STUDY OF SUPERCONDUCTIVTY OF LEAD NANO STRUCTURE

SUBMITTED IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE IN PHYSICS
AT
ADDIS ABABA UNIVERSITY
ADDIS ABABA, ETHIOPIA
JUNE 2009

By

Fikreselassie Teklay Brhane

ADDIS ABABA UNIVERSITY
DEPARTMENT OF
PHYSICS

The undersigned hereby certify that they have read and recommend to the School of Graduate Studies for acceptance a thesis entitled "**STUDY OF SUPERCONDUCTIVTY OF LEAD NANO STRUCTURE**" by **Fikreselassie Teklay Brhane** in partial fulfillment of the requirements for the degree of **Master of Science in Physics**.

Dated: June 2009

Advisor: _____
Professor Singh.P

Examiner: _____
professor Vadim N. Mal'nev

_____
Dr.Gebregizabher kahsay

ADDIS ABABA UNIVERSITY

Date: **June 2009**

Author: **Fikreselassie Teklay Brhane**

Title: **STUDY OF SUPERCONDUCTIVTY OF LEAD NANO STRUCTURE**

Department: **Physics**

Degree: **M.Sc.** Convocation: **June** Year: **2009**

Permission is herewith granted to Addis Ababa University to circulate and to have copied for non-commercial purposes, at its discretion, the above title upon the request of individuals or institutions.

Signature of Author

Table of Contents

List of Figures

Abstract

Quantum confinement of electrons in clean nanowires and nanofilms results in the formation of a series of subbands that move in energy with changing wire/film thickness. When the bottom of such a subband moves through the Fermi surface, the density of states changes and a size-dependent superconducting resonance appears, leading to quantum-size oscillations in the critical temperature T_c and the order parameter $\triangle$. Our theoretical formulation is based on a numerical solution of the Bogoliubovde Gennes equations in the clean limit.

Acknowledgements

I would like to thank professor singh.p , my advisor, for his many suggestions and constant support during this research. His limitless and invaluable effort in guiding, supervising, encouraging for the accomplishment of this thesis gives me a great pleasure. It is him who gave me courage in doing my graduate thesis in this way.I would like to thank Yikdem Mengesha for his support which I don't have words to express.

Introduction

Superconductivity is phenomenon first discovered by Kameringh Onnes in mercury at temperature T_c (4.2K for mercury)in 1911[1,2]. For many years superconductors were thought to consist simply of a vanishing of all electrical resistance below transition temperature. A major advance was the discovery of the Meissner effect in 1933, which showed that a superconductor is perfect diamagnet; magnetic flux is excluded from all but from thin surface layer[1,2]. In1935 F.London and L.London proposed phenomenological theory of the electromagnetic properties in which the diamagnetic aspects were assumed basic . F .London suggested quantum theoretic approach to a theory in which it was assumed that there is some how coherence or rigidity in the superconducting state such that the wave function is not modified very much when a magnetic is applied [2,3]. The concept of coherence has been emphasized by Pipard who, on the basis of experiments on penetration phenomena proposed a non local modification of the London equation in which coherence distance, ε_o is introduced[2] .In 1950 Fröhlich suggested electron-phonon mechanism of superconductivity for the first time[15] .His suggestion was confirmed experimentally by the discovery of the isotope effect i.e. the proportionality of T_c to $m^{\frac{-1}{2}}$ for isotopes of the same element[1,3]. In 1957 Bardeen ,Cooper and Schrieffer proposed microscopic theory of superconductivity which has successfully explained many properties of superconductors[1,2].Since

the first discovery of superconductivity at 4.2 K, the quest for new superconducting materials has led to a slow increase in T_c over the decades. Finally the highest T_c seemed to have reached a plateau in Nb_3Ge ($T_c = 23K$) . Thus the discovery of superconductivity at T_c = 35 K of (LBCO) in 1986 (a mixed oxide of lanthanum, barium, and copper) by Bednorz and M $\ddot{u}$ller came as a big surprise[1]. Another big jump to T_c =90 K in the (YBCO) class of materials followed immediately, and yet higher T_c values have been achieved in the (BSCCO) and (TBCCO) systems. These high-temperature superconductors are distinct from the low-temperature or conventional superconductors which can be well understood in terms of the BCS theory. The mechanism of high T_c super- conductivity is still not known. Thus extensive research in the area of superconductivity still continues today. In this thesis we study the superconductivity of nano size lead. For this study we have used the microscopic Bogoliubov -de Genness equation.The thesis is organized into five chapters. chapter one discusses basic concepts of superconductivity. Chapter two discusses the derivation of Bogoliubov -de Genness equation and the pairing potential $\triangle(r)$ .Chapter three deals with the mechanism of superconductivity in nano structures and how the microscopic bogoliubov -de genness equation is used to investigating superconductivty of nano structures. Chapter four contains the result and discussion,and chapter five gives the conclusion.

Chapter 1

SUPERCONDUCTIVTY

1.1 EXPERIMENTAL SURVEY

Kamerlingh onnes liquified helium in 1908 , shortly after wards , he began investigating the conductivity of metals at new temperature below 4k[1] .To reduce resistance caused by impurities , he studied mercury of high purity and was not surprise when he found no measurable resistance .However ,it soon became clear that the experiment was not in accord with the expectation .The addition of impurities to mercury did not increase its resistance .Further more , the resistance did not decrease smoothly to zero but dropped almost discontinuity to zero .He concluded that mercury enters into new state , on the account of its remarkable electrical properties , may called the "superconducting state". The complete disappearance of resistance is most remarkably demonstrated by experiments with persistent current in the superconduction rings. Kamerlingh onnes also discovered that Superconductivity was destroyed when a superconductor was placed in sufficiently strong magnetic field . The minimum magnetic field required to destroy superconductivity is called critical magnetic field H_C .The temperature dependence of this critical magnetic field H_C is empirically

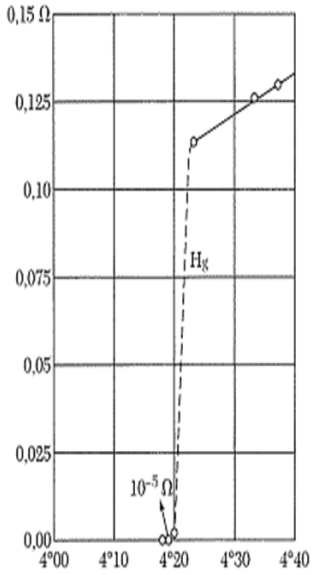

Figure 1.1: temperature vs resistivity[12]

given by

$$H_c(T) = H_c(0)[1 - (\frac{T}{T_c})^2] \tag{1.1.1}$$

If a superconductor really can be described by infinite conductivity ,the the electric field inside is always zero and,

$$\dot{B} = 0 \tag{1.1.2}$$

The magnetic induction is constant , and the the magnetic induction inside depends on the past history of the state and is not a unique function of the external condition . This means that there is not a single superconducting state in a given external field ,but an infinite number which could be meta stable.

