STUDY OF SUPERCONDUCTIVITY OF ALKALI METAL DOPED A_3C_{60}(A=K,Rb AND Cs) SUPERCONDUCTORS

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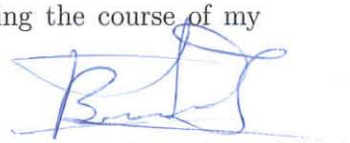

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Abstract

The mechanism of superconductivity in A_3C_{60}(A=K, Rb and Cs) appears to be one of difficult question in the theory of superconductivity. In this Work we try to show electronic(exciton) and phonon-exciton combined mechanism of superconductivity in A_3C_{60} superconductors.

In the first part of our work we try to show exclusively excitonic mechanism can not properly explain superconductivity in A_3C_{60}(A=K, Rb and Cs) superconductors. As a result of this and the existence of small isotope effect we try to explain mechanism of superconductivity in these compounds by phonon-exciton combined mechanism. Our result shows phonon-exciton mechanism is capable of explaining the whole range of T_c values for all of these superconductors. The isotope effect and reduced gap values are in good agreement with the experimental values. Also it is inferred that A_3C_{60} superconductors are BCS type assisted by excitonic effect.

Introduction

Superconductivity which is the state of zero resistance was first realized by Kammerling Onnes in 1911 .He found that the electrical resistivity of pure mercury(Hg) dropped abruptly to zero upon cooling to below $4.2K$ during studies of metals behavior at low temperature. He concluded that mercury had passed into a new state and gave the name superconductivity to this new phenomenon. The temperature at which the resistance vanishes is known as transition temperature (T_c). Following Onnes discovery, many other materials including metals , alloys and the complex ceramics were investigated in the search of superconductivity. After the discovery of superconductivity many other properties of superconductors were discovered. It was shown by Miessner and Ochsenfeld , that superconductor is not merely a perfect conductor but also a perfect diamagnet.

Besides, the experimental investigations, the theoretical efforts were also made to understand the microscopic origin of superconductivity. Understanding of the phenomenon took around 45 years to be able to reach a logical conclusion.Frohlich in 1950 found that two electrons in a metal could effectively attract each other , attraction being mediated by phonons. Following Frohlich's idea Bardeen,Cooper and Schrieffer in 1957 put forward a theory known as BCS theory based on bound electron pair ,

called cooper pairs and the coherent superposition of these pairs into a single macroscopic quantum state . This theory was able to explain many of superconductivity properties. After the discovery of high T_c superconductivity , the prime objectives of condensed matter physicist and material scientists have been to raise the transition temperature to make materials technologically useful.

The highest temperature to beat at present is $155K$ and the search for room temperature superconductivity is going on. A general review of superconductivity findings all the years is shown on figure(1). It has been realized that BCS theory based on electron phonon interaction is not capable of explaining such high T_c values in cuprates and alkali metals doped C_{60} superconductors. Hence, a number of theories have been proposed by several workers which invoke phonons, excitons, biexcitons [1], polarons, spin fluctuations [2] etc. to explain superconductivity in high transition temperature superconductors and other unusual properties of these systems. But so far there is no general consensus on mechanism of superconductivity in alkali metal doped C_{60} compounds and cuprates. As a result we try to investigate the superconductivity mechanism in A_3C_{60}(A=K, Rb and Cs) compounds. In chapter one the review of work carried out by several workers through the years, which is closely connected to the present investigation is presented.

In our investigation we have used double time temperature dependent green function formalism to study a model Hamiltonian invoking an exciton mechanism. A description of this mathematical technique is given in chapter two. The theoretical formulation of the problem is contained in chapter three. In this section we consider the effect of electronic excitation (excitons) for pair formation.The model Hamiltonian has been described and equation of motion have been obtained by employing the

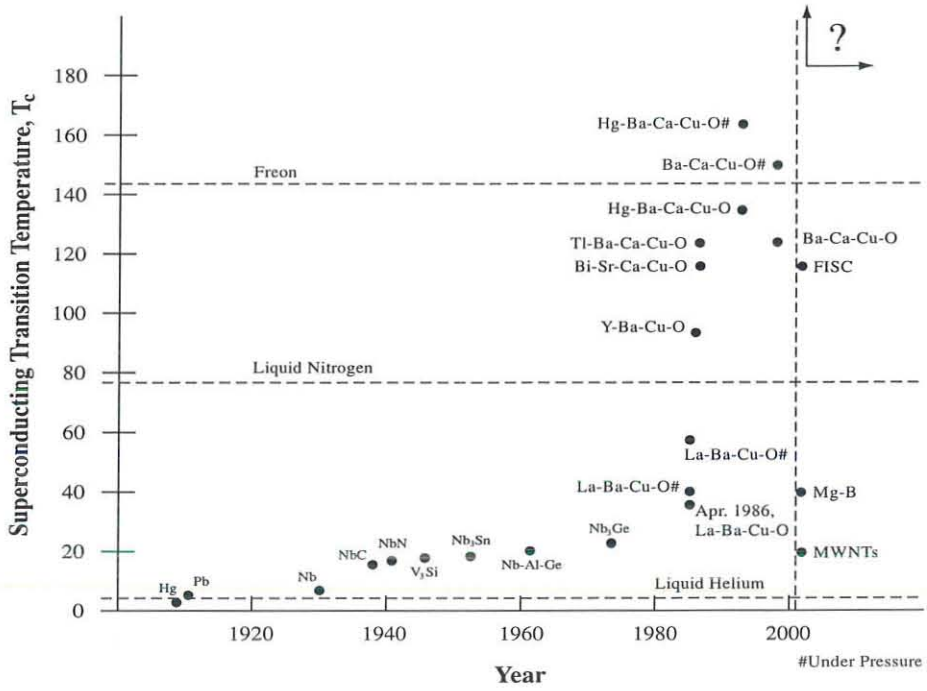


Figure 1: Discovery of superconductvity all the years.

Green function formalism. The equation is solved in order to obtain T_c and the gap parameter $\triangle$. Also we try to obtain the values of T_c , α and reduced gap $\frac{2\triangle}{K_B T_c}$ for this system from phonon-exciton mechanism. In section four we discuss the results comparing with the experimental values and from graphs . Finally we have summarized our results in chapter five.

Chapter 1

Review Of Literature

The fullerenes(C_{60},C_{70}....) have attracted much interest since their discovery by Kroto et al. [3] in 1985.This interest increased dramatically when Kratschmer et al. [4]in 1990 produces C_{60} in large enough quantities to be able to make solids of a size which allowed traditional solid state experiments.Very soon Haddon et al. [5] found that intercalation of alkali metal atoms in solid C_{60} leads to metallic behavior. Shortly afterwards it was found that some of these alkali-doped C_{60} compounds are superconducting with a transition temperature T_c which is only surpassed by the cuprates [6].The greatest interest in the superconductivity of the alkali-doped C_{60} compounds is particularly due to the large value of T_c and the question wether such a large value of T_c can be caused by the coupling to phonons alone or not.

There had been a great effort over the last ten years to characterize and understand both the normal and superconducting state properties of fullerides .The present review deals only with C_{60} compounds, since no other superconducting fullerides are known so far.

1.1 Structure and Electronic Properties Of C_{60}

The Buckminster fullerene C_{60} a molecule with 60 Carbon atoms that occupy the vertices formed by the intersections of 20 hexagonal and 12 pentagonal faces to build a cage (Fig.1.1). All of the atoms in the molecule are equivalent, and molecular shape is very close to a sphere. The molecule belongs to the I_h symmetry group, and the high symmetry provides a high degeneracy in the electronic structure. Each carbon atom has three C-C bonds and is surrounded by two hexagons and one pentagon.It possesses a π electron and three σ electrons that form an sp^2 hybrid orbital.

The highest occupied molecular orbital(HOMO)is that of the π states, with $5-fold$ degeneracy and h_u symmetry, while the lowest unoccupied molecular orbital(LUMO) has $3-fold$ degeneracy and t_{1u} symmetry [7].The electronic structure of the crystal is determined mainly by the bonding interactions within individual molecules, and the band width is determined by electron hopping between the C_{60} molecules.

C_{60} molecules aggregate to form a cubic crystal with fcc structure and a lattice constant of $1.42nm$ at room temperature. The nearest-neighbor molecular center-to-center distance is $1.002nm$, implying a van der waals separation of $0.29nm$ for a calculated diameter of $0.71nm$. The band structure of the C_{60} crystal calculated in the Local Density Approximation(LDA) is characterized by an energy gap between the valence band corresponding to HOMO of the molecule and the conduction band corresponding to LUMO [8]. Fig.1.2 shows the energy levels of the C_{60} molecule, and the band structure of the fcc C_{60} crystal. The electronic structure expresses the fact that the C_{60} crystal is a semiconductor with a direct gap [8]. The calculated energy gap between the h_u and t_{1u} orbitals is $\simeq 1.5ev$. If the system had perfect spherical

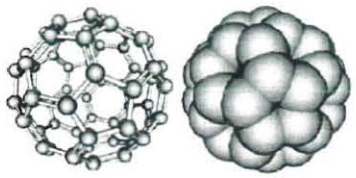


Figure 1.1: Two Schematic views of C_{60} Molecule.

