\}^{-2}\right] \tag{13}$$

which acquires larger values for larger unit cell dimensions, the smaller sound velocity also gives larger transition temperatures. Since we may replace *c* by $2Rn$, larger *n* gives larger T_c. Here *R* is the distance between Cu^{2+} and O^{2-} ions in an octahedron.

In the case of a hexagonal lattice a = *b* and $v_l/v_t \sim 1.3$ so that

$$\ln T_c \simeq -\frac{v_l^2}{\rho_F V \omega_D^2 (2.6a+c)^2} + \ln(1.14\hbar\Omega_D/k_B) \tag{14}$$

A plot of $\ln T_c$ versus $(2.6a + c)^{-2}$ is then predicted to be linear. In Fig.1 we show such a plot from the experimental values for two classes of compounds.

It is seen that the experimental behavior is in reasonable agreement with the expression (14).

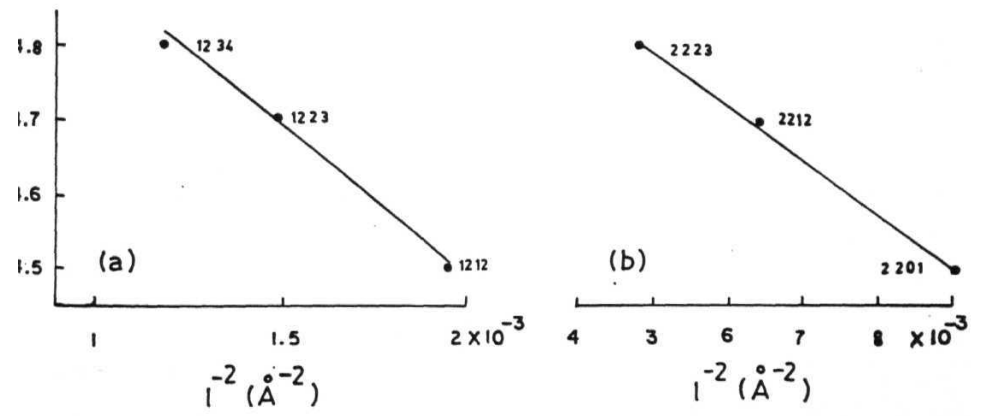

Fig. 1. The ln T_c with I^2 where / = 2.6 $a+c$ showing linear dependence as predicted by eq.(14) for (a) $Tl_1Ba_2Ca_{n-1}Cu_nO_{2n+3}$ and (b) $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$, class of compounds. The data is taken from Sleight (ref. 2).

In the case of cubic unit cells, as in the case of carbon superconductors A_3C_{60} *(A =* K, Rb, Cs*),* $a = b =$ c so that (13) gives

$$\ln T_c \simeq -\frac{v_l^2}{(3.6)^2 \rho_F V \omega_D^2 a^2} + \ln(1.14\hbar\omega_D/k_B) \qquad (15)$$

which shows that $\ln T_c$ versus a"^{2} is linear. Therefore, the larger is the unit cell, the larger is the transition temperature. Such a theoretical prediction made by (15) is in complete accord with the measurements [12] of T_c in A_3C_{60} with $A = K_3, K_2Rb, KRb_2, Rb_3$ and Rb_2Cs.

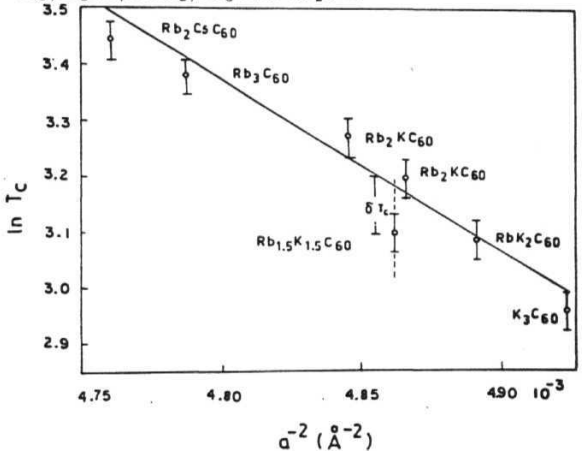

Fig. **2.** Plot of $\ln T_c$ with a"^{2} for various carbon alkalimetal superconductors. The crystallographic unit cell size and the experimental values of T_c are taken from Fleming et.al (ref.12). Thus the theoretical prediction of eq.(15) agrees with the experimental data. Here the straight line represents $\ln T_c =$ 18.37-3.125 x $10^3 a^{-2}$ with a in $\mathring{A}$ units and T_c in K. The dashed line indicates T_c as deviated from a^{-2} but there is no T_c that is independent of the size of the unit cell showing that there are defects in the lattice periodicity.

In Fig. 2 we show the $\ln T_c$ versus a"^{2} as deduced from the experimental data particularly because of the random distribution of K and Rb atoms. We observe that the theory (15) agrees with the measurments within the errors in the T_c values. The dependence of T_c on the ionic size is thus predicted from the present microscopic theory.

An effort is made to see if there is any dependence which is independent of the lattice constant. Actually the inverse of the area of a face of the cube appears in (15) while the original BCS theory is independent of such an area. In case, there were transition temperatures, independent of the area of the cube face then the same indicates that the BCS type coupling is applicable. In Fig.2 we see that there is no T_c that is independent of area except that the transition temperature near the combination $K_{1.5}Rb_{1.5}C_{60}$ has a small contribution to T_c that is deviated from a"^{2} but such a magnitude is of the order of $\delta T_c \sim 2.25K$ only. Actually, the operator part of the BCS theory, i.e., the form of the electron (fermion) and the phonon (boson) operators and the spin-singlet zero-momentum pair wave function is correct but the wave vector dependence of the coupling constant requires modification. Such a modification as given here requires the consideration of randomly vacant oxygen sites. **The V^{BCS} is therefore replaced by $(3.6)^2V\omega_D^2a^2/v_l^2$ in which $(3.6)^2\omega_D^2a^2/v_l^2$** is a dimensionless coupling parameter. The effect of this parameter is that the transition temperatures become very large as a increases. For very large cells Va^2 becomes very large and the T_c increases accordingly. This means that T_c increases to 00 as $a \rightarrow$ 00. Thus a glass can have a T_c larger than that of a crystal because it is difficult to grow crystals of very large unit cell

dimensions. We will see that oscillations are set in to prevent the T_c from becoming very large.

Oscillations in T_c.