In (1933)Meissner and Ochsenfeld measured the field surrounding a superconductor

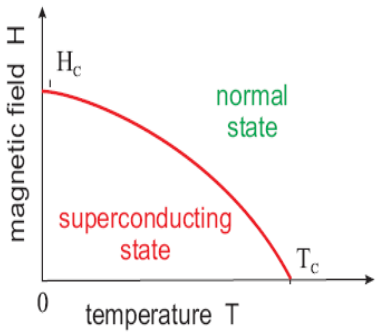

Figure 1.2: Magnetic field vs temperature[1,2,4]

and concluded that in all circumstance the magnetic field induction B inside was zero[1] .This important effect known as the Meissner effect which showed that the superconducting state in a given magnetic field is a single stable state to which the laws of thermodynamics apply . This result showed that a superconductor behaves as a perfect diamagnet. Strictly speaking a superconductor is not a perfect diamagnet because the magnetic field penetrates to a distance of the order of 10^{-6} to 10^{-5} cm . Many properties of a superconductor can be understood on the basis of perfect diamagnetism .

1.2 LONDON'S ELECTROMAGNETIC EQUATION

To account for the electromagnetic properties of superconductors in particular to account for the Meissner effect and the existence of persistent current F .and H .London proposed that ohm's law which relates current density and electric field in normal metals be replaced by other relation connecting the superconducting current and fields

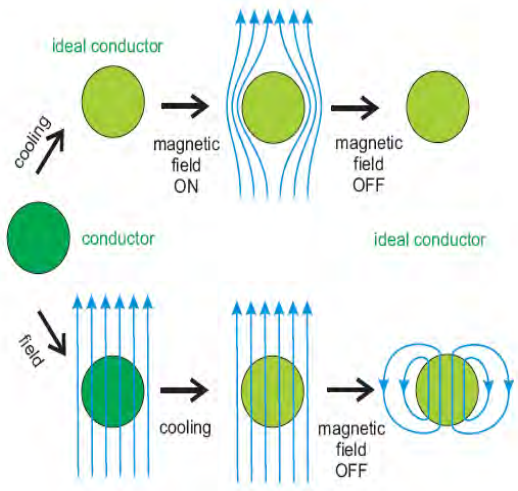

Figure 1.3: a perfect conductor in a magnetic field[4]

in a superconductor[1,3].They used two-fluid model , of the total density of electrons there is a fraction n_s that represents the superconducting electrons .These electrons are not scattered by either impurities or lattice vibration i.e phonons .Thus ,they do not contribute to the resistivity , moreever these electrons are freely accelerated by an electric field. If v_s is their super fluid velocity , one can write the equation of motion as

$$M\frac{dv_s}{dt} = eE \tag{1.2.1}$$

and the superconducting current density is

$$J_s = n_s e v_s \tag{1.2.2}$$

Then

$$\frac{dJ_s}{dt} = \frac{n_s e^2}{m}E \tag{1.2.3}$$

$$\frac{dJ_s}{dt} = \wedge E \tag{1.2.4}$$

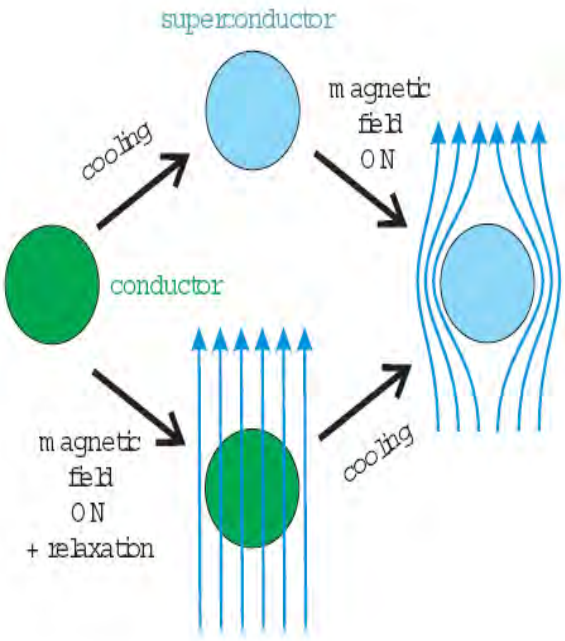

Figure 1.4: a superconductor in a magnetic field[4]

where $\wedge = \frac{n_s e^2}{m}$ .This is simply Newton's second law for superconducting electrons . Let us find a relation between J_s and magnetic field $\hat{H}$ in a superconductor .The free energy of a superconductor is given

$$F = \int F_s + E_{kin} + E_{mag} \tag{1.2.5}$$

The kinetic energy (E_{kin}) is connected with the current density $J_s = n_s e v_s$, and it is written as

$$E_{kin} = \frac{1}{2}\int n_s m v_s^2 dv = \frac{1}{2}\int \frac{m J_s^2}{n_s e^2} \tag{1.2.6}$$

Taking into account the Maxwell's equation,

$$\nabla X \vec{H} = \frac{4\pi}{c} J_s \tag{1.2.7}$$

The kinetic energy will be

$$E_{kin} = \frac{1}{8\pi} \int \lambda^2 (\nabla X \vec{H})^2 \tag{1.2.8}$$

where we have defined

$$\lambda^2 = \frac{mc^2}{4\pi n_s e^2} \tag{1.2.9}$$

The magnetic energy density is $\frac{H^2}{8\pi}$ .The free energy of the superconductor is thus

$$F = F_o + \frac{1}{8\pi} \int [\vec{H}^2 + \lambda^2 (\nabla X \vec{H})^2] dv \tag{1.2.10}$$

Where F_o is the free energy of a superconductor at $\vec{H}$ =0 . Let us find the value of $\vec{H}$ corresponding to the minimum vale of F. Assuming a small variation $\vec{H} \rightarrow \vec{H} + \delta\vec{H}$, we find a change in F as

$$\delta F = \frac{1}{8\pi} \int (2\vec{H}\delta\vec{H} + 2\lambda^2 \vec{\nabla} X \vec{H}.\vec{\nabla} X \delta\vec{H}) dv \tag{1.2.11}$$

$\vec{H}$ corresponds to minimum value of F, that is

$$\delta F = 0 \tag{1.2.12}$$

Using

$$\vec{a}.\vec{\nabla} X \vec{b} = \vec{b}.\vec{\nabla} X \vec{a} - div(\vec{a} X \vec{b}) \tag{1.2.13}$$