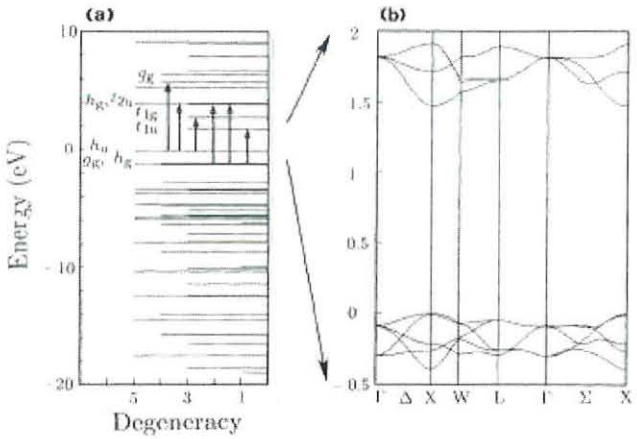


Figure 1.2: (a)Electronic energy levels of an isolated C_{60} molecule (b)Band structure of fcc C_{60} around the energy gap. The optically allowed transitions with excitation energies less than $6ev$ are indicated by arrows.

symmetry, the energy levels would be characterized by an angular momentum number ℓ, and the optically allowed transitions would be from ℓ to $\ell \pm 1$ states. The energy levels of the C_{60} molecule possess a clear correspondence to the ℓ state. For example, the second- and third-highest occupied states (g_g and h_g) correspond to the $\ell = 4$ states in the case of spherical symmetry, and h_u corresponds to the $\ell = 5$ states. The allowed optical transitions are shown by arrows in Fig.1.2:$h_u \rightarrow t_{1g}$, $h_g \rightarrow t_{iu}$, $h_u \rightarrow h_g$, $g_g \rightarrow t_{2u}$, $h_g \rightarrow t_{2u}$, and $h_u \longrightarrow g_g$. Since the energy levels of the C_{60} molecule corresponds to the energy bands of the C_{60} crystal, we can expect the optical spectral of the fcc C_{60} crystal to be similar to those of the C_{60} molecule. The calculated excitation energies for these optically allowed transition are $2.9ev$, $3.1ev$, $4.1ev$, $5.1ev$, $5.2ev$ and $5.9ev$, respectively and these energies are in qualitative agreement with the observed peaks in photoabsorption measurements [9]. Both the valence-band top and the conduction-band bottom are located at the X point Fig.1.2.

The transition between the two is, however, optically forbidden since both the conduction and the valence bands have " ungerade " symmetry under the inversion operation. It is expected that rotation of the fullerenes affects the dispersion of the energy bands since the fullerene molecule is not perfectly spherical due to the presence of the internal bond network. With regard to the electrical transport properties,the C_{60} crystal is an insulator with a resistivity of $10^6\Omega$.cm or higher at room temperature. The lower resistivity is found in crystals kept away from oxygen gas with the activation energy in the range of $0.15 - 0.5ev$, much less than energy gap, indicating that C_{60} is not an intrinsic semiconductor. The resistivity is raised significantly in an ambient atmosphere due to carrier trapping caused by the absorption of O_2 [10].

1.2 Structure and Electronic Properties Of A_3C_{60}

In the fcc C_{60} lattice there are two tetrahedral and one octahedral interstitial sites per C_{60}. Tetrahedral and octahedral sites have sufficient room to accommodate spheres of radii $0.11nm$ and $0.21nm$ respectively. Since the ionic radii of Potassium and Rubidium are $0.13nm$ and $0.14nm$, respectively, the alkali atoms could be accommodated at the interstitial sites of fcc C_{60}.These sites are shown in figure 1.3. It is found that solid C_{60} weakly condensed via a van der Waals-like force is transformed upon alkali-atoms doping into a strongly bonded ionic metals, and a unified linear relation between T_c and the density of states (DOS) near the Fermi level (ε_F) in alkali-doped fullerides.

The lattice structure is fcc for A_3C_{60} and bct for A_4C_{60}.The difference in lattice structure favors A_3C_{60} to be metal and A_4C_{60} to be insulator.A unique advantage of the alkali-doped fullerides lies in the capability of varying systematically the lattice constant, which is an important parameter determining T_c , by changing the chemical species of the dopant atoms and/or applying pressure. In fact, T_c increases from $19.3K(K_3C_{60})$ to $29.4K(Rb_3C_{60})$ with increasing lattice constant a, and other data for alloy systems $A_{3-x}A'_xC_{60}$ corroborate this positive correlation between T_c and a [43]. The pressure dependent of T_c has also been measured for K_3C_{60} and Rb_3C_{60} , and a negative coefficient is observed for T_c [43].

For K_xC_{60}, significant electron transfer from the K atom to the C_{60} molecule takes place , i.e, electrons are transferred from the K $4s$ orbital to the C_{60} t_{1u} conduction band. The triply degenerate t_{1u} bands can accommodate up to six electrons. Thus, KC_{60} ,K_2C_{60} and K_3C_{60} possess unfilled bands and all are expected to be metallic and

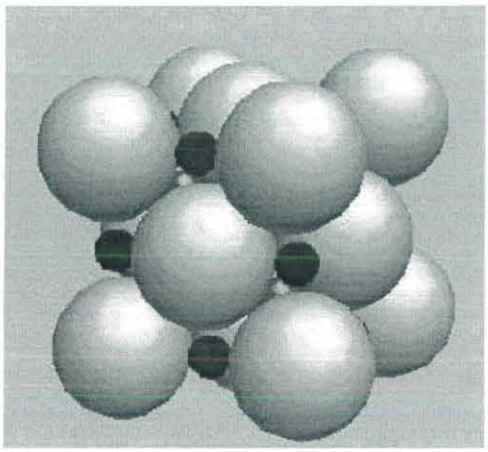


Figure 1.3: Structur of A_3C_{60}(A=K, Rb and Cs)

ionic, provided that a simple band model is applicable . The electrical conductivity increases with the dopant concentration and shows a maximum for K_3C_{60}. On the other hand , the molecular solid character leads to certain simplifications, for instance the electronic properties are expected to be dominated by the three-fold degenerate t_{1u} orbital.

1.3 Superconductivity in A_3C_{60}

Since the observation of superconductivity in K_3C_{60}, with $T_c = 19K$ [6] and Rb_3C_{60}, $T_c = 29K$ [11], superconductivity has been observed in dozens of other compounds of C_{60}. The transition temperature spans a range of up to $33K$. Further, in 1995 Plastra et al. found that Cs_3C_{60} was a pressure induced superconductor that exhibited at $14.3kbar$ the highest superconducting critical temperature $T_c = 40K$ among fullerene superconductors [12]. According to their observation, the T_c appeared by applying

pressure and increased with an increase in pressure. This increase in T_c is contrary to the model that a band broadening by applying pressure reduces the density of state on the Fermi level, $N(\varepsilon_F)$, and T_c as expected from the BCS theory.

The symmetry of the order parameter and the magnitude of the energy gap are the two most fundamental properties of superconductors. Since the original discovery in 1991 [5] great progress has been made in understanding superconductivity in A_3C_{60} compounds. There is a general agreement about the s-wave nature of the order parameter [13]. A very successful line of studies was carried out on the relationship between the superconducting transition temperature(T_c) and the lattice spacing by two different methods : pressure dependence and substitutional doping [14]. Modest pressure in the range of $10 - 20kbar$ can cause relatively large changes in the lattice parameters. According to the experiments these are accompanied by a significant variation of the transition temperature. On the other hand, using different alkali metals results in different lattice parameters. The combination of these two methods allowed for a continuous coverage of the lattice parameter range from 13.9 to $14.5A^0$ [15].The observed drop of the transition temperature at smaller lattice spacing is generally attributed to the increase of band width [14] which in turn leads to lower density of state at the Fermi level.

The superconducting energy gap is of great interest since a value of the reduced gap $\frac{2\triangle}{K_BT_c}$ which is substantially larger than the BCS value(3.53) indicates that strong coupling effects are important. A review of the literature reveals some disparity between the various measurements of the superconducting energy gap in K_3C_{60} and Rb_3C_{60}. An early measurement of $\triangle$ was performed using point contact tunneling in STM, giving $\frac{2\triangle}{K_BT_c} = 5.3$ for Rb_3C_{60} [16]. Later STM measurements on single crystals

have given reduced gaps $\frac{2\Delta}{K_B T_c} = 5.4$ [17] and $\frac{2\Delta}{K_B T_c} = 2.0 - 4.0$ [47]. From measurements using NMR the values 3.0 for K_3C_{60} and 4.1 for Rb_3C_{60} [18],4.3 [19] and 3.4 ± 0.2 [20] for K_3C_{60} were deduced. Recent NMR measurements were found to be in good agreement with the BCS value for the gap [21]. Using muon spin relaxation, Kiefl et al. [22] obtained the value 3.6 for Rb_3C_{60} . Recent optical measurements have given the values 3.44 for K_3C_{60} and 3.45 for Rb_3C_{60} [23, 24].Finally, the reduced gap was measured in photoemission, giving the value 4.1 for Rb_3C_{60} [25]. We note that the data obtained from different experiments show a substantial variation. Most recent results, however, tend to scatter around the weak coupling limit and are consistent with this limit, if a reasonable uncertainty is assumed for these experiments. These experimental results are summarized in table 1.

Material	Op[a]	NMR[b]	μSR[c]	TJ[d]	PE[e]
K_3C_{60}	3.44 [23]	3.0 [18]		5.3 [16]	
		4.3 [19]			
		3.4 ± 0.2 [20]			
Rb_3C_{60}	3.45 [24]	4.1 [18]	3.6 ± 0.3 [22]	5.2 ± 0.3	4.1 [25]
				5.4, $2.0 - 4.0$ [17, 47]	

Table 1. Energy gap measurements in A_3C_{60} compounds, reported in terms of the ratio $\frac{2\Delta}{K_B T_c}$

op^a: optical spectroscopy, TJ^d: tunnelling(STM)

NMR^b:nuclear magnetic resonance, PE^e:photoemission

μSR^c: muon spin rotation

The isotope effect may provide interesting information about the mechanism for superconductivity. In the BCS theory for a system with only one type of ions with

the mass M , the transition temperature behaves as $T_c \sim M^{-\alpha}$, where $\alpha = 0.5$. For the A_3C_{60} compounds , the C_{60} phonons are expected to be the important ones, and one is therefore interested in the isotope effect when ^{12}C is substituted by ^{13}C. For the case of complete $(99o/o)$ substitution , it was found that $\alpha = 0.30 \pm 0.06$ for K_3C_{60} [26] and $\alpha = 0.30 \pm 0.05$ for Rb_3C_{60} [48]. Interesting and contradictory results have been obtained for incomplete substitution.Chen and Lieber [48] found that for a single peak mass distribution of C_{60} molecules $(Rb_3(^{13}C^{12}_{0.55}C_{0.45})_{60})$, the value of α was consistent with the result for complete substitution. On the other hand, they found that a two peak mass distribution $(Rb_3(^{13}C_{60})_{0.5}(^{12}C_{60})_{0.5})$ gave a much larger value of $\alpha(\sim 0.8)$. A value of α which is larger than 0.5 is unusual, but it was also observed by three other groups. These values are $\alpha = 1.4 \pm 0.5$ for Rb_3C_{60} $33o/o$ substitution [27], $\alpha = (1.2-1.43) \pm 0.2$ for K_3C_{60} and $\alpha = (2-2.25) \pm 0.25$ for Rb_3C_{60} $60o/o$ substitution obtained [28] and $\alpha = 1.45 \pm 0.3$ for $82o/o$ substitutions [20]. However, these results were observed for distributions of C_{60} masses with essentially only one peak, while the $\alpha > 0.5$ was obtained for a two peak distribution [48].