We find that the transition temperature oscillates as a function of number of layers *n* of *Cu* — *O* atoms per unit cell. Actually the approximation of small wave vectors taken to write (4) is not valid and there are both acoustical as well as optical branches in the dispersion relation.. Therefore, we write the interaction without the approximation of small wave vectors for acoustical phonons leaving out the energetically unfavourable optical phonons. The two sine waves of (3) may be written as

$$\sin(kR_i)\sin(k.R_j) = 2\pi \sum_{l=0}^{\infty} \sum_{m=-2l}^{m=2l} i^{2l} \Big[j_{2l}(k|R_i - R_j|) Y_{2l}^{m}(\theta_k, \phi_k) Y_{2l}^{m*}(\theta, \phi) - j_{2l}(k|R_i + R_j|) Y_{2l}^{m}(\theta_k, \phi_k) Y_{2l}^{m*}(\theta', \phi') \Big] \quad \textbf{(16)}$$

where $(\theta_k, \phi_k), (\theta, \phi)$ and (θ', ϕ') describe the direction of fc$_t$, $R_i - R_j$ and *Ri* + R_j respectively with j_{2l} as the spherical Bessel **function,**

$$j_m(x) = (\frac{\pi}{2x})^{1/2} J_{n+(1/2)}(x) \quad \textbf{(17)}$$

The unit vector along *k* is e_k = *k*/\k\. Considering that the product of the unit vectors, $e_k, e_{k'}$ transforms like $Y_n^m(\theta_k, \phi_k)$ with *n* = 0 and 2, only the terms with / = 0, 1 in (16) have to be retained. The average value over the direction of propagation and polarization is found to be,

$$A_l = \sum_{ij} \langle e_k e_{k'} \sin(k.R_i)\sin(k'.R_j) \rangle$$

$$= \frac{\delta k k'}{6} \sum_{ij} [j_o(kR_{ij}) + j_2(kR_{ij})] - \frac{1}{2} j_2(kR_{ij}) e_{ijk} e_{ijk'} \quad \textbf{(18)}$$

for the longitudinal and

$$A_t = \frac{\delta k k'}{12} \sum_{ij} [2j_o(kR_{ij}) - j_2(kR_{ij})] + \frac{1}{4} j_2(kR_{ij}) e_{ijk} e_{ijk'} \quad (19)$$

for the transverse branch. Therefore we write,

$$A(k) = A(k_l R) + 2(\frac{v_l}{v_t})^3 A(k_t R) \quad \textbf{(20)}$$

The dominant normal modes of CuO_6 octahedran transform as E_g **and** T_{2g} irreducible representations of the octahedral group. Considering these modes which are planer in the *xy, yz* and *zx* planes separately and orthogonal, the distance between two oxygen atoms of the CuO_6 octahedron is either *2R* or $\sqrt{2}R$ so that,

$$\begin{aligned} A(k_l) &= 1 - j_o(2k_l R) + 2j_2(2k_l R) + 6j_2(\sqrt{2}k_l R) \\ A(k_t) &= 1 - j_o(2k_t R) - 2j_2(2k_t R) - 3j_2(\sqrt{2}k_t R) \end{aligned} \quad (21)$$

which have to be linearly combined to describe the totally symmetric mode. In the approximation of $v_t \sim v_l$, we add the contributions from two transverse branches and one longitudinal branch so that we define, $B(k) = A(k_l) + 2A(k_t)$ in which case $j_2(x)$ cancells and we get

$$B(k) = 3[1 - j_o(2kR)] \quad \textbf{(22)}$$

which is better than the value used in (4) and clearly displays the Γ_1 symmetry. It emphasises the wave nature of the lattice waves [11]. Since

$j_o(x) = (\sin x)/x$, the interaction oscillates as a function of distance. These oscillations are sustained due to reasonable periodicity of the lattice. The conduction band is also subject to the reasonable periodic boundary conditions in spite of the oxygen defects. The matrix element of the electron-phonon interaction in this approximation becomes,

$$|M_q|^2 = |v_{kq}|^2 \left(\frac{3\hbar}{2M\omega_q}\right)[1 - j_o(2qR)] \tag{23}$$

Considering the lattice waves along different directions in the unit cell, we can write,

$$|M_q|^2 = |v_{kq}|^2 \left(\frac{\hbar}{2M\omega_q}\right)[3 - j_o(qa) - j_o(qb) - j_o(qc)] \tag{24}$$

In the case of a hexagonal lattice a = *b* so that

$$|M_q|^2 = |v_{kq}|^2 \left(\frac{\hbar}{2M\omega_q}\right)[3 - 2j_o(qa) - j_o(qc)] \tag{25}$$

In our simple model for layered superconductors, with *n* as the number of layers, we write *2Rn* in place of *c* so that for a layered superconductor

$$|M_q|^2 = |v_{kq}|^2 \left(\frac{\hbar}{2M\omega_q}\right)[3 - 2j_o(qa) - j_o(2Rnq)]$$

The larger the n, the larger is the matrix element of the electron-phonon interaction but the wave vector $q \sim \omega_D/v$ also plays an important role. We write the attractive potential as,

$$-\frac{|M_q|^2}{\hbar\omega} = -\frac{|v_{kq}|^2}{2M\omega_D^2}\left[3 - 2j_o\left(\frac{\omega_D a}{v}\right) - j_o\left(\frac{2Rn\omega_D}{v}\right)\right] \tag{27}$$

which is to be compared with $-V_{BCS}$ given by (10). We have thus introduced lattice wave propagation with a defect or wave vector dependence on the

coupling constant of the electron-phonon interaction. This effect causes a dependence of the attractive potential on the phonon velocity v and the lattice constants, a and $2Rn$ and hence n, the number of layers of $Cu - O$. The *BCS* potential given by (10) is valid near $q \sim \omega_D/v \sim 0$ only. The gap equation is then of the form

$$\Delta = \frac{2\hbar\omega_D}{\exp\left[-\rho_F^{-1}V_{BCS}^{-1}\{3 - 2j_o(\omega_D a/v) - j_o(2Rn\omega_D/v)\}^{-1}\right] - 1} \tag{28}$$

which shows that larger gap arises for larger values of n, the number of layers of CuO_6 octahedra. The transition temperature is now given by

$$T_c \simeq 1.14(\hbar\omega_D/k_B)\exp\left[-\rho_F^{-1}V_{BCS}^{-1}\left\{3 - 2j_o\left(\frac{\omega_D a}{v}\right) - j_o\left(\frac{2Rn\omega_D}{v}\right)\right\}^{-1}\right] \tag{29}$$

which gives larger T_c for larger n. For n = 4, the T_c was found to decrease instead of increasing with respect to the value at n = 3. This decrease is caused by the oscillatory nature of the Bessel function in (29). The T_c as a function of n shows oscillations and tends to saturate.

The maxima of j_o correspond to minima of T_c. The n = 0 corresponds to a maximum in j_o and hence minimum in T_c, which means that there is no $Cu - O$ at all. At n = 1 there is neither a maximum nor a minimum but at $2Rn\omega_D/v$= 37r/2, there is a minimum in j_o and hence a maximum in T_c. The next maximum in j_o occurs at $2Rn\omega_D/v$= 57r/2 which means that there is a minimum in T_c. The next minimum in $j_o$occurs at 77r/2 which is a maximum for T_c. We thus predict maximum T_c for n = 3 and 7 but the value of T_c at n = 7 is smaller than at n = 3. The function of importance which occurs in the expression for T_c saturates for large values of n but it may show

oscillations depending upon the value of $2R\omega_D/v$ chosen. The expression (6) corresponds to a smaller wave vector approximation of the proper matrix **element** (23) which oscillates [13].