And combining eqn (1.2.11) and (1.2.12),we obtain

$$\int [\vec{H} + (\lambda^2 \vec{\nabla} X \nabla X \vec{H})].\delta\vec{H} dv - \int [div \nabla X \vec{H} X \delta\vec{H}] = 0 \tag{1.2.14}$$

for arbitrary $\delta\vec{H}$ we have to satisfy

$$\vec{H} + \lambda^2 \vec{\nabla} X \vec{\nabla} X \vec{H} = 0 \tag{1.2.15}$$

.This is the second London 's equation .Using

$$\nabla X\vec{H} = \frac{4\pi}{c}J_s \tag{1.2.16}$$

and

$$\vec{H} = \vec{\nabla}X\vec{A} \tag{1.2.17}$$

We can write eqn (1.2.2) as

$$J_s = \frac{-c}{4\pi\lambda^2}\vec{A} \tag{1.2.18}$$

eqn (1.2.18) is correct only in the so-called london guage choice of the vector potential

$$div\vec{A} = 0 \tag{1.2.19}$$

$$\vec{A}\vec{n} = 0 \tag{1.2.20}$$

Where $\vec{n}$ is the vector along the normal to superconductor surface .eqn (1.2.18) and eqn (1.2.19) specify the continuity of current and absence of a supercurrent source , while (1.2.20) assures that no supercurrent can pass through the boundary of a superconductor. using eqn(1.2.18)and eqn (1.2.6),eqn (1.2.4)can be written as

$$J_s = \frac{-}{c\wedge}\vec{A} \tag{1.2.21}$$

$$\wedge = \frac{4\pi\lambda^2}{c^2} \tag{1.2.22}$$

1.3 THE MEISSNER EFFECT

We now apply the London 's equation and discuss the penetration depth of magnetic field $\vec{H}$ into a superconductor . We choose the simplest geometry ,the surface of the specimen in x-y plane. We have

$$\vec{H} + \lambda^2\vec{\nabla}X\vec{\nabla}X\vec{H} = 0 \tag{1.3.1}$$

$$\nabla X\vec{H} = \frac{4\pi}{c}J_s \tag{1.3.2}$$

$$div\vec{H} = 0 \tag{1.3.3}$$

1.If $H \parallel Z$, we obtain $\frac{dH}{dZ} = 0$, H=constant ,consequently, $\vec{\nabla}X\vec{H}$= 0,$J_s = 0$,from london equation ,H=0.The field can not be normal to superconductor surface. 2.If $H \parallel X$, div H=0 automatically met, and we get $j \parallel y$ so,the Maxwell equation is

$$\frac{dH}{dZ} = \frac{4\pi}{c}J_s \tag{1.3.4}$$

and the london

$$\frac{d^2H}{dz^2} - \lambda^{-2}H = 0 \tag{1.3.5}$$

The boundary conditions are $H(0) = H_o, H(\infty) = 0$, the solution is

$$H(z) = H_o e^{\frac{-z}{\lambda}_L} \tag{1.3.6}$$

And the screening current

$$j_s = c\frac{H_o}{4\pi\lambda}e^{\frac{-z}{\lambda}_L} \tag{1.3.7}$$

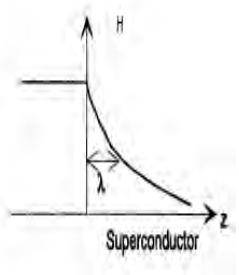

Figure 1.5: magnetic field pentration in to asuperconductor

1.4 BCS THEORY

The phenomenological theory we discussed so far does not explain or describe what a superconducting state is, even it failed to describe the distinguishing characteristics of superconducting state ,exponential variation of specific heat at temperature below T_c, the existence of energy gap ,and the so- called isotope-effect .

The problem was solved is 1957 when Bardeen ,Cooper ,and Schrieffer formulated a microscopic theory of superconductivity ,which explained many properties of superconductors[1,2] .BCS theory gave as excellent account especially of electron- phonon interaction at temperature very near to zero . It was the isotope -effect that gave a hint that somehow lattice vibrational exciation (phonon), were involved in the formation of superconductivity .

Before the development of BCS theory of superconductivity, cooper (1956) showed that two electron interacting near the fermi surface form a bound state regardless of how weak the interaction is , so long as it is attractive i.e the fermi sea is unstable against the formation of at least one bound pair[14] . These pairs (bound states) commonly called cooper pairs , have characteristic length of order of ε_o, which is introduced as the phenomenological theory. The electrons in the bound state have opposite spins and momenta $(\vec{k}\uparrow, -\vec{k}\downarrow)$.

BCS theory is based on the attractive electron - electron interaction which results from the electron- phonon interaction i.e a first electron polarizes the medium by attracting the positive ion ; these excess positive ions , in turn , attract the second electron(which lowers its energy) , giving an effective attraction between electrons as it is shown in fig (1.5).

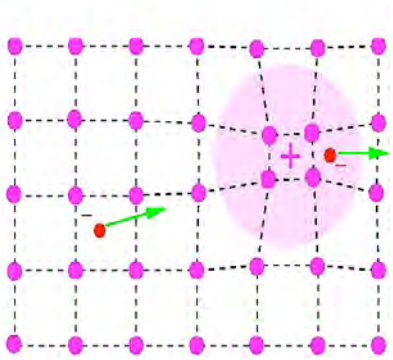

Figure 1.6: Electron -phonon interaction

In the electron - phonon interaction , electrons are scattered from a Bloch state by absorption or emission of a phonon of wave vector of q . As it is shown in fig (1.6) the attractive electron -electron interaction is due to the virtual exchange of phonons . The energy difference between these interacting electrons should be less than phonon energy $\hbar w_q$. For superconductivity to occur this attractive electron- electron interaction should dominate the screened coulomb electron- electron interaction.

The the electron - phonon interaction is given by

$$H' = i \sum_{kq} D_q c^{\dagger}_{k+q} c_k (a_q - a^{\dagger}_{-q}) \tag{1.4.1}$$

where $c^{\dagger}$,c are fermion operators and $a^{\dagger}$,a are boson operators ;D_q is a number , and for convenience we take it equal to D, a real constant .The the total hamiltonian of electron , phonons , and their interaction is[16,22]

$$H = \sum_{q} w_q a^{\dagger}_q a_q + \sum \varepsilon_k c^{\dagger}_k c_k + i \sum_{kq} D_q c^{\dagger}_{k+q} c_k (a_q - a^{\dagger}_{-q}) \tag{1.4.2}$$

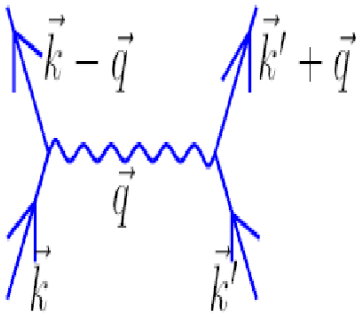

Figure 1.7: Attractive electron -electron interaction due to exchange of virtual phonons

Using canonical transformation of the hamiltonian,the reduced hamiltonian is given by

$$H = \sum_{k\alpha} \epsilon_k n_{k\alpha} + \sum_{kk'} v_{kk'} c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \tag{1.4.3}$$

Where $n_{k\alpha}$ is the number operator which count the number of electron in a single state.