Finally $\alpha = 0.37 \pm 0.05$ for mass distribution of $15o/o^{12}C_{60}$ and the rest $(^{13}C^{12}_{0.9}C_{0.1})_{60}$ was obtained [29]. For the partially substituted compounds , the experimental situation thus appears to be unclear. The results are summarized in table(2). The theoretical considerations have so far , however , been made for completely substituted systems , where $\alpha = 0.3$ should be the best available experimental result. The theoretical treatment of partially substituted compounds remains a challenging problem. The problem of isotope effect has been studied by Singh and Kishare , Pandey et al. and Singh et al. [38].

The isotope effect with respect to the alkali dopants have also been studied. It was found that within the experimental error there is no isotope effect [30, 31]. This is consistent with experimental results that applying pressure on Rb_3C_{60} so that the lattice parameter is reduced to that of K_3C_{60} leads to about the same T_c for both systems [32]. This strongly suggests that the alkali ions have a very weak influence on T_c except for the indirect influence via the lattice parameter.

Material	$^{13}C(o/o)$	α	Ref
Rb_3C_{60}	99	0.30 ± 0.05	48
Rb_3C_{60}	33	1.4 ± 0.5	27
Rb_3C_{60}	60	$(2 - 2.25) \pm 0.25$	28
Rb_3C_{60}	82	1.45 ± 0.3	20
$Rb_3(^{13}C^{12}_{0.55}C_{0.45})_{60}$	55	0.3	48
$Rb_3(^{13}C_{60})_{0.5}(^{12}C_{60})_{0.5}$	50	0.8	48
K_3C_{60}	99	0.30 ± 0.06	26
K_3C_{60}	60	$(1.2 - 1.43) \pm 0.2$	28

Table2.Carbon isotope effect in A_3C_{60} compounds.

1.4 Mechanism of superconductivity on A_3C_{60}

The high temperature superconductivity of alkali metal doped C_{60}, up to $40K$ in Cs_3C_{60} [12], has sparked much investigation into the mechanism of superconductivity and nature of the normal state. Proximity to a Mott-Hubbard transition [33] could call into question the role of standard electron-phonon mechanism. Theories of superconductivity in the fullerides have ranged from the conventional phonon-mediated electron pairing [34] to more unconventional electronic mechanisms [35].

There are proposals that explain the mechanism of superconductivity based on phonon-mediated electronic processes. The phonon mechanism can be further subdivided into models that rely upon intramolecular phonons [34, 36] and those which incorporate intermolecular translational modes [37] and librons [49] or alkali-C_{60} optical phonons [39]. The electronic processes are concerned with an appreciable on-site coulomb energy and the narrow band [40], and some what complicated Fermi surfaces with valley degeneracy [41].

With regard to the electronic process, electron correlation effects within single C_{60} molecules are considered to play a central role in electron pairing [40]. The attractive interaction has been evaluated on the basis of the Hubbard model for a single C_{60} molecule and the possibility of singlet superconductivity that depends on the effective intra-ball electron-electron repulsion and the inter-ball hopping amplitude. It was argued also that the isotope substitution effect in a superconductivity transition can be explained based on the phonon-mediated attraction with on-site coulomb repulsion [42].

Chapter 2

Mathematical Techniques

In the present investigation we have used a model Hamiltonian consisting of electrons , excitons and their interaction . Using Green function technique Zubarev [44] we obtain the expressions for superconducting transition temperature T_c and order parameter ($\triangle$).

2.1 Indirect Electron-Electron Interaction Via Phonons

The attractive interaction is caused by the electron-phonon interaction . The importance of this fact was first noticed by Frohlich [45]. Discovery of the isotope effect on T_c supported his assertion that the electron phonon interaction plays an essential role in superconductivity . This is because the dependence of T_c on the mass of the constituting atom signifies that the lattice modes must be involved in superconductivity.

The electron-phonon interaction of the deformation-potential type in superconductors [46] is given by the following Hamiltonian:

$\hat{H} = \hat{H}_0 + \hat{H}'$

$$\hat{H}_0 = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_q \hbar\omega_q b^\dagger_q b_q \tag{2.1}$$

$\hat{H}' = i \sum_{k,q,\sigma} \chi_q a^\dagger_{k+q\sigma} a_{k\sigma} (b_q - b^\dagger_{-q})$

where $\hat{H}_0$ is the Hamiltonian of electrons and phonons without mutual interaction, and $\hat{H}'$ represents the coupling interaction ; $a^\dagger_{k\sigma}(a_{k\sigma})$ is the creation(annihilation) operators of an electron specified by the wave vector k and the spin σ, and ϵ_k is the one-electron energy , and ε_F the Fermi energy at absolute zero ; $b^\dagger_q(b_q)$ are the creation(annihilation) operators of a phonon labelled by the wave vector q ; $\hbar\omega_q$ is the energy of the phonon ; and χ_q is the coupling constant of the electron-phonon interaction.

In first order , $\hat{H}'$ causes electron-phonon scattering. In second order it leads to the above mentioned exchange of a phonon between electrons . This process is illustrated in Figure 2.1 . This simply shows that one electron polarizes the lattice and the other electron interacts with the polarization . In order to get the expression of the attractive interaction , one performs the following canonical transformation which eliminates the first-order term in χ_q :

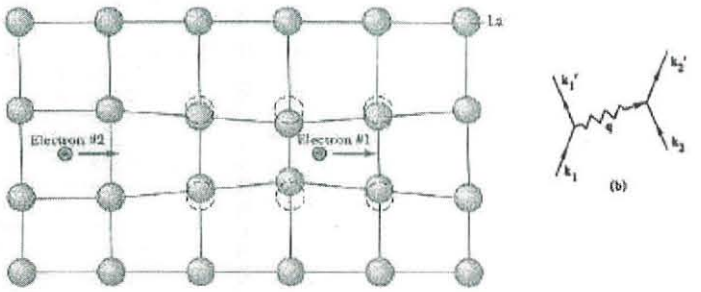
$$\tilde{H} = e^{-iu} \hat{H} e^{iu} \tag{2.2}$$

with

$$U = \sum_{k,q,\sigma} \chi_q a^\dagger_{k+q\sigma} a_{k\sigma} \left[\frac{b_q}{\epsilon_k - \epsilon_{k+q} + \hbar\omega_q} - \frac{b^\dagger_{-q}}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_q} \right] \tag{2.3}$$

Thus , U satisfies $i[\hat{H}_0, U] = -\hat{H}'$. Neglecting terms of the order of χ_q^3 , we obtain $\tilde{H} = \hat{H}_0 + \frac{i}{2}[\hat{H}', U]$

$$\tilde{H} = \hat{H}_0 + \sum_{k,k',q,\sigma,\sigma'} |\chi_q|^2 a^\dagger_{k+q\sigma} a_{k\sigma} a^\dagger_{k'-q\sigma} a_{k'\sigma'} \frac{\hbar\omega_q}{(\epsilon_{k'} - \epsilon_{k'-q})^2 - (\hbar\omega_q)^2} \tag{2.4}$$



(a)

Figure 2.1: (a)A schematic diagram of an electron polarizing positive ions in its vicinity to create an attractive potential for a second electron following the first electron.(b)A schematic diagram of an electron-electron interaction transmitted by a phonon of wave vector $\vec{q}$, such that $\vec{k_1} + \vec{k_2} = \vec{k_1'} + \vec{k_2'}$.

So that the electron-electron interaction may be written as

$\hat{H}' = \sum_{k,k',q,\sigma,\sigma'} |\chi_q|^2 a^\dagger_{k+q\sigma} a_{k\sigma} a^\dagger_{k'-q\sigma} a_{k'\sigma'} \frac{\hbar\omega_q}{(\epsilon_{k'}-\epsilon_{k'-q})^2-(\hbar\omega_q)^2}$

Just such an attractive interaction is present in $\tilde{H}$ whenever $|\epsilon_{k'} - \epsilon_{k'-q}| < \hbar\omega_q$. This may allow pairs of electrons to form a bound state of lower energy than that of the two free electrons.The existence of Cooper pairs in which two electrons of opposite wave number and spin form a bound state, provides the foundation for the BCS theory.

2.2 Green's Function Formalism

The mathematical technique we used is the Green function technique Zubarev [44].In quantum field theory the Green functions are the so called propagators.This name is based on the idea that, in order to fined the important physical properties of a system, it is essential to know, not the detailed behavior of each particle in the system, but rather just the average behavior of one or two typical particles. Green functions or propagators play the most important part in the quantum field-theoretic treatment of the many-body problem. There are different types of Green functions : advanced, retarded, causal, zero-temperature, finite-temperature, real-time,imaginary-time, and so on. In our discussion we Confine ourselves to only retarded Double-time Green function.