Discussions and conclusions.

Usually there is a canonical transformation [14,15] in the *BCS* theory as first performed by Bogoliubov [16,17]. It absorbs part of the interaction into the unperturbed Hamiltonian by shifting the single-particle energies so that the potential in the resulting Hamiltonian is small compared with the unperturbed Hamiltonian. In our problem, the effect of this transformation is to slightly renormalize $|v_{kq}|$ of (10) without affecting the phonon part of the coupling constant. However, the gap equation and the equation of T_c are usually coupled. McMillan [18] has given an approximate solution of the coupled Eliashberg equations as

$$T_c = \frac{<\omega>}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right] \qquad \textbf{(30)}$$

for a special case of the phonon spectrum. Here $<\omega>$ is the average phonon frequency, $X = \rho_F V$ and μ^* is the Coulomb pseudo-potential parameter. Our effect of treating the sine waves occurs in the attractive potential V and hence in A. Thus A in (30) oscillates as a function of n, the number of layers of the $Cu-O$ atoms. Similarly, $<\omega>$ is slightly renormalized due to the electron-phonon interaction. The oscillations in T_c which are clearly visible in (29) are slightly masked in (30) but the oscillations do occur. This theory of oscillations is also applicable to spin triplets [19,20].

We can calculate the effect of the optical phonons as a trivial extension of

that of the acoustic phonons which for the present purpose is not necessary. It is possible to treat the phonons exactly by computing all the frequencies so that the acoustic and optic phonons need not be distinguished separately in terms of only two branches that is why in the modern theory of superconductivity, the Eliasberg function $\alpha^2 F(\omega)$ is introduced to describe the electron-phonon interaction. However, the wave vector dependence arising in the coupling constant due to lattice defects such as vacancies in the lattice has not been treated in the exact calculations. This aspect was also missed in most of the classical works on the electron-phonon interaction in metals. The problem is that only the electronic wave vectors are integrated in the calculation of T_c and the phonon is eliminated so that if any phonon wave vector dependence is introduced the same comes out of the integral and affects the attractive potential only. Besides, the Bogoliubov transformation has not been done in the Eliasberg formalism for the calculation of the transition temperature. This will introduce a wave vector dependence in the potential which has not been solved for the coupled equations.

In conclusion, we find that the transition temperature of high temperature superconductors increases with increasing the number of $Cu — O$ layers per unit cell and oscillates for $n > 3$. Thus a large T_c occurs for $n = 3$ but the value for $n = 4$ is smaller. Due to the use of the Bessel functions we are able to predict that the next high value of T_c occurs for $n = 7$ but this value is smaller than at $n = 3$. This conclusion is important for the manufacture of intercalated compounds of high transition temperatures. We have found that the coupling constant of the electron-phonon interaction in

the theory of superconductivity oscillates as a function of number of layers of *Cu —0* atoms. These oscillations are important for the understanding of transition temperatures of high-temperature superconductors. A linearization of the BCS expression for the transition temperature in terms of the Bessel functions has also been reported in literature [21].

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Chapter 4

Theory of detection of x-rays by superconductors

Two new processes occur in a superconducting film when it is used as a detector of x-rays. One of these processes is the scattering of the x-ray by a single electron which gives rise to the broadening of the x-ray line. Another process describes the breaking of a Cooper pair by the x-ray which also contributes to the width of the x-ray. The line width arising from the single electron process depends on T^4 whereas that arising from the pair breaking process varies almost as T^6 at low temperatures. Lines occur at $\hbar\omega_q \pm 2\mathrm{A}$, and at $\hbar\omega_q$ where $\hbar\omega_q$ is the energy of the x-ray and 2Δ is the gap of the superconductor

Recently,the superconducting tunnel junctions have been used to measure the nonequilibrium quasiparticle population caused by the x-rays absorbed into the superconducting thin films. This energy breaks the Cooper pairs and the resulting quasiparticles tunnel across the barrier until they recombine to form Cooper pairs. A measurement of this current gives a measure of the x-ray energy. It is possible to achieve energy resolution better than 10 eV for 6 KeV x-rays [1]. Niobium based x-ray detector being developed [2] for the European Space Agency requires a highly theoretical approach combined with advanced device process developement. The latest work demonstrates an exceptional energy resolution of 53 eV when cooled to 1.5 K. The superconducting films of NbN/BN have been shown to exhibit photoresponse to visible light [3]. It has been pointed out by Jochum et al [4] that new detectors have initiated important discoveries. Kraus et al[5] have pointed out that the rate of relaxation of particles down to the gap edge is,

$\gamma \propto E^3/\tau_o$

where E is the energy of excitations and τ_o is a time constant characteristic of the material. Several properties of the detectors of x-rays using superconducting junctions have been reported [6-9] but the quantum theory of widths and shifts has not yet been solved. The phonon scattering has been considered to be important [10-14] for the processes to take place but Burstein et al [15] have considered the use of superconductors as detectors of microwaves in which the photons play an important role. In the B.C.S. theory [16], the phonon operators of the Hamiltonian are eliminated to derive the attractive interaction between the electrons so that the phonon effects are found in the coupling constant. Thus the pair formation and breaking by phonons is stronger than by photons but the frequency of the x-ray is very large so that the two, phonon and photon resonances are far apart and hence do not interfere. Therefore it is of interest to determine the spectrum of the scattered

x and 7-rays. The solar x-rays can be detected using the superconductors. However, a monochromatic source of x-rays and a detector, both with an energy resolution of the order of the superconducting gap is not yet available. When ever such a technology is developed it will be necessary to have a calculation of shifts and widths, particularly because the widths determine the resolution of the instrument. Hence our calculation is of interest in the area of astrophysics and astronomy also. Further, the prospects of developing superconducting tunnel junctions as efficient detectors of x-rays[24] makes the study of detection of x-rays using superconductors more interesting.

In this work, we construct the Hamiltonian for the interaction of x-rays with Cooper pairs in a superconductor. As the x-ray hits the Cooper pair, it breaks the pair into two electrons and the x-ray is scattered. The spectrum of the scattered x-ray consists of several frequencies. One of the frequencies is the same as that of the incident x-ray, $\hbar\omega_q$,as in the Rayleigh scattering and there are sidebands at $\hbar\omega_q \pm 2\Delta$.We have performed the Bogoliubov transformation on the pair breaking interaction which we have used to calculate the self energy of the x-ray. This self energy corresponds to a broadening of the x-ray. We find that in a three dimensional superconductor, this broadening depends on temperature as T^4 for the electron scattering process and as T^6 for the pair breaking process at low temperatures.