1.4.1 BCS GROUND STATE

According to BCS theory in the ground states at absolute zero temperature of a superconductor is a linear combination of staes in which pairs $(\vec{k}\uparrow, -\vec{k}\downarrow)$ are occupied or unoccupied. In the ground state all the electrons participate in the paring and all the cooper pair collective form macroscopic condensate due to strong correction among the cooper pair.This is the origin of zero resistivity and stiffness against magnetic fields of a superconductor . In the ground state ,electrons near the fermi surface are only strongly affected by the electron -phonon interaction. The reduce hamiltonian

is defined by

$$H = \sum_{k\alpha} \epsilon_k n_{k\alpha} + \sum_{kk'} v_{kk'} c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \tag{1.4.4}$$

Creation and annihilation operator for pair may be defined in terms of the single particle operators as follows

$$b_k = c_{-k\uparrow} c_{k\downarrow} \tag{1.4.5}$$

$$b^{\dagger}_k = c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} \tag{1.4.6}$$

$$n_{k\alpha} = c^{\dagger}_{k\alpha} c_{k\alpha} \tag{1.4.7}$$

The number operator

$$n_{k\alpha} = n_{k\uparrow} + n_{k\downarrow} \tag{1.4.8}$$

can be replaced by

$$n_{k\alpha} = 2 b^{\dagger}_k b_k \tag{1.4.9}$$

Then the reduced Hamiltonian is given by

$$H_{red} = \sum_{k} 2\epsilon_k b^{\dagger}_k b_k + \sum_{kk'} v_{kk'} b^{\dagger}_k b_k \tag{1.4.10}$$

BCS theory is a mean-field theory, and for zero temperature, it applies the variational principle. The trial wave function for the many-body ground state, $|\Psi_o>$ is taken

$$|\Psi_o> = \prod_k (u_k + v_k b^{\dagger}_k)|0> \tag{1.4.11}$$

where $|0>$ is a null state. The u_k is the probability amplitude that the pair state $(\vec{k}\uparrow, -\vec{k}\downarrow)$ is unoccupied, and v_k is the probability amplitude that this pair state is occupied. They are variational parameters and satisfy the normalization condition $u_k^2 + v_k^2 = 1$, so that the total wave function is normalized. As is clear from eqn (1.4.12), BCS theory is based on grand canonical ensemble, and the number of particles in

the system is not conserved. One imposes the constraint that on average the number of electrons is N:

$$< \Psi_o|\hat{N_{OP}}|\Psi_o >=< \Psi_o| \sum_k n_{k\alpha}|\Psi_o >= N \tag{1.4.12}$$

The $\hat{N_{OP}}$ is the number operator which counts the number of electrons in the many-body system. Using the Lagrange multiplier,μ i.e.chemical potential, one minimizes the ground-state energy:

$$\delta W = \delta < \Psi_o|H_{RED} - \hat{N_{OP}}|\Psi_o >= 0 \tag{1.4.13}$$

Substituting the Hamiltonian (1.4.11) and the wave function (1.4.12) into this equation(1.4.14), and applying the commutation relations of $b_k^\dagger$ and b_k , one has

$$W = \sum_k 2(\epsilon_k - \mu)v_k^2 + \sum_{kk'} v_{kk'}v_k u_k v_{k'}u_{k'} \tag{1.4.14}$$

Minimizing this energy in terms of and v_k and u_k , with the normalization condition, one obtains

$$\begin{aligned} u_k^2 &= \frac{1}{2}(1 + \frac{\epsilon_k}{E_k}) \\ v_k^2 &= \frac{1}{2}(1 - \frac{\epsilon_k}{E_k}) \end{aligned} \tag{1.4.15}$$

where E_k is defined by

$$E_k = [(\epsilon_k - \mu)^2 + \triangle_k^2]^{\frac{1}{2}} \tag{1.4.16}$$

and $\triangle_k$ satisfies the relation

$$\triangle_k = -\sum_k v_{kk'} \frac{\triangle_{k'}}{2E_K} \tag{1.4.17}$$

From BCS theory

$$V_{kk'} = -v, if|\xi_k|and|\xi_k| \leq \hbar w_D$$

$$0, otherwise \tag{1.4.18}$$

and

$$\triangle_k = \triangle, if|\xi_k|and|\xi_k| \leq \hbar w_D,$$

$$0, otherwise \tag{1.4.19}$$

For $\triangle_k = \triangle$, eqn (1.4.19) will be

$$1 = \frac{v}{2}\sum_k \frac{1}{E_k} \tag{1.4.20}$$

Converting the above equation into integration ,it becomes

$$1 = \frac{v}{2}\int_{-\hbar\omega_D}^{\hbar\omega_D} N(\varepsilon)\frac{d\varepsilon}{\sqrt{\Delta^2+\varepsilon^2}} \tag{1.4.21}$$

replacing $N(\varepsilon)$ by N(0) which is the density of states at the Fermi level because $\hbar w_D << \xi_F$, and enq (1.4.21) becomes

$$1 = vN(0)\int_0^{\hbar\omega_D} \frac{d\varepsilon}{\sqrt{\Delta^2+\varepsilon^2}} \tag{1.4.22}$$

for weak coupling,$N(0)v << 1$,and the integration gives

$$\Delta = 2\hbar\omega_D \exp[\frac{-1}{vN(0)}] \tag{1.4.23}$$

where $\triangle(r)$ is the energy gap parameter .Using (1.4.15,1.4.16,1.4.18,),the energy difference between the normal and the superconducting state is given by

$$U_s(0) - U_n(0) = \frac{-1}{2}N(0)\triangle^2 \tag{1.4.24}$$

1.4.2 EXCITED STATES

The excitation spectrum of the superconductor can be conveniently treated by introducing a linear combination of the fermion creation and annihilation operators. This is known as the Valatin-Bogoliubov transformation:[17,18]

$$c_{k\uparrow} = u^* \gamma_{k0} + v_k \gamma_{k1}^\dagger \tag{1.4.25}$$

$$c_{-k\downarrow} = -v^* \gamma_{k0} + u_k \gamma_{k1}^\dagger \tag{1.4.26}$$

are used ,and the reduced BCS hamiltonian is given by

$$H = \sum (\xi_k - E_k + \triangle_k b_k^\dagger) + \sum_k E_k (\gamma_{k0}^\dagger \gamma_{k0} + \gamma_{k1}^\dagger \gamma_{k1}) \tag{1.4.27}$$

and

$$\triangle_k = \frac{-1}{2} \sum_{k'} v_{kk'} \frac{\triangle_{k'}}{E_{k'}} (1 - 2f(E_{k'}) \tag{1.4.28}$$

Following the the same procedure we used to derive the $\triangle$,we find critical temperature T_c to be

$$T_c = 1.14 \frac{\hbar w_D}{k_B} e^{\frac{-1}{N(0)V}} \tag{1.4.29}$$

where N(0) is the density of state at the fermi surface ,and the V is coupling constant.The temperature dependence of $\triangle$ is given by

$$\triangle(T) = 1.74 \triangle(0) (1 - \frac{T}{T_c})^{\frac{1}{2}} \tag{1.4.30}$$

For finite temperature, the BCS theory is formulated on the basis of the statistical method for a grand canonical ensemble. One of the predictions deducted from the BCS theory that agrees perfectly with experiments, is the temperature dependence of the energy gap. Now we have seen that the quasi particle excitation can be simply