$G_r(t,t') = \ll A(t), B(t') \gg_r$

$$G_r(t,t') = -i\theta(t-t') < [A(t), B(t')] > \tag{2.5}$$

Where $\ll A(t), B(t') \gg$ are short notation for the corresponding Green function and $< \ldots\ldots >$ indicates for average over a grand canonical ensemble ,that is, for any operator . $\theta(t-t')$ is heaviside step function and $A(t)$,$B(t')$ are the Heisenberg representation of operators A and B expressed in terms of product of quantized field functions.

$$A(t) = \exp(iHt)A(0)\exp(-iHt), \hbar = 1 \tag{2.6}$$

$$\theta(t,t') = \begin{cases} 1 & for \quad t>t' \\ 0 & for \quad t<t' \end{cases} \tag{2.7}$$

$[A(t), B(t')]$ indicates the commutator or anticommutator.

$$[A(t), B(t')] = A(t)B(t') - \eta B(t')A(t) \tag{2.8}$$

$$\eta = \begin{cases} +1 \quad for \quad Bosons \\ \\ -1 \quad for \quad Fermions \end{cases}$$

In order to obtain equation of motion for Green function differentiating eq.(2.5) with respect to t we get

$i\frac{dG_r(t,t')}{dt} = i\frac{d}{dt} \ll A(t), B(t') \gg_r$

$$i\frac{dG_r(t,t')}{dt} = \frac{d}{dt}\theta(t-t') < [A(t), B(t')] > + \ll i\frac{d}{dt}A(t), B(t') \gg \tag{2.9}$$

Taking use of between Heaviside step function $\theta(t)$ and Dirac δ-function

$\theta(t) = \int_{-\infty}^{t} \delta(t)dt$, therefore $\frac{d\theta(t)}{dt} = \delta(t)$

It is known that A(t) and B(t) satisfy equation of the form $i\frac{dA}{dt} = [A, H]$

now equation of motion becomes:

$$i\frac{dG_r(t-t')}{dt} = \delta(t-t') < [A(t), B(t')] > + \ll A(t)H - HA, B(t') \gg \tag{2.10}$$

To solve eq.(2.10) it is convenient to work with Fourier transform of this equation. A careful analysis shows that the function depends on t and t' through $(t-t')$. Thus we can write $G_r(t,t') = G_r(t-t')$

Now let $G_r(\omega)$ be the fourier transform of $G_r(t-t')$ such that

$$G_r(t-t') = \int_{-\infty}^{\infty} G_r(\omega)e^{-i\omega(t-t')}d\omega \tag{2.11}$$

$$G_r(\omega) = \frac{1}{2\Pi}\int_{-\infty}^{\infty} e^{i\omega(t-t')}G_r(t-t')d(t-t') \tag{2.12}$$

and from the analytical property of $G_r(\omega)$ we have

$$< B(t')A(t) >= -\frac{1}{\Pi}\int_{-\infty}^{\infty} \frac{ImG_r(\omega+i\epsilon)}{e^{\beta\omega}+1}dt \tag{2.13}$$

Using the delta function

$\delta(t-t') = \frac{1}{2\Pi}\int_{-\infty}^{\infty} e^{-i\omega(t-t')}d\omega$

Eq.(2.12) can be transformed to the following form

$$\omega G(\omega) =< [A(t), B(t^{'})] >_{\omega} + \ll [A(t), H], B(t^{'}) \gg_{\omega} \tag{2.14}$$

Eq.(2.14) follows since the Fourier transform of G(t) is

$G(t) = \int G(\omega) \exp(-i\omega t) d\omega$

from which it can be shown that

$\frac{\partial G}{\partial t} = -i\omega \times$Fourier transform of G(t)

For future use we write eq.(2.14) in the form :

$$\omega \ll A, B \gg_{\omega} =< [A, B] > + \ll [A, H], B \gg_{\omega} \tag{2.15}$$

Since $\ll A, B \gg$ denotes the Fourier transform of the Green function involving the operators A and B , it satisfies the equation of motion(2.15), where the double brackets $\ll ... \gg$ indicate the Fourier transforms of the corresponding Green function. The single brackets $< ... >$ indicate the thermal average over a canonical ensemble, that is,

$< F >= \frac{Tre^{-\beta H} F}{Tre^{-\beta H}}$

where $\beta = \frac{1}{K_B T}$, and H is the Hamiltonian of the system considered. The correlation function $< B(t^{'}) A(t) >$ is related to the Green function by

$$< B(t^{'}) A(t) >= ilim_{\varepsilon \longrightarrow 0} \int_{-\infty}^{\infty} \frac{[\ll A, B \gg_{\omega + i\varepsilon} - \ll A, B \gg_{\omega - i\varepsilon}] e^{i\omega(t - t^{'})}}{e^{\beta\omega} - \eta} d\omega \tag{2.16}$$

where $\beta = (K_B T)^{-1}$ and K_B is the Boltzman constant. In order to obtain the supre-rconducting properties we have defined the following correlations in our formalism.

$\triangle = \sum_k V < a^{\dagger}_{-k\downarrow} a^{\dagger}_{k\uparrow} >= \sum_k V < a_{-k\downarrow} a_{k\uparrow} >$

where $\triangle$ is the superconducting order parameter, this can also be found by relation.

$$\triangle = \frac{V}{\beta} \sum_{k,n} << a^{\dagger}_{-k\downarrow} a^{\dagger}_{k\uparrow} >> \tag{2.17}$$

The value of transition temperature T_c is calculated by using the condition that, $\triangle \longrightarrow 0$, $T \longrightarrow T_C$ For a BCS case we have

$$G^{\uparrow\uparrow}_{kk} = [\frac{\omega + \epsilon_k}{\omega^2 - \epsilon_k^2 - \triangle^2}] \tag{2.18}$$

and

$$G^{\downarrow\uparrow}_{-kk} = -[\frac{\triangle}{\omega^2 - \epsilon_k^2 - \triangle^2}] \tag{2.19}$$

The Green function $<< a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >>$ is given by
$<< a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >>= \frac{\triangle \tanh(\frac{\beta}{2}\sqrt{(\epsilon_k^2+\triangle^2)})}{\sqrt{(\epsilon_k^2+\triangle^2)}}$
substituting this in eq.(2.17)and converting summation over k into an integral with cut off energy $\pm\hbar\omega_D$from the Fermi level

$$\triangle = N(0)V \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{\triangle \tanh(\frac{\beta}{2}\sqrt{(\epsilon_k^2 + \triangle^2)})}{2\sqrt{(\epsilon_k^2 + \triangle^2)}} d\epsilon_k \tag{2.20}$$

or

$$\frac{1}{N(0)V} = \int_0^{\hbar\omega_D} \frac{\tanh(\frac{\beta}{2}\sqrt{(\epsilon_k^2 + \triangle^2)})}{\sqrt{(\epsilon_k^2 + \triangle^2)}} d\epsilon_k \tag{2.21}$$

as $T \longrightarrow T_c$, $\triangle \longrightarrow 0$, then eq.(2.21) becomes

$\frac{1}{N(0)V} = \int_0^{\hbar\omega_D} \frac{\tanh(\frac{\epsilon_k}{2K_B T_c})}{\epsilon_k} d\epsilon_k$
Integrating

$$T_c = 1.14\theta_D \exp(-\frac{1}{N(0)V}) \tag{2.22}$$

which is the well known BCS expression.

Chapter 3

Formulation Of The Problem

In this chapter we try to obtain an expression for T_c and $\triangle$ from exclusively excitonic coupling and also we calculate the value of T_c, reduced gap $\frac{2\triangle}{k_B T_c}$ and α for $A_3C_{60}(A = K, Rb, andCs)$ from phonon-exciton combined mechanism.

3.1 Exciton Mechanism

Consider the following Hamiltonian

$$\hat{H} = \hat{H}_o + \hat{H}' \tag{3.1}$$

where the first term is the Hamiltonian of the total energy of noninteracting electrons and excitons , and the second term is the Hamiltonian of electron-exciton interaction.

$$\hat{H}_o = \sum_{k,\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{k,q} \hbar\omega_{ex} b^\dagger_q b_q \tag{3.2}$$

$$\hat{H}' = i \sum_{k,k',q,\sigma,\sigma'} X_q (a^\dagger_{k\sigma} a_{k'\sigma'} b_q + h.c) \tag{3.3}$$

where $a^\dagger_{k\sigma}(a_{k\sigma})$ is the creation(annihilation) operators of an electron specified by the wave vector k and the spin σ, and ϵ_k is the one-electron energy measured relative

to the chemical potential , $b_q^\dagger(b_q)$ are the creation(annihilation) operators of exciton labelled by the wave vector q ; $\hbar\omega_{ex}$ is the energy of the exciton ; and χ_q is the coupling constant of the electron-exciton interaction. Here $\hat{H}'$ does not immediately show us that there is an indirect electron-electron interaction through excitons. To make this interaction apparent and to get pairing interaction we make a canonical transformation .

The system Hamiltoniam can be canonically transformed to :

$$\tilde{H_{int}} = e^{-iU}\hat{H}e^{iU} \tag{3.4}$$

Expanding using power series and rearranging the above hamiltonian becomes

$$\tilde{H_{int}} = \hat{H}_o + \frac{i}{2}[\hat{H}', U] + ... \tag{3.5}$$

We choose U in such a way that its commutator with $\hat{H}_0$ cancels the term $\hat{H}'$,that means

$i[\hat{H}_o, U] = -\hat{H}'$

Let $U = i\sum_{k,k',\sigma,\sigma',q} X_q(Aa^\dagger_{k\sigma}a_{k'\sigma'}b_q - Ba^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q)$

where A and B are constants to be calculated.