We consider the x-rays interacting with the conduction electrons so that the unperturbed Hamiltonian of the system is described as,

$$H_o = \sum_q \hbar\omega_q \beta_q^\dagger \beta_q + \sum_{k,\sigma} \epsilon_{k,\sigma} (c_{k\sigma}^\dagger c_{k\sigma} + c_{-k,-\sigma}^\dagger c_{-k,-\sigma}) \tag{1}$$

where $\hbar\omega_q$ is the single particle energy of one x-ray. The $\beta_q^\dagger$ and β_q are the boson creation and annihilation operators for the x-ray. The single particle energy of the electrons of wave

vector k and spin σ in the conduction band is $\epsilon_{k\sigma}$. The wave vector of the x-ray is $q = \omega/c$ where c is the velocity of light. The attractive interaction between the electrons is given by

$$H_a = -V \sum_{k,k'}{}' c^\dagger_{k',\sigma} c^\dagger_{-k',-\sigma} c_{-k,-\sigma} c_{k,\sigma} \tag{2}$$

This interaction is useful for the formation of spin singlet zero momentum pairs as in the B.C.S. theory [16,17] and is diagonalized by the

$$c_k = u_k d_k + v_k d^\dagger_{-k} \tag{3}$$

where k is associated with spin σ and $-k$ with $-\sigma$. The coefficients u_k and v_k are real, where u_k is an even function of k and v_k is an odd function of k, $u_k = u_{-k}, v_k = -v_{-k}$ with $u_k^2 + v_k^2 = 1$. The gap is written in terms of pair operators,

$$\begin{aligned} \Delta_k &= V \Sigma'_{k'} c_{-k,-\sigma} c_{k,\sigma} , \\ \Delta^*_k &= V \Sigma'_k c^\dagger_{k,\sigma} c^\dagger_{-k,-\sigma} . \end{aligned} \tag{4}$$

The interaction of the x-ray photon with the conduction electrons is described by

$$\begin{aligned} H'_{pe} &= i \sum_{k,k',q'} G_{k,k',q'} c^\dagger_{k'} c_k \beta^\dagger_{q'} \delta(k - k' - q') \\ &+ i \sum_{k,k'',q} G_{k,k'',q} c^\dagger_{k''} c_{-k} \beta_q \delta(k'' - q + k) + h.c. \end{aligned} \tag{5}$$

where $G = gV^{-1/2}$ with

$$g = \frac{e\hbar}{mc} \left(\frac{\hbar\omega_q}{\kappa} \right)^{1/2} \tag{6}$$

where κ is the dielectric constant of the medium and m is the mass of the electron. One of the terms in the second-order energy operator of the above interaction is given by

$$\begin{aligned} H'_2 &= - \sum_{k,k',k'',q,q'} (\epsilon_{k'} - \epsilon_k + \hbar\omega_q)^{-1} G_{k,k',q} G_{k,k'',q} c^\dagger_{k''} c_{-k} c^\dagger_{k'} c_k \beta^\dagger_{q'} \beta_q \\ &\delta(q - k' - k'' - q') + h.c. \end{aligned} \tag{7}$$

Using anti commutators for the electron operators, the product of the electronic operators in the above can be written as

$$c^{\dagger}_{k''}c_{-k}c^{\dagger}_{k'}c_{k} = \delta_{-k,k''}c^{\dagger}_{k'}c_{k} - c_{-k}c^{\dagger}_{k''}\delta_{k,k'} + c_{-k}c^{\dagger}_{k'}\delta_{k,k''} - c_{-k}c_{k}c^{\dagger}_{k''}c^{\dagger}_{k'} \tag{8}$$

from which leaving out the first three terms which describe single particle electron scattering by photons, we write the interaction corresponding to pair formation and breaking as

$$H'_2 = \sum_{k,k',k'',q,q'} (\epsilon_{k'} - \epsilon_k + \hbar\omega_{q'})^{-1} G_{k,k',q'} G_{k,k'',q} c_k c_{-k} c^{\dagger}_{k'} c^{\dagger}_{k''} \beta^{\dagger}_{q'} \beta_q \delta(q - q' - k' - k'') \tag{9}$$

Including the sum over intermediate states, one more contribution to the above interaction occurs which we calculate and include in the above so that

$$\begin{aligned} H''_2 &= \sum_{k,k',k'',q,q'} \left[(\epsilon_{k'} - \epsilon_k + \hbar\omega_{q'})^{-1} + (\epsilon_{k''} - \epsilon_{-k} - \hbar\omega_q)^{-1}\right] G_{k,k',q'} G_{k,k'',q} \\ &\times c_k c_{-k} c^{\dagger}_{k'} c^{\dagger}_{k''} \beta^{\dagger}_{q'} \beta_q \delta(q - q' - k' - k'') + h.c. \end{aligned} \tag{10}$$

This means that the x-ray photons can break pairs of electrons into single electrons and pairs can be made by shining x-rays on electrons but the electromagnetic energy, $H^2/8\pi$, is small compared with $k_B T_c$. Hence this mechanism is too small to predict the transition temperatures but it can be effective for detecting x-rays, due to different frequency regime. Since the wave vector dependence in the coupling constant is small, we write the above interaction as,

$$H' = \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} \beta_q \beta^{\dagger}_{q'} c_{k,\sigma} c_{-k,-\sigma} c^{\dagger}_{k',\sigma} c^{\dagger}_{k'',-\sigma} \delta(q - q' - k' - k'') + h.c. \tag{11}$$

where $h.c.$ stands for the hermitian conjugate of the previous terms. Using the commutators for bosons and anticommutators for fermions, the above interaction can be written as,

$$H = H'_o + H_a + H'_a + H'_s + H'_p \tag{12}$$

$$H'_o = \sum_\sigma \sum_{k,q} D_{k,q} - \sum_\sigma \sum_{k,q} D_{k,q}\beta^\dagger_q\beta_q - \sum_\sigma \sum_{k,q} D_{k,q}(c^\dagger_{k\sigma}c_{k\sigma} + c^\dagger_{-k,-\sigma}c_{-k,-\sigma}) \tag{13a}$$

$$H'_a = \sum_\sigma \sum_{k,k',q} D_{k,k',q}c^\dagger_{k',\sigma}c^\dagger_{-k',-\sigma}c_{-k,-\sigma}c_{k,\sigma} \tag{13b}$$

$$H'_s = \sum_\sigma \sum_{k,k'',q,q'} D_{k,k'',q,q'}\beta^\dagger_{q'}\beta_q c^\dagger_{k'',-\sigma}c_{-k,-\sigma}\delta(q - q' - k - k'') + \sum_\sigma \sum_{k,k',q,q'} D_{k,k',q,q'}\beta^\dagger_{q'}\beta_q c^\dagger_{k',\sigma}c_{k,\sigma}\delta(q - q' - k' + k) + h.c. \tag{13c}$$

$$H'_p = \sum_\sigma \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'}\beta^\dagger_{q'}\beta_q c^\dagger_{k',\sigma}c^\dagger_{k'',-\sigma}c_{k,\sigma}c_{-k,-\sigma}\delta(q - q' - k' - k'') + h.c. \tag{13d}$$