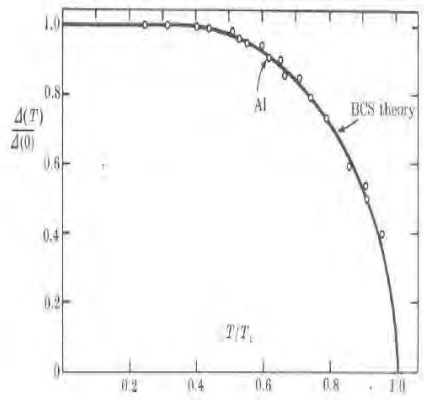

Figure 1.8: Temperature dependance of measured energy gap for various conventional superconductors. The curve is the BCS prediction[3]

described as fermions created by the $\gamma_k^\dagger$,which are in one to one correspondence with the $c_k^\dagger$ of the normal metal, then we can obtain the superconducting density of state N_s by equating

$$N_s dE = N_n d\xi \tag{1.4.31}$$

Since we are interested in energies ξ only a few milli electron volts from the fermi energy,we can takeN_ξ= , N(0) a constant .This leads directly to the simple result

$$\frac{N_s(E)}{N_n(0)} = \frac{d\xi}{dE} = \frac{E}{E^2 - \triangle^2}, E > \triangle$$

$$0, E < \triangle \tag{1.4.32}$$

The $\triangle_k$ is called the pairing potential or order parameter .One must solve $\triangle_k$ self consistently .

1.5 SUPERCONDUCTIVITY IN THIN FILM

Since 1960 researchers have explored the possibility that the superconducting properties of thin films may be superior to, or at least different from, those of bulk materials[5]. As the thickness of a thin film is reduced to the nano meter scale, the films surface and interface confine the motion of the electrons leading to the formation of discrete electronic states known as quantum well states .This quantum size effect changes the over all electronic structures of the thin film at small thickness, physical properties are thus expected to vary , often dramatically with thickness. Recent experimental studies have demonstrated such variation with film thickness for properties such as electronic density , electron -phonon coupling, surface energy, and thermal stability .The variations are expected to follow a damped oscillatory curve that is superimposed on a N^{γ} baseline (where N is the number of atomic layers in the film and the exponent γ is often close to 1). The superconducting transition temperature for a metal such as lead depends on the density of states and on electron-phonon coupling. It should thus also vary with film thickness. An oscillatory dependence of T_c on film thickness is a far more convincing proof for quantum size effects. Some prior studies suggested such oscillatory behavior , but the report by Guo et al[5]. is the first definitive and quantitative demonstration. Using atomically uniform films of lead with exactly known numbers of atomic layers deposited on a silicon (111) surface (see the figure 19), the authors observed oscillations in T_c that correlated well with the confined electronic structure. Their work has elevated this type of measurement to a new level of precision and sophistication. As the search for better superconducting materials continues, quantum size effects are an important avenue toward this goal. The oscillatory variation of the superconducting temperature for those metal can be

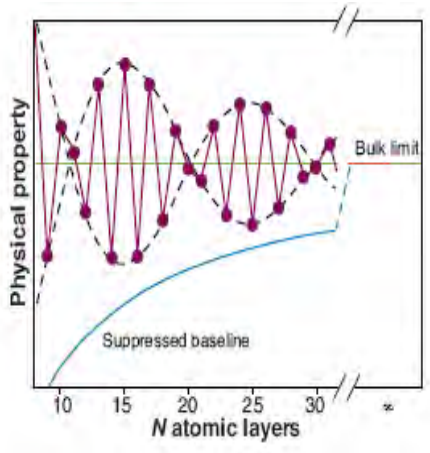

Figure 1.9: physical properties vs thickness[5]

understood qualitatively by means of a simple model of the quantum size effect in which the film is modeled by infinite or periodic boundary condition in the plane , freely moving carriers within the plane and the requirement that charge carrier do not leave the film at its surface .This corresponds to an infinite potential well in the vertical direction across the thickness of the film. Under these conditions the energy spectrum splits in to subbands denoted by a quantum number S.The density of state in such a thin film is of the form

$$D(\epsilon) = \frac{m}{\pi\hbar^2 t}[\frac{2t}{\lambda_F}] \tag{1.5.1}$$

where $[\frac{2t}{\lambda_F}]$ is the integer part of $\frac{2t}{\lambda_F}$ .Hence $D(\epsilon)$ decreases with increasing t as long as S= $[\frac{2t}{\lambda_F}]$ which is the number of filled subbands ,that stay the same .Here λ_F is the Fermi wave length and t, is the film thickness .At certain values of t a new susband opens up i.e $S \rightarrow S+1$ and the density of states increase by $\frac{m}{\pi\hbar^2 t}$ .This leads to a saw tooth like oscillation of the density of states as a function of t . The period of these

oscillation $\triangle t$ is given by

$$\triangle t = \frac{\lambda_F}{2} \tag{1.5.2}$$

Superconductivity is modified as a consequence of the dependence of the density of state on thickness . Electrons which are paired have equal and opposite momenta and belong to the same subband denoted by S .The oscillation in the density of state then leads to oscillation of the gap $\triangle$ and of T_c as a function of thickness .BCS models gives

$$T_c = 1.14\hbar w_D \exp[\frac{-1}{vD(\varepsilon)}] \tag{1.5.3}$$

and,

$$\triangle = 2\hbar w_D \exp[\frac{-1}{D(\varepsilon)v}] \tag{1.5.4}$$

where v is coupling constant, w_D is the Debye frequency and $D(\epsilon)$ is the density of state .The critical temperature and the gap would decrease monotonically with increasing film thickness, but the increase in S at certain thickness which causes jumps in these parameters . A saw tooth like variation of T_c and $\triangle$ as a function of thickness with the amplitude of the oscillation decreases with increasing film thickness is observed .

1.6 NANO MATERIALS

1.6.1 Definition

In their broadest definition, nanostructured materials show structural features with sizes in the range from 1nm to a few hundred nanometers in atleast one dimension. Nanostructured material is associated with a specific novel property or a significant improvement in a specific property resulting from the nanoscale structuring. For instance, opaque substances become transparent (copper); inert materials become

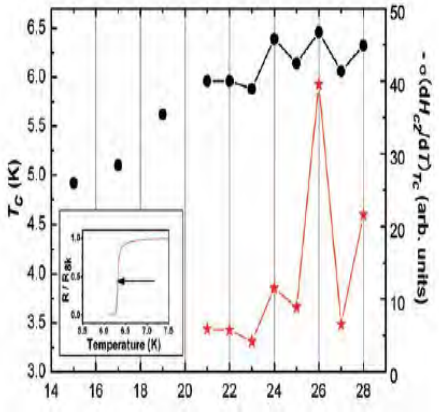

Figure 1.10: the oscillation the transition temperature T_c of Pb [4]

catalysts (platinum); stable materials turn combustible (aluminum); solids turn into liquids at room temperature (gold); insulators become conductors (silicon). A material such as gold, which is chemically inert at normal scales, can serve as a potent chemical catalyst at nanoscales. Much of the fascination with nanotechnology stems from these quantum and surface phenomena that matter exhibits at the nanoscale. As a consequence, the type of nanostructuring used must be based on a spatial dependence of some parameter related to the property under consideration. This parameter could be, for example, the material density, transport parameters, or the dielectric constant. Two main technological approaches may be defined:

1. The top-down manufacturing paradigm consists in down scaling the patterning of materials to nanometer sizes. This allows the generation of materials which are coherently and continuously ordered from macroscopic down to nanoscopic sizes. 2.The bottom-up paradigm is based on the atomically precise fabrication of entities of increasing size. It is the domain of macromolecular and supra molecular chemistry

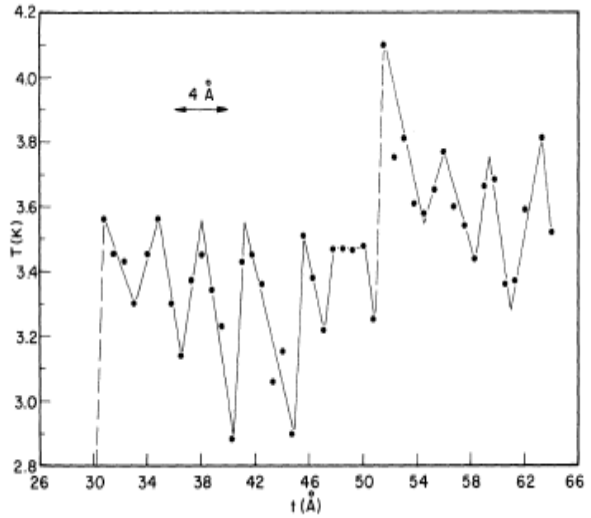

Figure 1.11: the oscillation the transition temperature T_c of Sn [7]

(dendrimers, engineered DNA, etc.) and of cluster and surface physics (epitaxy, self assembly, etc.). Most of the common nano materials can be classified in terms of dimensionality, according to the number of orthogonal directions X, Y, Z in which the structural patterns referred to above have dimensions $L_{X,Y,Z}$ smaller than the nano scopic limit L_0 . This leads to the classical definitions of dimensionality summarized in Table 1.1 below.The structure of the density of states (DOS) in nano structures is strongly dependent on the dimensionality. A free 3D motion yields a band characterized by three wavevectors k_x, k_y, k_z . The corresponding DOS depends smoothly on the energy E, as $(E - E_0)^{1/2}$, where E_0 is the energy of the bottom of the band. Confinement into a 2D system splits the band into subbands, and leaves only two continuously varying wave vectors k_x, k_y in each subband. The DOS for each subband is then constant above the energy E_0^N of its bottom state. The overall DOS is discontinuous,with a stepwise structure that is characteristic of quantum

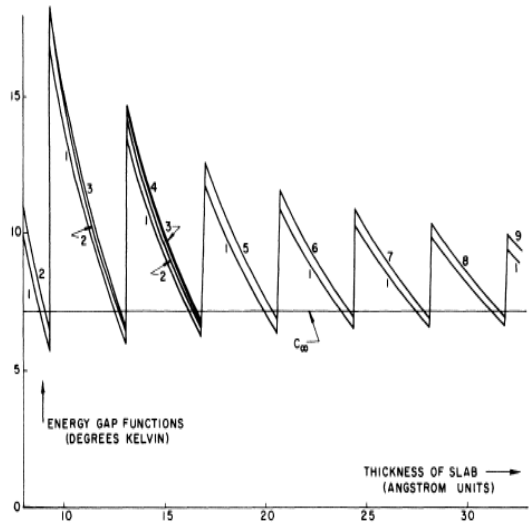

Figure 1.12: the superconducting energy gap vs thicknnes[8]

wells. Confinement in one additional dimension splits each 2D subband further into a set of 1D subbands. Each 1D subband is characterized by only one continuously varying wave vector k_x , and two quantum numbers N, M. The DOS corresponding to the subband N, and M has a variation of the form $(E - E_0^{N,M})^{-1/2}$, with a divergence at the bottom of the subband $E_0^{N,M}$. The DOS of a quantum wire thus has a more pronounced structure than does a 2D well, with a larger number of subbands, each one starting as a peak . Finally, confinement in all three dimensions creates a completely discrete, atom-like set of states. The DOS of a quantum dot thus consists of a series of $\delta functions$. The sharpening of the DOS at specific energies induced by quantum confinement is the origin of many improvements in the properties of nano structured materials compared with bulk materials.

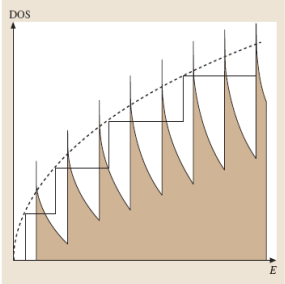

Figure 1.13: Density of state for 3D free electron (dashed line)2D quatum well (solid line),and 1D quntum wire (shaded line) as function energy[9]

1.6.2 SPECIFIC PROPERTIES

The specific properties of nano structured materials can have two different possible origins: Size effects, which result from the spatial confinement of a physical entity inside an element of the nanoscale structural pattern. Such an element is called a low-dimensional system. An example is the confinement of electron wave functions inside a region whose size is smaller than the electron mean free path. This class of effects may give birth to completely new properties. Boundary effects, which are a consequence of the significant volume fraction of matter one located near surfaces, interfaces, or domain walls. Processes that take place only at such locations may be highly favored, and properties specific to structural boundaries may also be greatly enhanced.

1.6.3 ELECTRONIC QUANTUM SIZE EFFECT

Confined electronic systems are quantum systems in which carriers, either electron or holes, are free to move only in a restricted number of dimensions. In the confined dimension, the sizes of the structural elements are of the order of a few de Broglie

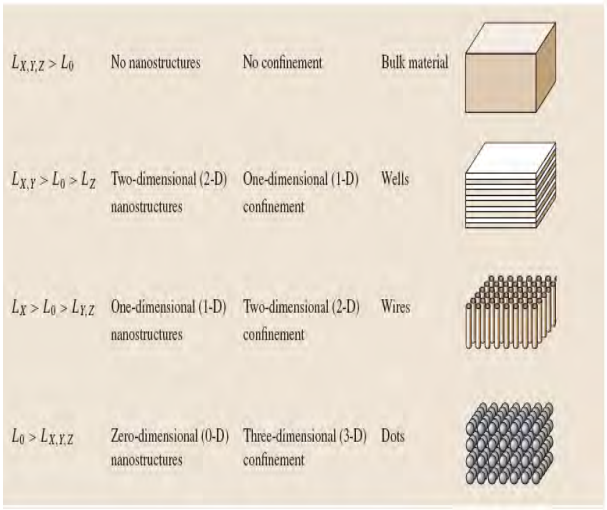

Figure 1.14: Types of nano structures[8]