$[\hat{H}_o, U] = \sum_{k,\sigma}\epsilon_k[a^\dagger_{k\sigma}a_{k\sigma}, U] + \sum_q \hbar\omega_{ex}[b^\dagger_q b_q, U]$

The first term becomes:

$$\begin{aligned}\sum_k \epsilon_k[a^\dagger_{k\sigma}a_{k\sigma}, U] &= i\sum_{k,p,k',\sigma,\sigma',\sigma'',q}\epsilon_k X_q A[a^\dagger_{k\sigma}a_{k\sigma}, a^\dagger_{p\sigma'}a_{k'\sigma''}b_q] - \\ &\quad i\sum_{k,p,k',\sigma,\sigma',\sigma'',q}\epsilon_k X_q B[a^\dagger_{k\sigma}a_{k\sigma}, a^\dagger_{k'\sigma'}a_{p\sigma'}b^\dagger_q] \\ &= i\sum_{k,p,k',\sigma,\sigma',\sigma'',q}\epsilon_k X_q A[a^\dagger_{k\sigma}a_{k\sigma}, a^\dagger_{p\sigma'}a_{k'\sigma''}]b_q - \\ &\quad i\sum_{k,p,k',\sigma,\sigma',\sigma'',q}\epsilon_k X_q B[a^\dagger_{k\sigma}a_{k\sigma}, a^\dagger_{k'\sigma''}a_{p\sigma'}]b^\dagger_q\end{aligned}$$

$$= i\sum_{k,p,k',\sigma,\sigma',\sigma'',q} \epsilon_k X_q A\{[a^\dagger_{k\sigma}a_{k\sigma}, a^\dagger_{p\sigma'}]a_{k'\sigma''}b_q + a^\dagger_{p\sigma'}[a^\dagger_{k\sigma}a_{k\sigma}, a_{k'\sigma''}]b_q\} -$$

$$i\sum_{k,p,k',\sigma,\sigma',\sigma'',q} \epsilon_k X_q B\{[a^\dagger_{k\sigma}a_{k\sigma}, a^\dagger_{k'\sigma''}]a_{p\sigma'}b^\dagger_q + a^\dagger_{k'\sigma''}[a^\dagger_{k\sigma}a_{k\sigma}, a_{p\sigma'}]b^\dagger_q\}$$

$$= i\sum_{k,p,k',\sigma,\sigma',\sigma'',q} \epsilon_k X_q A[a^\dagger_{k\sigma}\{a_{k\sigma}, a^\dagger_{p\sigma'}\}a_{k'\sigma''}b_q - a^\dagger_{p\sigma'}\{a^\dagger_{k\sigma}, a_{k'\sigma''}\}a_{k\sigma}b_q] -$$

$$i\sum_{k,p,k',\sigma,\sigma',\sigma'',q} \epsilon_k X_q B[a^\dagger_{k\sigma}\{a_{k\sigma}, a^\dagger_{k'\sigma''}\}a_{p\sigma'}b^\dagger_q - a^\dagger_{k'\sigma''}\{a^\dagger_{k\sigma}, a_{p\sigma'}\}a_{k\sigma}b^\dagger_q]$$

$$= i\sum_{k,p,k',\sigma,\sigma',\sigma'',q} \epsilon_k X_q A\{a^\dagger_{k\sigma}\delta_{kp}\delta_{\sigma\sigma'}a_{k'\sigma''}b_q - a^\dagger_{p\sigma'}\delta_{kk'}\delta_{\sigma\sigma''}a_{k\sigma}b_q\} -$$

$$i\sum_{k,k',p,\sigma,\sigma',\sigma'',q} \epsilon_k X_q B\{a^\dagger_{k\sigma}\delta_{kk'}\delta_{\sigma\sigma''}a_{p\sigma'}b^\dagger_q - a^\dagger_{k'\sigma''}\delta_{kp}\delta_{\sigma\sigma'}a_{k\sigma}b^\dagger_q\}$$

$$= i\sum_{p,\sigma',\sigma'',q} X_q A(\epsilon_p - \epsilon_{k'})a^\dagger_{p\sigma'}a_{k'\sigma''}b_q + i\sum_{k',\sigma',\sigma'',q} X_q B(\epsilon_p - \epsilon_{k'})a^\dagger_{k'\sigma''}a_{p\sigma'}b^\dagger_q$$

The second term becomes:

$$\sum_q \hbar\omega_{ex}[b^\dagger_q b_q, U] = i\sum_{k,k',q,q'} \hbar\omega_{ex}X_q A[b^\dagger_q b_q, a^\dagger_{k\sigma}a_{k'\sigma'}b_{q'}] - i\sum_{k,k',q,q'} \hbar\omega_{ex}X_q B[b^\dagger_q b_q, a^\dagger_{k'\sigma'}a_{k\sigma}b_{q'}]$$

$$= -i\sum_{k,k',\sigma,\sigma',q,q'} \hbar\omega_{ex}X_q A a^\dagger_{k\sigma}a_{k'\sigma'}\{b^\dagger_q b_q, b_{q'}\} + i\sum_{k,k',\sigma,\sigma',q,q'} \hbar\omega_{ex}X_q B a^\dagger_{k'\sigma'}a_{k\sigma}\{b^\dagger_q b_q, b^\dagger_{q'}\}$$

$$= i\sum_{k,k',\sigma,\sigma',q,q'} \hbar\omega_{ex}X_q A a^\dagger_{k\sigma}a_{k'\sigma'}[b^\dagger_q, b_{q'}]b_q + i\sum_{k,k',\sigma,\sigma',q,q'} \hbar\omega_{ex}X_q B a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q[b_q, b^\dagger_{q'}]$$

for $q = q'$

$$= -i\sum_{k,k',\sigma,\sigma',q} \hbar\omega_{ex}X_q A a^\dagger_{k\sigma}a_{k'\sigma'}b_q + i\sum_{k,k',\sigma,\sigma',q} \hbar\omega_{ex}X_q B a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q$$

Since $i[H_o, U] = -\hat{H}'$, the commutation $[H_o, U]$ becomes:

$[H_o, U] = i\sum_{k,k',\sigma,\sigma',q} X_q A(\epsilon_k - \epsilon_{k'} - \hbar\omega_{ex})a^\dagger_{k\sigma}a_{k'\sigma'}b_q + i\sum_{k,k',\sigma,\sigma',q} X_q B(\epsilon_k - \epsilon_{k'} + \hbar\omega_{ex})a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q$

From this A and B will be,

$A = i(\epsilon_k - \epsilon_{k'} + \hbar\omega_{ex})^{-1}$and , $B = i(\epsilon_k - \epsilon_{k'} - \hbar\omega_{ex})^{-1}$

Now substituting the values of A and B in U, U can be written as

$U = \sum_{k,k',\sigma,\sigma',q} X_q\{\frac{a^\dagger_{k\sigma}a_{k'\sigma'}b_q}{(\epsilon_k - \epsilon_{k'} - \hbar\omega_{ex})} - \frac{a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q}{(\epsilon_k - \epsilon_{k'} + \hbar\omega_{ex})}\}$

To simplify eq.(3.5),let us evaluate the commutation $[\hat{H}', U]$:

$$[\hat{H}', U] = i\sum_{k,k',\sigma,\sigma',q} |X_q|^2 \{ \frac{[a^\dagger_{k\sigma}a_{k'\sigma'}b_q, a^\dagger_{k\sigma}a_{k'\sigma'}b^\dagger_{q'}]}{(\epsilon_k - \epsilon_{k'} - \hbar\omega_{ex})} - \frac{[a^\dagger_{k\sigma}a_{k'\sigma'}b_q, a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_{q'}]}{(\epsilon_k - \epsilon_{k'} + \hbar\omega_{ex})} -$$

$$\frac{[a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q, a^\dagger_{k\sigma}a_{k'\sigma'}b_{q'}]}{(\epsilon_k - \epsilon_{k'} - \hbar\omega_{ex})} + \frac{[a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q, a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_{q'}]}{(\epsilon_k - \epsilon_{k'} + \hbar\omega_{ex})} \} \tag{3.6}$$

Of the many terms in the commutator, we examine particularly the set that arises from commuting the boson operators(excitons). As a result the first and last terms become zero.

The second term will be :

$$\begin{aligned}
[a^\dagger_{k\sigma}a_{k'\sigma'}b_q, a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_{q'}] &= -a^\dagger_{k'\sigma'}a_{k\sigma}\{a^\dagger_{k\sigma}a_{k'\sigma'}b_q, b^\dagger_{q'}\} \\
&= -a^\dagger_{k'\sigma'}a_{k\sigma}a^\dagger_{k\sigma}a_{k'\sigma'}[b_q, b^\dagger_{q'}] \\
&= -a^\dagger_{k'\sigma'}a_{k\sigma}a^\dagger_{k\sigma}a_{k'\sigma'}\delta_{qq'} \\
&= -a^\dagger_{k\sigma}a_{k'\sigma'}a^\dagger_{k'\sigma'}a_{k\sigma}
\end{aligned}$$

The third term:

$$\begin{aligned}
[a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q, a^\dagger_{k\sigma}a_{k'\sigma'}b_{q'}] &= -a^\dagger_{k\sigma}a_{k'\sigma'}\{a^\dagger_{k'\sigma'}a_{k\sigma}b^\dagger_q, b_{q'}\} \\
&= a^\dagger_{k\sigma}a_{k'\sigma'}a^\dagger_{k'\sigma'}a_{k\sigma}[b_{q'}, b^\dagger_q] = a^\dagger_{k\sigma}a_{k'\sigma'}a^\dagger_{k'\sigma'}a_{k\sigma}\delta_{qq'} \\
\text{as q}\rightarrow q' \quad &= a^\dagger_{k\sigma}a_{k'\sigma'}a^\dagger_{k'\sigma'}a_{k\sigma}
\end{aligned}$$

Substituting the above commutation results in eq.(3.6), we get :

$$[\hat{H}', U] = i\sum_{k,k',\sigma,\sigma'} |X_q|^2 \{ \frac{a^\dagger_{k\sigma}a_{k'\sigma'}a^\dagger_{k'\sigma'}a_{k\sigma}}{(\epsilon_k - \epsilon_{k'} + \hbar\omega_{ex})} - \frac{a^\dagger_{k'\sigma'}a_{k\sigma}a^\dagger_{k\sigma}a_{k'\sigma'}}{(\epsilon_k - \epsilon_{k'} - \hbar\omega_{ex})} \}$$

$$= -2i\sum_{k,k',\sigma',\sigma} \frac{|X_q|^2\hbar\omega_{ex}}{(\epsilon_k - \epsilon_{k'})^2 - (\hbar\omega_{ex})^2} a^\dagger_{k\sigma}a_{k'\sigma'}a^\dagger_{k'\sigma'}a_{k\sigma}$$

Putting this result in eq.(3.5), the transformed Hamiltonian becomes:

$$\tilde{H}_{int} = \hat{H}_o + \sum_{k,k',\sigma,\sigma'} \frac{|X_q|^2\hbar\omega_{ex}}{(\epsilon_k - \epsilon_{k'})^2 - (\hbar\omega_{ex})^2} a^\dagger_{k\sigma}a^\dagger_{k'\sigma'}a_{k\sigma}a_{k'\sigma'} \tag{3.7}$$

where

$\hat{H}_o = \sum_{k,\sigma} \epsilon_k a^\dagger_{k\sigma}a_{k\sigma} + \sum_q \hbar\omega_{ex} b^\dagger_q b_q$