where the first term in (13a) is a constant. The second term describes a small negative shift in the x-ray energy. The third term gives the reduction in the single particle energy of electrons in the conduction band. The term given by (13b) is a positive pairing interaction and hence its effect is to reduce the strength of attractive interaction given by (2). The expression (13c) shows that the x-rays are scattered by single electrons and (13d) shows that pairs are broken by the x-rays. Upon rearranging the various terms, the Hamiltonian of the system becomes,

$$H = H_{oo} + H'_a + H'_s + H'_p \tag{14}$$

where

$$H_{oo} = \sum_\sigma \sum_{k,q} D_{k,q} + \sum_q \hbar\omega'_q\beta^\dagger_q\beta_q + \sum_{k,\sigma} \epsilon'_{k,\sigma}(c^\dagger_{k,\sigma}c_{k,\sigma} + c^\dagger_{-k,-\sigma}c_{-k,-\sigma}) \tag{15}$$

$$H'_a = -V' \sum_{k,k'} c^\dagger_{k',\sigma}c^\dagger_{-k',-\sigma}c_{-k,-\sigma}c_{k,\sigma} \tag{16}$$

with

$$\hbar\omega'_q = \hbar\omega_q - \sum_\sigma \sum_k D_{k,q} \tag{17a}$$

$$\epsilon'_{k,\sigma} = \epsilon_{k,\sigma} - \sum_q D_{k,q} \tag{17b}$$

and

$$V' = V - \sum_q D_{k,k',q} \tag{17c}$$

in which the first term is a constant and the single particle energy of the x-ray has been slightly reduced. Similarly, the single particle energy of the electrons is also reduced by a small amount. The transformation (3) substituted in (16) gives the ground state energy with single particle energies shifted by the pair breaking energy [17]. The transformed form of the scattering interaction of (13c) is found to become,

$$\begin{aligned} H'_s &= \sum_\sigma \sum_{k,q,q'} D_{k,q,q'} v_k^2 \beta^\dagger_{q'} \beta_q + \sum_\sigma \sum_{k,k'',q,q'} D_{k,k'',q,q'} (u_k u_{k''} \beta^\dagger_{q'} \beta_q d^\dagger_{k''} d_{-k} \\ &+ v_k v_{k''} \beta^\dagger_{q'} \beta_q d^\dagger_k d_{-k''}) \delta(q - q' - k - k'') + h.c. \end{aligned} \tag{18}$$

There are terms with k replaced by $-k$ and also charge non-conserving terms containing factors of the type $d_{-k''} d_{-k}$ or $d^\dagger_k d^\dagger_{k''}$ but all such terms cancell each other so that there is no charge non-conserving interaction. The pair breaking Hamiltonian may be expressed as

$$H'_p = H'_p(o) + H'_p(1) + H'_p(2) + H'_p(3) + H'_p(4) \tag{19}$$

where

$$\begin{aligned} H'_p(o) &= \sum_\sigma \sum_{k,k',q} D_{k,k',q} u_k u_{k'} v_k v_{k'} (d^\dagger_k d_k - d^\dagger_{-k} d_{-k}) \beta^\dagger_q \beta_q \\ &+ 2 \sum_\sigma \sum_{k',k'',q,q'} D_{k',k'',q,q'} v_{k''} v^3_{k'} d^\dagger_{k'} d_{-k''} \beta^\dagger_{q'} \beta_q \delta(q - q' - k' - k'') + h.c. \end{aligned} \tag{20}$$

Upon decoupling, it is seen that this interaction gives a shift in the single particle frequency of the x-ray which depends on the number density of electrons. The second term in (20)

gives the electron scattering within a band. Next we write the terms which contain a pairing operator of the form $d_k d_{-k}$ which annihilates a fermion pair as,

$$\begin{aligned} H'_p(1) &= \sum_{\sigma} \sum_{k,k'',q} D_{k,k'',q} u_k^2 u_{k''} v_{-k''} d_k d_{-k} \beta_q^\dagger \beta_q \\ &+ \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k''q,q'} u_k v_k v_{k'} v_{k''} d_{-k'} d_{-k''} \beta_{q'}^\dagger \beta_q \delta(q - q' - k' - k'') \\ &- \sum_{\sigma} \sum_{k,k',q} D_{k,k',q} u_{k'} v_{k'} v_k^3 d_{-k}^\dagger d_k^\dagger \beta_q^\dagger \beta_q \\ &- \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} u_k u_{k'} u_{k''} v_k d_{k'}^\dagger d_{k''}^\dagger \beta_{q'}^\dagger \beta_q \delta(q - q' - k' - k'') + h.c. \end{aligned} \tag{21}$$

We now write the interaction terms in which pairs are broken into two particles by the x-ray as,

$$\begin{aligned} H'_p(2) &= \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} u_k^2 u_{k'} u_{k''} d_{k'}^\dagger d_{k''}^\dagger d_k d_{-k} \beta_{q'}^\dagger \beta_q \delta(q - q' - k' - k'') \\ &- \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} v_k^2 v_{k'} v_{k''} d_{-k}^\dagger d_k^\dagger d_{-k'} d_{-k''} \beta_{q'}^\dagger \beta_q \delta(q - q' - k' - k'') + h.c. \end{aligned} \tag{22}$$

The terms which do not conserve the quasiparticle number unless pairs are formed are given below,

$$\begin{aligned} H'_p(3) &= \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} \big[u_k v_k v_{k'} v_{k''} d_{-k}^\dagger d_{-k'} d_{-k''} d_{-k} \beta_{q'}^\dagger \beta_q \\ &+ u_k v_k v_{k'} v_{k''} d_k^\dagger d_{-k'} d_{-k''} d_k \beta_{q'}^\dagger \beta_q + u_k u_{k'} u_{k''} v_k d_{k'}^\dagger d_{k''}^\dagger d_{-k}^\dagger d_{-k} \beta_{q'}^\dagger \beta_q \\ &+ u_k u_{k'} u_{k''} v_k d_{k'}^\dagger d_{k''}^\dagger d_k^\dagger d_k \beta_{q'}^\dagger \beta_q \big] \delta(q - q' - k' - k'') + h.c. \end{aligned} \tag{23}$$

Now we write those terms which are quadratic in pair breaking upon interaction with the

$$H'_p(4) = \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} \left[u_k^2 v_{k'} v_{k''} d_{-k'} d_{-k''} d_k d_{-k} - u_{k'} u_{k''} v_k^2 d^\dagger_{k'} d^\dagger_{k''} d^\dagger_{-k} d^\dagger_k \right] \beta^\dagger_{q'} \beta_q \delta(q - q' - k - k'') + h.c. \quad (24)$$

This completes the definition of our Hamiltonian. Considering the single particle energies and the attractive interaction as given by (16), we find that the coherence factors are given by,

$$u_k^2 = \frac{1}{2}\left[1 + \frac{\epsilon'_k}{(\epsilon'^2_k + \Delta^2)^{1/2}}\right]$$

and

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon'_k}{(\epsilon'_k + \Delta^2)^{1/2}}\right] \quad (25)$$

where the single particle energy is given by (17) which is slightly shifted from that in the conduction band due to shining with x-rays.