wavelengths of the carriers or less. Depending on their dimensionality, these structures can be quantum dots (0-D), quantum wires (1-D), or quantum wells (2-D). One of the most dramatic effects, called the quantum size effect, consists in a redistribution of the energy spectrum of the system, the density of states becoming discrete along the confinement direction. In the most simple "particle in a box" model of a quantum well, the energies of the corresponding eigen states are

$$E_N, k_x, k_y = N^2 \frac{\hbar^2 \pi^2}{2md^2} + \frac{\hbar^2}{2m}(k_x^2 + k_y^2) \tag{1.6.1}$$

where m is the effective mass of the carrier, d is the confinement dimension, and N is a quantum number. The first term appears because of the quantized motion in the z direction, whereas the second term represents the energy of the free x, y motion, characterized by wave vectors k_x, k_y . Each value of N defines a semi infinite subband of energy levels. Although the "particle in a box" model is simplistic compared with real systems, this limiting case is often successful in describing the essential features of

quantum size effects . The importance of the quantum size effect is mainly determined by the energy differences $E_{N+1} - E_N$. Quantum size effects become observable when this separation exceeds the thermal energy of the carriers, so that adjacent sub bands are differently populated. Since the energy difference $E_{N+1} - E_N$ increases with N, it could be anticipated that quantization effects would be more important for processes involving higher sub bands[9].

Chapter 2

Mathematical formulation

2.1 Bogoliubov -de Gennes equation

We consider the case where an electron experiences an arbitrary external potential $U_0(r)$ (this will be important to describe the effects of impurities, specimen surface (sample surface) ,and magnetic[11] field. We define the creation and annihilation operators $\Psi^\dagger$ and Ψ respectively in real space as.

$$\Psi^\dagger(r\alpha) = \sum_k e^{-ik.r} a^\dagger_{k\alpha} \tag{2.1.1}$$

$$\Psi(r\alpha) = \sum_k e^{ik.r} a_{k\alpha} \tag{2.1.2}$$

Here $a^\dagger_{k\alpha}$ and $a_{k\alpha}$ are the creation and annihilation operators defined in the momentum space in the BCS theory .The $\Psi^\dagger(r\alpha)\Psi(r\alpha)$ creates (removes) an electron with spin $\alpha = \uparrow$ *or* $\downarrow$ from position $\overrightarrow{r}$. The operators Ψ satisfy the anticomutation rules .

$$\{\Psi(r\alpha), \Psi(r'\beta)\} = 0 \tag{2.1.3}$$

$$\{\Psi^\dagger(r\alpha), \Psi^\dagger(r'\beta)\} = 0 \tag{2.1.4}$$

$$\{\Psi^\dagger(r\alpha), \Psi(r'\beta)\} = \delta_{\alpha\beta}\delta(r - r') \tag{2.1.5}$$

the operator associated with the number of particle is

$$N = \sum_{k\alpha} a^{\dagger}_{k\alpha} a_{k\alpha} = \sum_{\alpha} \int dr \Psi^{\dagger}(r\alpha)\Psi(r\alpha) \tag{2.1.6}$$

Assuming a point like(pair wise) interaction in real space to describe s- wave coupling with coupling constant v, the Hamiltonian $\widehat{H}$ can be written as

$$\hat{H} = \hat{H}_o + \hat{H}_1 \tag{2.1.7}$$

$$\hat{H}_o = \sum_{\alpha} \int dr \Psi^{\dagger}(r\alpha)[\frac{(\hat{p} - \frac{e}{c}A)^2}{2m} + U_o(r)]\Psi(r\alpha) \tag{2.1.8}$$

$$\hat{H}_1 = \frac{-v}{2} \sum_{\alpha\beta} \int dr \Psi^{\dagger}(r\alpha)\Psi^{\dagger}(r\beta)\Psi(r\alpha)\Psi(r\beta) \tag{2.1.9}$$

where $\hat{p}$ is the momentum operator. The $\hat{H}_o$ above is a sum of the kinetic energy and single particle potential energy with the mass of an electron m_e . $U_o(r)$ includes crystal potential and surface potential(confining potential).The $\hat{H}_1$ models the electron-phonon interaction among cooper pairs. It will be useful to define

$$H_O - E_F N = \sum_{\alpha} \int dr \Psi^{\dagger}(r\alpha) H_e \Psi(r\alpha) \tag{2.1.10}$$

where

$$\hat{H}_e = \frac{1}{2m}(-i\hbar\nabla - \frac{eA}{c})^2 + u_o(r) - E_F \tag{2.1.11}$$

In the mean field approximation one writes the interaction in terms of effective two - body interaction.

$$\hat{H_{eff}} = \int dr[\sum_{\alpha} \Psi^{\dagger}(r\alpha)H_e\Psi(r\alpha) + U(r)\Psi^{\dagger}(r\alpha)\Psi(r\alpha) + \triangle(r)\Psi^{\dagger}(r\uparrow)\Psi^{\dagger}(r\downarrow) + \triangle^*(r)\Psi(r\downarrow)\Psi(r\uparrow)] \tag{2.1.12}$$

The U(r) is the Hartree - Fock potential arising from the pair interaction .The last two terms in eqn (2.1.12) are called anomalous term representing the pair scattering

.It can be noted that both of the two terms change the number of particles by two. The $\triangle(r)$ is the order parameter or the pairing potential, now depending on $\overrightarrow{r}$ .H_{eff} is quadratic from in $\Psi^{\dagger} and \Psi$ .we can diagonalize it by performing a unitary transformation .

$$\Psi^{\dagger}(r\uparrow) = \sum_{n} \gamma^{\dagger}_{n\uparrow} u^{*}_{n}(r) - v_{n}(r)\gamma_{n\downarrow} \tag{2.1.13}$$

$$\Psi^{\dagger}(r\downarrow) = \sum_{n} \gamma^{\dagger}_{n\downarrow} u^{*}_{n}(r) + v_{n}(r)\gamma_{n\uparrow} \tag{2.1.14}$$

$$\Psi(r\uparrow) = \sum_{n} \gamma_{n\uparrow} u_{n}(r) - v^{*}_{n}(r)\gamma^{\dagger}_{n\downarrow} \tag{2.1.15}$$

$$\Psi(r\downarrow) = \sum_{n} \gamma_{n\downarrow} u_{n}(r) + v^{*}_{n}(r)\gamma^{\dagger}_{n\uparrow} \tag{2.1.16}$$

where $\gamma^{\dagger}_{n\uparrow}$ creates a particle is the state n with spin up and $\gamma^{\dagger}_{n\downarrow}$ annihilates hole with spin down. u_n and v_n are electron and hole like wave fuctions of the quasi particle with quantum number n .Using the above unitary transformation the diagonalized effective Hamiltonian is given as

$$H_{eff} = \varepsilon_g + \sum_{n\alpha} \varepsilon_n \gamma^{\dagger}_{n\alpha}\gamma_{n\alpha} \tag{2.1.17}$$

Where ε_g is the ground state energy ε_n is energy eigen value of the quasi particle excitations .γ and $\gamma^{\dagger}$ are new operator (quasi particle operators still satisfying the fermions anticommutation relation) .