To get attraction interaction

$|\epsilon_k - \epsilon_{k'}| \ll \hbar\omega_{ex}$ as a result $\tilde{H}_{int}$ is reduced to :

$\tilde{H}_{int} = \hat{H}_o - \sum_{k,k',\sigma,\sigma'} \frac{|X_q|^2}{\hbar\omega_{ex}} a^\dagger_{k\sigma} a^\dagger_{k'\sigma'} a_{k\sigma} a_{k'\sigma'}$

$\tilde{H}_{int} = \hat{H}_o + \hat{H}''$

where

$\hat{H}'' = -\sum_{k,k',\sigma,\sigma'} \frac{|X_q|^2}{\hbar\omega_{ex}} a^\dagger_{k\sigma} a^\dagger_{k'\sigma'} a_{k\sigma} a_{k'\sigma'}$

Since in A_3C_{60} superconductors, it is found that the paring mechanism is s-wave and BCS type, we reduce the summation over σ and σ' in $\hat{H}''$ into :

$\hat{H}'' = -\sum_{k,k',q} \frac{|X_q|^2}{\hbar\omega_{ex}} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}$

Now we need to find equation of motion for $\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg$

$$\omega \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg = \ll [a^\dagger_{-k\downarrow}, \tilde{H}_{int}], a^\dagger_{k'\uparrow} \gg_\omega \tag{3.8}$$

To solve eq.(3.8) let us evaluate the commutation $[a^\dagger_{-k\downarrow}, \tilde{H}_{int}]$,

$[a^\dagger_{-k\downarrow}, \tilde{H}_{int}] = [a^\dagger_{-k\downarrow}, \hat{H}_o] + [a^\dagger_{-k\downarrow}, \hat{H}'']$

$[a^\dagger_{-k\downarrow}, \hat{H}_o] = \sum_{k,p,\sigma} \epsilon_p [a^\dagger_{-k\downarrow}, a^\dagger_{p\sigma} a_{p\sigma}] + \sum_{k,q} \hbar\omega_{ex} [a^\dagger_{-k\downarrow}, b^\dagger_q b_q]$

$= -\sum_{k,p,\sigma} \epsilon_p \{a^\dagger_{-k\downarrow}, a_{p\sigma}\} a^\dagger_{p\sigma} + 0$

$= -\sum_{k,p,\sigma} \epsilon_p a^\dagger_{p\sigma} \delta_{-kp} \delta_{\downarrow\sigma}$

$= -\epsilon_{-k} a^\dagger_{-k\downarrow}$

$[a^\dagger_{-k\downarrow}, \hat{H}''] = -\sum_{k,k',p} \frac{|X_q|^2}{\hbar\omega_{ex}} [a^\dagger_{-k\downarrow}, a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{k'\downarrow} a_{-k'\uparrow}]$

$[a^\dagger_{-k\downarrow}, a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{k'\downarrow} a_{-k'\uparrow}] = [a^\dagger_{-k\downarrow}, a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow}] a_{k'\downarrow} a_{-k'\uparrow} + a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} [a^\dagger_{-k\downarrow}, a_{k'\downarrow} a_{-k'\uparrow}]$

$= a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} [a^\dagger_{-k\downarrow}, a_{k'\downarrow} a_{-k'\uparrow}]$

$= a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} \{a^\dagger_{-k\downarrow}, a_{k'\downarrow}\} a_{-k'\uparrow} - a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{k'\downarrow} \{a^\dagger_{-k\downarrow}, a_{-k'\uparrow}\}$

$= a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} \delta_{-kk'} \delta_{\downarrow\downarrow} a_{-k'\uparrow}$

$[a^\dagger_{-k\downarrow}, \hat{H}''] = -\sum_{k,k',p} \frac{|X_q|^2}{\hbar\omega_{ex}} a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} \delta_{-kk'} \delta_{\downarrow\downarrow} a_{-k'\uparrow}$

$[a^\dagger_{-k\downarrow}, \hat{H}''] = -\sum_{p} \frac{|X_q|^2}{\hbar\omega_{ex}} a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{k\uparrow}$

Substituting the results of the commutation in eq.(3.8) and using Wick's decoupling theorem $\ll a^{\dagger}_{-p\downarrow}a^{\dagger}_{p\uparrow}a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg = < a^{\dagger}_{-p\downarrow}a^{\dagger}_{p\uparrow} > \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg$

eq.(3.8) can be written as,

$\omega \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow} \gg = -\epsilon_{-k} \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow} \gg - \sum_p \frac{|X_q|^2}{\hbar\omega_{ex}} < a^{\dagger}_{-p\downarrow}a^{\dagger}_{p\uparrow} > \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg$

$$(\omega + \epsilon_{-k}) \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow} \gg = -\sum_p \frac{|X_q|^2}{\hbar\omega_{ex}} < a^{\dagger}_{-p\downarrow}a^{\dagger}_{p\uparrow} > \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg \tag{3.9}$$

Similarly to find equation of motion of $\ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg$,

$$\omega \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg = \delta_{kk'} + \ll [a_{k\uparrow}, \tilde{H}_{int}], a^{\dagger}_{k'\uparrow} \gg \tag{3.10}$$

$[a_{k\uparrow}, \tilde{H}_{int}] = [a_{k\uparrow}, \hat{H}_o] + [a_{k\uparrow}, \hat{H}'']$

$[a_{k\uparrow}, \hat{H}_o] = \sum_{p,k} \epsilon_p [a_{k\uparrow}, a^{\dagger}_{p\sigma}a_{p\sigma}] + \sum_{k,q} [a_{k\uparrow}, b^{\dagger}_q b_q]$

$= \sum_{p,k} \epsilon_p [a_{k\uparrow}, a^{\dagger}_{p\sigma}] a_{p\sigma}$

$= \sum_{p,k} \epsilon_p \delta_{kp}\delta_{\uparrow\sigma} a_{p\sigma}$

$= \epsilon_k a_{k\uparrow}$

$[a^{\dagger}_{-k\downarrow}, \hat{H}''] = -\sum_{k,k',p} \frac{|X_q|^2}{\hbar\omega_{ex}} [a_{k\uparrow}, a^{\dagger}_{p\uparrow}a^{\dagger}_{-p\downarrow}a_{k'\downarrow}a_{-k'\uparrow}]$

$[a_{k\uparrow}, a^{\dagger}_{p\uparrow}a^{\dagger}_{-p\downarrow}a_{k'\downarrow}a_{-k'\uparrow}] = [a_{k\uparrow}, a^{\dagger}_{p\uparrow}a^{\dagger}_{-p\downarrow}]a_{k'\downarrow}a_{-k'\uparrow} + a^{\dagger}_{p\uparrow}a^{\dagger}_{-p\downarrow}[a_{k\uparrow}, a_{k'\downarrow}a_{-k'\uparrow}]$

$= [a_{k\uparrow}, a^{\dagger}_{p\uparrow}a^{\dagger}_{-p\downarrow}]a_{k'\downarrow}a_{-k'\uparrow}$

$= \{a_{k\uparrow}, a^{\dagger}_{p\uparrow}\}a^{\dagger}_{-p\downarrow}a_{k'\downarrow}a_{-k'\uparrow} - a^{\dagger}_{p\uparrow}\{a_{k\uparrow}, a^{\dagger}_{-p\downarrow}\}a_{k'\downarrow}a_{-k'\uparrow}$

$= \delta_{kp}\delta_{\uparrow\uparrow}a^{\dagger}_{-p\downarrow}a_{k'\downarrow}a_{-k'\uparrow}$

$[a_{k\uparrow}, \hat{H}''] = -\sum_{k,k',p,q} \frac{|X_q|^2}{\hbar\omega_{ex}} \{\delta_{kp}\delta_{\uparrow\uparrow}a^{\dagger}_{-p\downarrow}a_{k'\downarrow}a_{-k'\uparrow}\}$

$[a_{k\uparrow}, \hat{H}''] = -\sum_{k',q} \frac{|X_q|^2}{\hbar\omega_{ex}} a^{\dagger}_{-k\downarrow}a_{k'\downarrow}a_{-k'\uparrow}$

Substituting the above commutation results in eq.(3.10) and using the Wick's decoupling theorem $\ll a^{\dagger}_{-k\downarrow}a_{k'\downarrow}a_{-k'\uparrow}, a^{\dagger}_{k'\uparrow} \gg = < a_{k'\downarrow}a_{-k'\uparrow} > \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow} \gg$ we get,

$\omega \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg = \delta_{kk'} + \epsilon_k \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg - \sum_{k'} \frac{|X_q|^2}{\hbar\omega_{ex}} < a_{k'\downarrow} a_{-k'\uparrow} > \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow} \gg$

$(\omega - \epsilon_k) \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg = \delta_{kk'} - \sum_{k'} \frac{|X_q|^2}{\hbar\omega_{ex}} < a_{k'\downarrow} a_{-k'\uparrow} > \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow} \gg$

For $k = k^{'}$

$(\omega - \epsilon_k) \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = 1 - \sum_{k} \frac{|X_q|^2}{\hbar\omega_{ex}} < a_{-k\downarrow} a_{k\uparrow} > \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg$

$$\ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = \frac{1}{\omega - \epsilon_k} \{1 - \sum_{k} \frac{|X_q|^2}{\hbar\omega_{ex}} < a_{-k\downarrow} a_{k\uparrow} > \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg \} \tag{3.11}$$

Let $\triangle = \sum_{k} \frac{|X_q|^2}{\hbar\omega_{ex}} < a_{-k\downarrow} a_{k\uparrow} >$,$\triangle^* = \sum_{p} \frac{|X_q|^2}{\hbar\omega_{ex}} < a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow} >$

For $\triangle = \triangle^*$, eq.(3.9) and (3.11) can be rewritten as,

$$\ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = \frac{1}{\omega - \epsilon_k} \{1 - \triangle \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg\} \tag{3.12}$$

For $\epsilon_k = \epsilon_{-k}$

$$(\omega + \epsilon_k) \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg = -\triangle \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg \tag{3.13}$$

Substituting eq.(3.12) in (3.13) we have the following expression,

$(\omega^2 - \epsilon_k^2) \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg = -\triangle \{1 - \triangle \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg\}$

$-\triangle = (\omega^2 - \epsilon_k^2 - \triangle^2) \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg$

$$\ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg = -\frac{\triangle}{(\omega^2 - \epsilon^2 - \triangle^2)} \tag{3.14}$$

The superconductivity gap parameter($\triangle$) can be defined as :

$\triangle = \frac{V}{\beta} \sum_{n,k} \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg$

Here, we see that the summation with respect to k and n extends overall allowed pair-states. As temperature is raised from zero , quasi-electrons are excited making the physical vacuum less perfect. The degree of perfection may be represented by the probability $\tanh(\frac{\beta E_k}{2})$.