The width of the x-ray as measured by the superconducting detector is given by $\hbar/\tau$ where r is the life time of the x-ray due to the interaction with the superconductor as calculated from the imaginary part of the self energy,

$$\frac{1}{\tau_q} = \frac{2}{\hbar} Im \Sigma_q \quad (26)$$

using Dirac's identity

$$\lim_{\epsilon \to 0} \frac{1}{x \pm i\epsilon} = \frac{P}{x} \mp i\pi\delta(x) \quad (27)$$

where the first term on the right hand side indicates that the Cauchy's principal value has to be evaluated for determining the real part. The width of the x-ray is caused by two important processes. One of these is the electron scattering process given by (18) and the other is the pair breaking process given by (22). The total width is given by $\hbar\delta\omega_q \sim \hbar\ (1/\tau_s + 1/\tau_p)$.

The method of calculation of the two mechanisms occuring here is similar to that used for the radiation damping from the magnon-photon interaction [18] and recombination in electron-hole droplets in semiconductors [19].

The first term of (18) gives rise to a shift of the energy of the x-ray as $\sum_{\sigma}\sum_{k,q} D_{k,q} v_k^2 n_q$ to which we add also the term $\sum_{\sigma}\sum_{k,q} D_{k,q} u_k^2 n_q$ where $n_q = [\exp(\hbar\omega_q/k_BT) - 1]^{-1}$ is the number density of the x-ray. This term does not contribute to the life time of the x-ray. Therefore, we calcualte the self energy of the x-ray due to the second term of (18) as

$$\Sigma_q^x(1) = \sum_{k,k'',q'} \frac{2G_1^2\zeta_1\delta(q - q' - k - k'')}{E - \hbar\omega_{q'} - \epsilon_{k''} + \epsilon_{-k}} \tag{28}$$

where

$$G_1 = D_q u_k u_{k''} \,, \tag{29a}$$

and

$$\zeta_1 = (1 + n_{q'})(1 - f_{k''})f_{-k} + n_{q'} f_{k''}(1 - f_{-k}) \tag{29b}$$

and f_k is a Fermi distribution

$$f_k = [\exp(\epsilon_k - \epsilon_F)/k_BT + 1]^{-1} \,.$$

A factor of 2 arises due to two spin configurations. Using the Dirac's identity (27), the imaginary part of the above is found to be,

$$Im\sum_q^x(1) = 2\pi \sum_{k,k'',q'} G_1^2\zeta_1\delta(q - q' - k - k'')\delta(\hbar\omega_q - \hbar\omega_{q'} - \epsilon_{k''} + \epsilon_{-k}) \tag{30}$$

where we took $\hbar\omega_q$ for E. We eliminate k'' using the first δ function and then near small k, $\hbar\omega_q \simeq \hbar\omega_{q'}$, so that the second δ function gives $\frac{1}{\hbar c}\delta(q - q')$. Then using (26) we find the life time of the x-ray as,

$$\frac{1}{\tau_1} \simeq \frac{2V\omega^2}{\pi\hbar^2 c^3} \sum_k G_1''^{\,2}\zeta_1''^{\,2} \tag{31}$$

where

$$G_1'' = D_q u_k^2 \,, \tag{32}$$

$$\zeta_1'' = f_{-k}(1 - f_{-k})(2n_q + 1) \tag{32b}$$

and V is the volume of the superconductor. In the case of a three dimensional superconductor the summation over k leads to T^3 dependence in the inverse life time. Another factor of T ariese from n_q so that the rate given by (31) varies as T^4 at low temperatures. There is one more term in the interaction due to the symmetry in the Bogoliubov transformation given by the third term of (18). This term is of the form $D_q v_k v_{q-q'-k}$ in place of (29a) so that when we add this contribution to (31) we obtain

$$\frac{1}{\tau_s} \simeq \frac{2V\omega^2}{\pi\hbar^2 c^3} \sum_L D_q^2 \zeta_1'' \,. \tag{33}$$

as the life time of the x-ray due to electron scattering from the processes of the form given by the second and third terms of (18). The first term of (20) does not contribute to the life time of the x-ray. The contribution of the second term is small compared with that calculated above. The contribution of all of the terms of (21) is real because of pair formation so that the imaginary part of the self energy is zero and only a shift occurs. This interaction becomes completely diagonalizable when pairs are introduced using the prescription given by (4). Sidebands are not produced by this interaction. Similarly (23) and (24) do not contribute to the width of the x-ray.

The broadening of the x-ray line due to pair breaking is given by the expression (22). The self energy of the x-ray due to the first term of (22) is found to be,

$$\Sigma_q^x(2) = \sum_\sigma \sum_{k,k',k'',q'} \frac{F_1^2 \eta_1 \delta(q - q' - k' - k'')}{E + 2\epsilon_k - \epsilon_{k'} - \epsilon_{k''} - \hbar\omega_{q'}})$$

where

$$F_1 = D_{k,k',k'',q'} u_k^2 u_{k'} u_{k''} \tag{35a}$$

$$\eta_1 = (n_{q'} + 1)(1 - f_{k'})(1 - f_{k''}) f_k f_{-k} + n_{q'} f_{k'} f_{k''}(1 - f_k)(1 - f_{-k}) \tag{35b}$$

in which $2\epsilon_k$ appears because we assumed $\epsilon_k = \epsilon_{-k}$ in the denominator. We evaluate the sum over k'' by using the δ function and then by using (26) and (27) we obtain the life time

of the x-ray due to pair breaking from the first term of (12) as,

$$\frac{1}{\tau_2} \simeq \frac{2V(\omega + \frac{2\Delta}{\hbar})^2}{\pi\hbar^2 c^3} \sum_{k,k'} F_1''^{\,2} \eta_1''^{\,2} \qquad \text{(36)}$$

where

$$F_1'' = D_{k,k'} u_k^2 u_{k'} u_{(2\Delta/\hbar c)+k'} \qquad \text{(37a)}$$

and

$$\eta_1'' = [n(2\Delta + \hbar\omega) + 1](1 - f_{k'})(1 - f_{-k'-2\Delta/\hbar c}) f_k f_{-k}$$

$$+ n(2\Delta + \hbar\omega) f_{k'} f_{-k'-2\Delta/\hbar c}(1 - f_k)(1 - f_{-k}) \qquad \text{(37b)}$$