In the low-temperature limit,this quantity approaches unity from below

$1 - 2\{(\exp(\beta E_k) + 1)^{-1}\} = \tanh(\frac{\beta E_k}{2}), (> 0)$

$\tanh(\frac{\beta E_k}{2}) \equiv \tanh(\frac{E_k}{2k_B T}) \longrightarrow 1$

We may therefore consider $\tanh(\frac{\beta E_k}{2})$ as the probability that the pair state$(k\uparrow, -k\downarrow)$ is available for the supercondensate formation at temperature T. As temperature is raised ,this probability becomes smaller. Thus, we may modify eq.(3.14)as follows

$\ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg = \frac{-\triangle}{(\omega^2 - \epsilon^2 - \triangle^2)}$

changing $\omega \longrightarrow i\omega_n$ and $E = \sqrt{(\epsilon^2 + \triangle^2)}$, we get

$\ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg = \frac{\triangle}{(\omega_n^2 + E^2)}$

From Matsubara's frequency, we have $\omega_n = (2n+1)\Pi\beta^{-1}$

$\ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg = \beta^2\big(\frac{\triangle}{(2n+1)^2\Pi^2 + E^2\beta^2}\big)$

but

$$\triangle = \frac{V}{\beta}\sum_{n,k} \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg \tag{3.15}$$

$\triangle = \triangle \sum_{k,n} V\beta\big(\frac{1}{(2n+1)^2\Pi^2 + E^2\beta^2}\big)$

For calculational convenience,the above equation can be rewritten using the following formula

$\frac{1}{2x}\tanh(\frac{x}{2}) = \sum_{n=-\infty}^{\infty} \frac{1}{(2n+1)^2\Pi^2 + x^2}$

$$\triangle = \sum_k V\frac{\triangle}{2E_k}\tanh(\frac{\beta E_k}{2}) \tag{3.16}$$

Eq.(3.16) is called the generalized energy gap equation at finite temperature. In the

bulk limit ,the sum over k can be converted into energy integral.Hence eq.(3.16) becomes

$1 = N(o)V \int_0^{\hbar\omega_{ex}} d\epsilon \frac{\tanh(\frac{\sqrt{(\epsilon^2+\triangle^2)}}{2k_BT})}{\sqrt{(\epsilon^2+\triangle^2)}}$

Where $V = \frac{<|X_q|^2>}{\hbar\omega_{ex}}$

$$\frac{1}{\lambda_{ex}} = \int_0^{\hbar\omega_{ex}} d\epsilon \frac{\tanh(\frac{\sqrt{(\epsilon^2+\triangle^2)}}{2k_BT})}{\sqrt{(\epsilon^2+\triangle^2)}} \tag{3.17}$$

Where $\lambda_{ex} = N(o)V$

This gap parameter($\triangle$) is temperature dependent. The limit temperature T_c at which $\triangle$ vanishes is defined by

$$\frac{1}{\lambda_{ex}} = \int_0^{\hbar\omega_{ex}} d\epsilon_k \frac{\tanh(\frac{\epsilon_k}{2k_BT_c})}{\epsilon_k} \tag{3.18}$$

In this limit, temperature T_c will be identified as the critical temperature at which the supercondensate disappears. Hence eq.(3.18) can be written as

$\frac{1}{\lambda_{ex}} = \int_0^{\frac{\hbar\omega_{ex}}{2K_BT_c}} dx \frac{\tanh(x)}{x}$

$\frac{1}{\lambda_{ex}} = [\ln(x)\tanh(x)]|_0^{\frac{\hbar\omega_{ex}}{2T_ck_B}} - \int_0^{\frac{\hbar\omega_{ex}}{2T_ck_B}} \sec h^2(x)\ln(x)dx$

For low temperature, we can replace $\tanh(\frac{\hbar\omega_{ex}}{2k_BT_c})$ by unity and extend the upper limit of the integral to infinity to find

$\frac{1}{\lambda_{ex}} = \ln(\frac{\hbar\omega_{ex}}{2k_BT_c}) - \int_0^{\infty} \sec h^2(x)\ln(x)dx$

The integral is equals to $\ln(0.44)$, from which we get :

$$K_B T_c = 1.14\hbar\omega_{ex} \exp(\frac{-1}{\lambda_{ex}}) \tag{3.19}$$

which is the well known BSC expression.

3.2 Superconductivity Energy gap

From eq.(3.17) above we have

$\frac{1}{\lambda_{ex}} = \int_0^{\hbar\omega_{ex}} \frac{\tanh(\frac{\beta E_k}{2})}{E_k} d\epsilon$, $E_k = \sqrt{(\epsilon^2 + \triangle^2)}$.

Let us first consider the limit $\beta = \infty$, that is , $T = 0$ and hence find the gap $\triangle(0)$ in the ground state . Therefore the above equation at $T = 0$ becomes,

$\frac{1}{\lambda_{ex}} = \int_0^{\hbar\omega_{ex}} \frac{1}{\sqrt{(\epsilon^2+\triangle^2)}} d\epsilon$,

This can be rewritten as

$\frac{1}{\lambda_{ex}} = \frac{1}{\triangle} \int_0^{\hbar\omega_{ex}} \frac{1}{\sqrt{(1+\frac{\epsilon^2}{\triangle^2})}} d\epsilon$

Since

$\int \frac{dx}{\sqrt{(a^2+x^2)}} = \ln|x + \sqrt{(a^2 + x^2)}| + c$ and $\sinh^{-1}(x) = \ln(x + \sqrt{(x^2 + a^2)})$

$\frac{1}{\lambda_{ex}} = \ln(\frac{\hbar\omega_{ex}}{\triangle} + \sqrt{(1 + \frac{(\hbar\omega_{ex})^2}{\triangle^2})})$

$\frac{1}{\lambda_{ex}} = \sinh^{-1}(\frac{\hbar\omega_{ex}}{\triangle})$

$\triangle(0) = \frac{\hbar\omega_{ex}}{\sinh(\frac{1}{\lambda_{ex}})}$

Since λ_{ex} is small quantity $\triangle(0)$ become

$$\triangle(0) = 2\hbar\omega_{ex} \exp(\frac{-1}{\lambda_{ex}}) \tag{3.20}$$

3.3 Phonon-exciton Combined Mechanism

From exclusively excitonic mechanism we have got T_c and $\triangle(0)$ values which are unappropriate to the experimental values. As a result we assume this exclusive excitonic mechanism is not the possible mechanism to explain superconductivity of alkali metals doped fullerene (C_{60}).

Since alkali metal doped C_{60} superconductors, A_3C_{60} ($A = K, Rb, Cs$) experimental values of $T_c = 19K$ for K_3C_{60} [6], $T_c = 29K$ for Rb_3C_{60} [11] and $T_c = 33 - 40K$ for Cs_3C_{60} has been observed [12]. Isotope coefficient experimental value, $\alpha = 0.30 \pm .06$ for K_3C_{60}[26] and $\alpha = 0.37 \pm 0.05$ for Rb_3C_{60}[29]. From these values we can understand that phonons participate in pair formation. As we can see from experimental values of α for A_3C_{60}, it is not the same as BCS type which is, $\alpha = 0.5$ for weak coupling and phonon mediated superconductors. Therefore the isotope effect still gives rise to some interesting experimental and theoretical questions.
It is also reported that electronic excitation may explain mechanism of superconductivity in this system , A_3C_{60}[35].
But from theoretical aspects it is difficult to explain the mechanism of superconductivity fully as phonon mediated[33].

Therefore, here we apply a combined mechanism .The contribution of electronic excitation is zero for isotope effect as there is no involvement of atomic mass. However, to take care of small isotope effect in A_3C_{60} superconductors, phonons are also included. Therefore, a combined phonon-exciton mechanism explains the T_c values very well as it is believed that for A_3C_{60} superconductors the coupling is strong as a result phonons alone can not explain such high critical temperature, as discussed by many

people [33, 35, 52]. Here, we try to calculate the following superconductivity parameters for this system. This are transition temperature(T_c), isotope effect coefficient(α) and the reduced gap ($\frac{2\triangle(0)}{K_B T_c}$). In the present mechanism pairing is achieved through the virtual exchange of excitons and phonons and it is singlet(s-wave) pairing. The critical transition temperature (T_c) is expressed as [1]

$$T_c = 1.14\omega_{ph}^{n_1}\omega_{ex}^{n_2}\exp[-(\lambda_{ph}^{*} + \lambda_{ex}^{*})^{-1}] \tag{3.21}$$

Where

$n_1 = \frac{\lambda_{ph}}{\lambda_{ph}+\lambda_{ex}}$, $n_2 = \frac{\lambda_{ex}}{\lambda_{ph}+\lambda_{ex}}$

and

$\lambda_{ph}^{*} = \frac{\lambda_{ph}}{\lambda_{ph}+1}$, $\lambda_{ex}^{*} = \frac{\lambda_{ex}}{\lambda_{ex}+1}$, $\lambda_{ex} = \frac{<|X_q|^2>}{\hbar\omega_{ex}}N(0)$

Here λ_{ex} is the electron-exciton coupling constant, λ_{ph} is the electron-phonon coupling constant, ω_{ex} and ω_{ph} are energies of excitonic and phononic excitations respectively .

Here we use the phonon energy $\hbar\omega_{ph} = 300K$ .This value is in agreement with the optical and tunneling studies [50] and calculation of Gunnarson et al. [51], where the low lying Raman modes of the C_{60} molecule proved to contribute significantly to the electron-phonon coupling. Also we use for exciton excitation energy $\omega_{ex} = 4000K$ taking $\lambda_{ph} = 0.3$ for different values of λ_{ex} we get T_c values for the three compounds as shown in table 3. This combined mechanism also helps us in understanding small values of isotope effect coefficient in A_3C_{60} superconductors . As we mentioned above, the contribution of electronic excitation is zero for isotope effect as there is no involvement of atomic mass.

Therefore

$$T_c \sim M^{\frac{-n_1}{2}} \tag{3.22}$$

Using the above model the isotope effect coefficient is given by

$$\alpha = \frac{n_1}{2} \tag{3.23}$$

By taking suitable values of the parameters of the system , values for α can be obtained for the three alkali-doped C_{60} superconductors, these are shown in table 3. Finally we calculate the reduced gap.From eq.(3.20) we have

$$\triangle(0) = 2\hbar\omega_{ph} \exp(\frac{-1}{\lambda_{ex} + \lambda_{ph}}) \tag{3.24}$$

Here we substitute $\lambda_{ex} + \lambda_{ph}$ in place of λ_{ex} since $\triangle(0)$ is a gross effect and there is a contribution from both phonons and excitons. Taking $\lambda_{ph} = 0.3$ and $\omega_{ph} = 300K$ for different values of λ_{ex} we calculate for the value of $\triangle(0)$ and it is given in table 3.

For $\omega_{ph} = 300K$, $\omega_{ex} = 4000K$ and $\lambda_{ph} = 0.3$ we get the following superconducting parameter values.

Compound	λ_{ex}	$T_c(k)$	α	$\triangle(0)(mev)$	$\frac{2\triangle}{K_B T_c}$	$2\triangle(0)mev$	$2\triangle^{exp}(0)mev$
Cs_3C_{60}	.12	36.7	.36	4.8	3.02	11.07	12.07
	.11	32.7	.37	4.5	3.20	9.86	10.01
Rb_3C_{60}	.10	28.5	.38	4.2	3.46	8.59	8.92
K_3C_{60}	.07	18.9	.41	3.5	4.25	5.7	5.8

Table 3. Calculated values of different superconducting parameters.

Chapter 4

Results and Discussion

In the first section of the previous chapter we have studied the effect of electronic excitation(excitons) on electron pair formation . For this purpose we have studied a model Hamiltonian which contains interactions involving electron-exciton.

We have reduced the model Hamiltonian of the system canonically to obtain BCS type attractive paring interaction. Using this reduced model Hamiltonian and applying the Green's function formalism we get an expression for $\triangle$ as a function of temperature . We also obtain an expression for transition temperature T_c from eq.(3.17). The order parameter $\triangle(0)$ at zero temperature has also been calculated.

The expression we get for T_c is similar to that of BCS type expression which is calculated for electron-phonon coupling. Our results clearly show that the excitons may also be responsible for the mechanism of superconductivity in alkali metal doped C_{60} superconductors if appropriate values of λ_{ex} and ω_{ex} are found it will be possible to produce the experimentaly observed values of T_c and reduced gap $\triangle$.

The other part of our study is section 3.3. In this part of our study we investigate the effect of electron-phonon and electron-exciton coupling on transition temperature T_c of A_3C_{60} . An exact calculation of electronic coupling constant λ_{ex} for the exciton

exchange discussed in the previous section is important but it has not been attempted in the present study and so is the evaluation of coupling constant χ_q .

In the absence of these values , rough estimates for T_c , α and reduced gap $(\frac{2\triangle}{K_B T_c})$ of different compounds of A_3C_{60} are made for appropriate values of the parameters from existing literature . T_c values seem to be in reasonable agreement to the experimental values see table (3) . The value of α that we get for Rb_3C_{60} is very close to the experimental result which was found by Ramirez et al. [29]. While our calculated value of reduced gap for K_3C_{60} is in good agreement with the experimental result of Sasaki et al. [19]. Most recent experimental results for reduced gap of this system , however , tend to scatter around the weak coupling limit [23, 24] if a reasonable uncertainty is assumed for these experiments and our result for Rb_3C_{60} is consistent with this limit.

From Rickayzen [53] calculation, the value of $\frac{\triangle(T)}{\triangle(0)}$ are well given by the equation:

$$\frac{\triangle(T)}{\triangle(0)} = \tanh[\frac{T_c}{T}\frac{\triangle(T)}{\triangle(0)}] \tag{4.1}$$

The following Figures show the variation of order parameter $\triangle(T)$ against temperature for different compounds of A_3C_{60} (A=K,Rb and Cs). From these figures it is clearly shown that on increasing temperature the superconducting energy gap decreases and become zero at transition temperature T_c this is because the cooper pairs break down when temperature increases and at T_c they completely disappear. Therefore, we can observe from the graphs the superconducting energy gap exists in the superconducting state and disappears at T_c and the normal state. The doted lines denote experimental points.

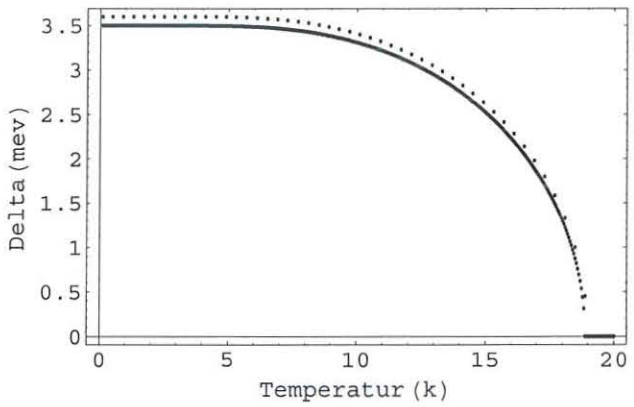


Figure 4.1: Energy gap Vs Temperature for K_3C_{60}

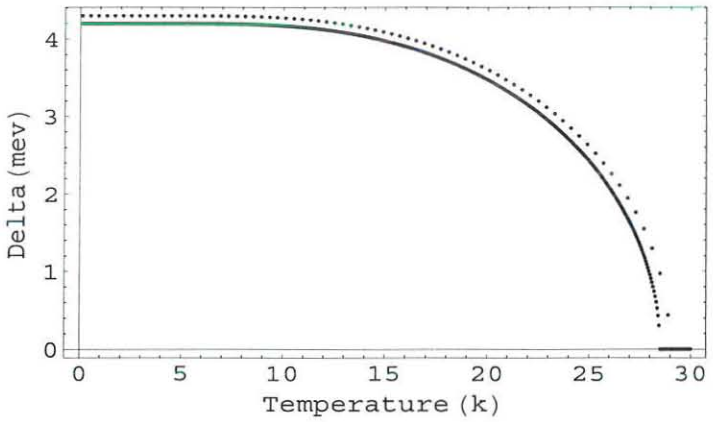


Figure 4.2: Energy gap Vs Temperature for Rb_3C_{60}.

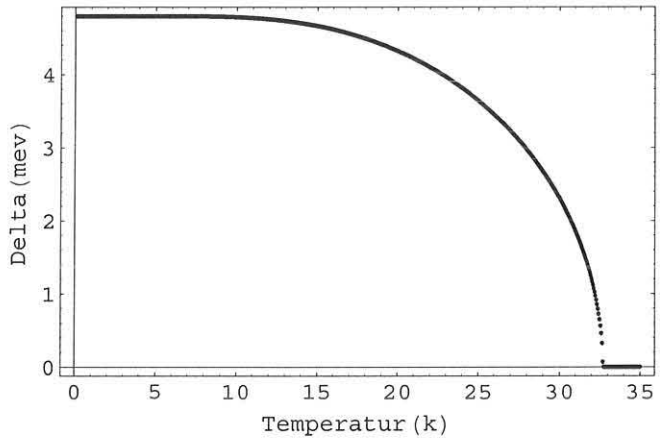


Figure 4.3: Energy gap Vs Temperature for Cs_3C_{60}

The curves are quite similar to the convectional superconductor theoretical curves.

Chapter 5

Conclusion

A model Hamiltonian consisting of electrons, excitons and their interaction is studied using quantum field theory formalism of Green function. It is concluded that the phonon-exciton combined mechanism plays an important role in the formation of cooper pairs to produce superconducting state in A_3C_{60} (A=K, Rb and Cs) as excitons and phonons are alone not able to explain properties of these C_{60} superconductors. The transition temperature(T_c), the isotope effect(α) and the reduced gap $\frac{2\triangle}{K_BT_c}$ are found to depend on the phonon and exciton excitation energy , also they depend on the phonon and exciton coupling constants. The isotope effect and reduced gap values are in good agreement with the experimental values. This exciton-phonon mechanism is capable of explaining the whole range of T_c values for all these superconductors. From the values of α and reduced gap it is inferred that A_3C_{60} superconductors are BCS type assisted by excitonic effect.

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DECLARATION

I hereby declare that this thesis is my original work and has not been presented for a degree in any other university. All sources of material used for the thesis have been duly acknowledged.

Name: Berhanu Tulu

Signature: ———————-

This thesis has been submitted for examination with my approval as University advisor.

Name: Professor P. Singh (PhD)

Signature: ———————-

Addis Ababa University

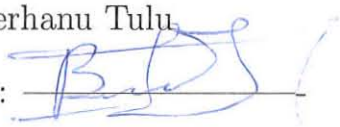
Department Of Physics

June 2005

DECLARATION

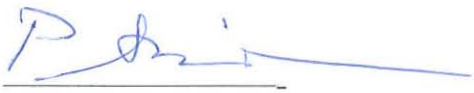
I hereby declare that this thesis is my original work and has not been presented for a degree in any other university. All sources of material used for the thesis have been duly acknowledged.

Name: Berhanu Tulu

Signature: 

This thesis has been submitted for examination with my approval as University advisor.

Name: Professor P. Singh (PhD)

Signature: 

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