Similarly, the second term of (22) gives,

$$\frac{1}{\tau_3} \simeq \frac{2V(\omega - \frac{2\Delta}{\hbar})^2}{\pi\hbar^2 c^3} \sum_{k,k'} F_1''^{\,2} \eta_2'' \,. \qquad \text{(38)}$$

where

$$F_2'' = D_{k,k'} v_k^2 v_{k'} v_{(2\Delta/\hbar c)+k'} \qquad \text{(39a)}$$

$$\eta_2'' = [n(\hbar\omega - 2\Delta) + 1](1 - f_k)(1 - f_{-k}) f_{-k'} f_{-k'+2\Delta/\hbar c}$$

$$+ n(\hbar\omega - 2\Delta) f_k f_{-k}(1 - f_{k'})(1 - f_{-k'+2\Delta/\hbar c}) \qquad \text{(39b)}$$

The total life time of the x-ray due to pair breaking is

$$\frac{1}{\tau_p} = \frac{1}{\tau_2} + \frac{1}{\tau_3} \qquad \text{(40)}$$

and the width of the x-ray is $\hbar\delta\omega = \frac{\hbar}{2}(\frac{1}{\tau_s} + \frac{1}{\tau_p})$ which is built up from the single quasiparticle scattering as well as pair breaking processes. The relaxation rates τ_2 and τ_3 suggest the occurance of three lines one each at ω and$\omega \pm 2\Delta/\hbar$. The temperature dependence in the pair breaking process is a bit stronger than T^6 at low temperatures. The calculations of τ_-^{-1} involves $\sum_{k\,k'}$ which for a three dimensional solid is equivalent to $//\ 2(m/\hbar^2)^3 \epsilon_k d\epsilon_k d\epsilon_{k'} \propto \epsilon^3$ in agreement with the E^3 dependence suggested by Kraus et al[5]. The resolution of the detector is limited by the line width determined from the life time of the x-ray (40).

The thermal and non-equilibrium response of superconductors as radiation detectors

has been studued by Zhang and Frenkel [20] and Epifani [21]. The x-ray operations of a thin film *Nb* superconducting strip particle detector is given by Parlato et.al [22] and by Gonsev et.al [23]. In the present work we have found the width of the x-ray as detected by a superconducting detector. Our calculation is thus of interest for the developement of superconducting films as detectors. Since lines occur at $\omega, \omega \pm 2A$, we predict that there are side bands which affect the resolution of the detector. Since the gap is proportional to the transition temperature, the smaller the gap the better is the resolution of the detector. Hence the smaller the transition temperature, the better is the resolution. In the case of large T_c the lines ω and $\omega \pm 2A$ will be well resolved.

We have found that the width of the x-ray line is determined by two processes. One of these is the process of electron scattering by x-rays and the other is the pair breaking. The width due to the former process depends on T^4 and that due to later is slightly stronger than T^6 at low temperatures. Both the mechanisms give zero line width at $T = 0$.

Since the x-ray frequency is much larger than the phonon frequency, creation of pairs by interaction of photons is possible at very low temperatures due to quantum mechanical effects.

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Chapter 5

Berry's phase factor accompanying orbit-lattice interaction

The orbit-lattice interaction gives rise to a Berry's phase factor in the wave function. This phase depends on the symmetry of the potential and on the band gap of the system. Thus in the case of a lattice distortion the exponent of the phase factor vanishes above a transition temperature.

It is known that Berry[l] has shown that the wave function of a system slowly transported round a circuit by varying a parameter R in its **Hamiltonian** $\mathcal{H}(\mathcal{R})$ acquires a phase **factor**, $e^{i\gamma}$ other than the usual phase factor $\exp(i\omega t)$. In the crystal field theory, the derivative of the potential with respect to the distance between atoms is calculated to obtain the orbit-lattice interaction which was used by van Vleck[2] to calculate the spin lattice relaxation time of paramagnetic ions interacting with lattice vibrations. It was also **found**[3-5] that there is always at least one vibration with respect to which the lattice is instable so that there is a distortion in the lattice in the ground state, which leads to missing symmetries in the ground state of the molecules, usually called the **Jahn-Teller** distortion. The effect of the vibration on the potential is obtained by varying the parameter R and evaluating the derivative of the potential at the equilibrium. Some time ago, we **found**[6-9] that such a variation of potential causes a shift in the energy of the paramagnetic ion which can be measured in terms of the change in the constants of the **spin-Hamiltonian** as a function of temperature which are related to the orbit-lattice interaction by the Wigner-Eckart theorem. In the case **of**[10] superconductors, the Berry's phase is calculated for an adiabatic motion and from that the Magnus force is deduced. Koizumi[ll] has discussed the electron-phonon interaction in Jahn-Teller crystals and has shown that Berry's formulation of the geometric phase that arises in adiabatic approximation leads to gauge potential terms in the Hamiltonian.

In this work, we calculate the Berry's phase for a system of single spin interacting with phonons in a lattice. We use the concept of symmetry breaking

which leads to Berry's phase in the wave functions, vanishing at a characteristic transition temperature.

Adiabatically, a system prepared in the state $|n(R(0))>$ evolves to the state $\backslash n(R(t))>$ after a time t with phase factor

$$|\psi(t)>= exp\{\frac{-i}{\hbar}\int_0^t dt' E_n(R(t))\}\ exp(i\gamma_{nB}(t))\ |n(R(t))> \qquad (1)$$

where the first exponential gives the usual dynamical phase and the second gives the Berry's phase, $exp(i\gamma_{nB})$ with $\gamma_{nB} = -/\ dS.V_n(R)$, where dS is the area element in the **R** space and

$$V_n(R) = Im\Sigma_{m\neq n}\frac{< n(R)|\frac{\partial}{\partial R}\mathcal{H}'(R)|m(R)><m(R)|\frac{\partial}{\partial R}\mathcal{H}'(R)|n(R)>}{[E_m(R)-E_n(R)]^2} \qquad (2)$$

A system of a single spin interacting with a continuum of phonons is described by the unperturbed Hamiltonian,

$$\mathcal{H}_0 = \Omega S_z + \Sigma_k \hbar\omega_k a_k^\dagger a_k \qquad (3)$$

where the first term gives the spin levels and the second describes the continuum of phonons with $\hbar\omega_k$ as the single particle energy of the phonons. The orbit-lattice interaction is obtained by finding the derivative of the Coulomb interaction between the electrons and the positively charged ions and multiplying the same by fluctuation in the distance between atoms. In the case of a lattice, the normal coordinates are generalised to take into account the oscillations of the entire lattice. Therefore,the interaction can be written as

$$\mathcal{H}' = \Sigma_{nm}\Sigma_k \frac{\partial}{\partial R} V_n^m \left(\frac{\hbar}{2M\omega_k}\right)^{1/2} (a_k + a_k^\dagger) \qquad (4)$$

In the case of an axial potential, $V_n^m(r)$ is written in terms of spherical harmonics $Y_2^0(r)$ and $Y_2^{\pm 2}(r)$. For cubic crystals [12] the potential is written in terms of $Y_4^0(r), Y_4^{\pm 4}(r)$ and $Y_6^{0,\pm 4}(r)$,etc. Thus n and m determine the symmetry of the crystal potential. The distance between the nearest neighbours is R, M is the mass of the crystal, $a_k(a_k^\dagger)$ are the annihilation(creation) operators for the phonons of wave vector k. The second order energy shift of a state $|M, n_k>$ is given by

$$S = \Sigma_{n,m}\Sigma_k \frac{n}{2M\omega_k} \times$$
$$[\frac{< M|\frac{\partial}{\partial R}V_n^m|M' >< M'|\frac{\partial}{\partial R}V_n^m|M >< n_k|a_k^\dagger|n_k - 1 >< n_k - 1|a_k|n_k >}{-\hbar\omega + \Omega(M' - M)}$$
$$+ \frac{< M|\frac{\partial}{\partial R}V_n^m|M' >< M'|\frac{\partial}{\partial R}V_n^m|M >< n_k|a_k|n_k + 1 >< n_k + 1|a_k^\dagger|n_k >}{\hbar\omega + \Omega(M' - M)}] \quad (5)$$

In the case of paramagnetic ions we consider the selection rule, $M' - M = \pm 1$ so that the above shift can be written as

$$S = \Sigma_{nm}\Sigma_k \frac{\hbar}{2M\omega_k} < M|\frac{\partial}{\partial R}V_n^m|M' >< M'|\frac{\partial}{\partial R}V_n^m|M > \times$$
$$[\frac{n_k}{\Omega - \hbar\omega} + \frac{n_k + 1}{\Omega + \hbar\omega}] \quad (6)$$

Usually in the case of paramagnetic ions, the splitting may be much larger than the single phonon frequency,$\Omega >> \hbar\omega$, so that the factor containing the phonon number density becomes proportional to the phonon correlation function. The above shift then reduces to,

$$S = \Sigma_k \frac{\hbar\Omega(2n_k + 1)V_M(R)}{2M\omega_k} \quad (7)$$

where

$$V_M(R) = \Sigma_{n,m} < M|\frac{\partial}{\partial R}V_n^m|M' >< M'|\frac{\partial}{\partial R}V_n^m|M > \Omega^{-2} \quad (8)$$

from which, it is found that

$$\int \frac{SRdR}{\Omega < \delta R^2 >} = \int V_M(R)RdR \quad (9)$$

where the integral encloses a finite area and

$$< \delta R^2 >= \Sigma_k \frac{\hbar}{2M\omega}(2n_k + 1) \quad (10)$$

which varies as T at low temperatures in two dimensions. From (9), the Berry's phase is given by

$$\gamma_{MB} = \int \frac{SRdR}{\Omega < \delta R^2 >} \quad (11)$$

In case (7) is a slowly varying function of R and $R^2/2 < \delta R^2 > \simeq$ c, the exponent of the Berry's phase becomes proportional to the shift,

$$\gamma_{MB} = \frac{Sc}{\Omega} \quad (12)$$

The form of the potential is given by Hutchings[12] so that we can extract the symmetry properties of the exponent of the Berry's phase. The potential is a function of the distance between atoms in such a way that the symmetry index, n appears in the exponent ,

$$V_n^m = V_n^m(0)R^{-(n+1)} \quad (13)$$

then the quantity $V_M(R)$ can be written approximately as ,

$$V_M(R) = \frac{(n+1)^2}{R^{2n+4}} < M|V_n^m(0)|M' >< M'|V_n^m(0)|M > \Omega^{-2} \quad (14)$$

which is seen to be dependent on $(n+1)^2$ and hence on the symmetry. Using (14) and the right hand side of (9) the exponent of Berry's phase is found to become,

$$\gamma_{MB} = \frac{(n+1) < M|V_n^m(0)|M' >< M'|V_n^m(0)|M >}{2\Omega^2}[\frac{1}{a_o^{2n+2}} - \frac{1}{R_o^{2n+2}}] \quad (15)$$

where the minimum distance is taken to be the Bohr radius a_o and the maximum is taken as the equilibrium distance between atoms, R_o.

In a symmetry conserving solution of the Hamiltonian, the average values of boson operators are zero,$< a_k >=< a_k^\dagger >= 0$ and $< a_k^\dagger a_k >= n_k$ gives the number density of phonons. In the case of lattice distortions, a gap in the single particle dispersion is introduced so that the average value of the operators is given by the gap energy and the energy of the interaction [13].

$$< a_k >=< a_k^\dagger >= \left(\frac{\Delta}{R\frac{\partial V}{\partial R}}\right)^{1/2} \delta_{k,Q} \quad (16)$$

where Q is the wave vector at which the distortion occurs and hence,

$$< a_k^\dagger a_k >= \frac{\Delta}{R\frac{\partial V}{\partial R}} \delta_{k,Q}. \quad (17)$$

Substituting this value in (7), we find that the shift is proportional to the gap energy,

$$S = \frac{\hbar\Omega[2(\Delta/R\frac{\partial V}{\partial R}) + 1]V_M R}{2M\omega_Q} \quad (18)$$

and hence the exponent of the phase factor from (12) also becomes proportional to the gap. Here *RdV/dR* is evaluated at the equilibrium.In the case of a transition from the normal to the superfluid liquid helium, the Berry's phase depends on the gap energy of the roton whereas in the normal

state it depends on the superfluid density.In the case of a superfluid of areal density,ρ_s, the exponent of the Berry's phase becomes[14],

$$\gamma_{bf} = -\pi \rho_s A \tag{19}$$

where A is the area enclosed by the loop, which goes to zero when ρ_s goes to zero. In the case of a superconductor [15] the Berry's phase round a closed loop is proportional to the magnitude of the magnetic field B and the area A enclosed by the loop projected in the direction of the magnetic field is,

$$\gamma_s = 2\pi(\frac{2e}{hc})BA \tag{20}$$

which is 2π times the number of flux quanta enclosed by the loop. In the case of the orbit-lattice interaction, the Berry's phase depends on the effective value of the gap energy,A of the distortion so that the phase describes a Goldstone boson [16-18],

$$\gamma_d \simeq 2\pi\Delta_{eff}/(R\frac{\partial V}{\partial R}) \tag{21}$$

while in the case of a symmetry conserving state, it depends on the phonon correlation function and hence on the number density of phonons which are the Goldstone bosons of zero mass. In the mean field theory the gap varies with the temperature as $A = \Delta_o(1 - T/T_c)^{1/2}$so that it is zero at $T = T_c$. Therefore, in the case of a lattice distortion, the exponent of the Berry's phase vanishes at a particular transition temperature, T_c, at which the distortion also vanishes.

We have found the Berry's phase in a system of an atom interacting with the continuum of phonons. The exponent of the phase depends on the

symmetry of the system and on the number density of phonons. In the case of a lattice distortion it depends on the band gap.

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Educational Qualifications

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Extra-Curricular Awards

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List of Publications

(a) in Journals/Books.

1. *Detection of x-rays by pair breaking in superconductors.*
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