$$\{\gamma^{\dagger}_{n\alpha}, \gamma_{m\beta}\} = \delta_{nm}\delta_{\alpha\beta} \tag{2.1.18}$$

$$\{\gamma_{n\alpha}, \gamma_{m\beta}\} = 0 \tag{2.1.19}$$

Using egn (2.1.17) and egn (2.1.18,2.19), one can write

$$[H_{eff}, \gamma_{n\alpha}] = -\varepsilon_n \gamma_{n\alpha} \tag{2.1.20}$$

$$[H_{eff}, \gamma^{\dagger}_{n\alpha}] = \varepsilon_n \gamma^{\dagger}_{n\alpha} \tag{2.1.21}$$

Taking the commutator $[H_{eff}, \Psi]$, using the definition for H_{eff} and the anti comutatation propertities of Ψ, we obtain

$$[\Psi(r\uparrow), H_{eff}] = [H_e + U(r)]\Psi(r\uparrow) + \triangle(r)\Psi^{\dagger}(r\downarrow) \tag{2.1.22}$$

$$[\Psi(r\downarrow), H_{eff}] = [H_e + U(r)]\Psi(r\downarrow) + \triangle(r)\Psi^{\dagger}(r\uparrow) \tag{2.1.23}$$

In this equality, we replace the Ψ's by γ's , and then we apply the anticommutation of γ 's. Comparing the coefficients of γ_n and $\gamma^{\dagger}_n$) on the two side of the equation ,we obtain the Bogoliubov -de Gennes equation is given by

$$\varepsilon_n u_n(r) = [H_e + U(r)]u_n(r) + \triangle(r)v_n(r) \tag{2.1.24}$$

$$\varepsilon_n v_n(r) = -[H_e + U(r)]v_n(r) + \triangle(r)u_n(r) \tag{2.1.25}$$

The $\begin{pmatrix} u_n \\ v_n \end{pmatrix}$ are eigen function of a linear system with corresponding eigen values ε_n

$$\varepsilon \begin{pmatrix} u \\ v \end{pmatrix} = \Omega \begin{pmatrix} u \\ v \end{pmatrix} \tag{2.1.26}$$

Ω is hermitian operator and the eigen functions $\begin{pmatrix} u \\ v \end{pmatrix}$ are orthogonal, and if $\begin{pmatrix} u \\ v \end{pmatrix}$ is the solution ε, $\begin{pmatrix} u^* \\ v^* \end{pmatrix}$ is the soln for the eigen value -ε . We now determine H_{eff} by requiring that the free energy F calculated from the states which diagonalized H_{eff} be stationary. By definition

$$F = < H > -TS \tag{2.1.27}$$

where H is the initial Hamiltonian, $H = H_O + H_1$ and the average $< H >$ is given by

$$< H >= \frac{\sum_{\Phi} < \Phi|H|\Phi > \exp(-\beta E_{\Phi})}{\sum_{\Phi} \exp(-\beta E_{\Phi})} \tag{2.1.28}$$

The matrix elements are taken with respect to the eigen functions $|\Phi>$ of H_{eff}

$$H_{eff}|\Phi>=\epsilon_{\Phi}|\Phi> \tag{2.1.29}$$

a general method to calculate $< H >$ is to replace the Φ 's by γ's according to (2.1.17), then to use the mean value rules

$$<\gamma^{\dagger}_{n\alpha}\gamma_{m\beta}>=\delta_{nm}\delta_{\alpha\beta}f_n \tag{2.1.30}$$

$$<\gamma_{n\alpha}\gamma_{m\beta}>=0 \tag{2.1.31}$$

$$f_n=\frac{1}{e^{\beta\epsilon_n}+1} \tag{2.1.32}$$

However it will not be necessary to perform this entire calculation. we write $< H >$ in the form of

$$\begin{aligned} < H >&=\sum_{\alpha}\int dr < \Psi^{\dagger}(r\alpha)H_e\Psi(r\alpha) > \\ &\frac{-v}{2}\sum_{\alpha\beta} < \Psi^{\dagger}(r\alpha)\Psi^{\dagger}(r\beta)\Psi(r\alpha)\Psi(r\beta) > \end{aligned} \tag{2.1.33}$$

the product $< \Psi^{\dagger}\Psi^{\dagger}\Psi\Psi >$ can be simplified by Wick theorem which makes use of only the fact that $\Psi^{\dagger}$ and Ψ are linear function of $\gamma^{\dagger}, and\gamma$ .the theorem gives

$$\begin{aligned} &< \Psi^{\dagger}(1)\Psi^{\dagger}(2)\Psi(3)\Psi(4) >=< \Psi^{\dagger}(1)\Psi(4) >< \Psi^{\dagger}(2)\Psi(3) > \\ &- < \Psi^{\dagger}(1)\Psi(3) >< \Psi^{\dagger}(2)\Psi(4) > - < \Psi^{\dagger}(1)\Psi^{\dagger}(2) >< \Psi(3)\Psi(4) > \end{aligned} \tag{2.1.34}$$

We now vary the amplitudes $\begin{pmatrix} u \\ v \end{pmatrix}$ to $\begin{pmatrix} \delta u \\ \delta v \end{pmatrix}$ and the occupation number f_n to δf_n . The free energy then varies by δF as :

$$\delta F=\int dr\{\sum_{\alpha}\delta[< \Psi^{\dagger}(r\alpha)H_e\Psi(r\alpha) >]-v\sum_{\alpha\beta} < \Psi^{\dagger}(r\alpha)\Psi(r\alpha) > \delta[< \Psi^{\dagger}(r\beta)\Psi(r\beta) >]$$

$$+v\sum_{\alpha} < \Psi^{\dagger}(r\alpha)\Psi(r\alpha) > \delta[< \Psi^{\dagger}(r\alpha)\Psi(r\alpha) >]$$

$$-v[< \Psi^{\dagger}(r\uparrow)\Psi^{\dagger}(r\downarrow) > \delta(< \Psi(r\downarrow)\Psi(r\uparrow) >) + c.c]\} - T\delta s \tag{2.1.35}$$

where we have assumed $< \Psi^{\dagger}(r\uparrow)\Psi(r\downarrow) >= 0$, as it is correct in our non magnetic case,Now notice that the equality

$$F_1 =< H_{eff} > -TS \tag{2.1.36}$$

It is stationary with respect to $\delta u_n, \delta v_n$,and δf_n since our excitations diagonalize H_{eff} exactly. Using $\Psi's$ in terms of γ , this condition becomes explicitly

$$0 = \delta < H_{eff} > -T\delta S = \int dr\{\sum_{\alpha} \delta < \Psi^{\dagger}(r\alpha)H_e + U(r)\Psi(r\alpha) > +$$

$$\triangle(r)\delta(< \Psi^{\dagger}(r\uparrow)\Psi^{\dagger}(r\downarrow) >) + c.c\} - T\delta S \tag{2.1.37}$$

Comparing eqn (2.1.35) and (2.1.36), we see that F will be stationary if we take as effects potentials

$$U(r) = -v < \Psi^{\dagger}(r\uparrow)\Psi(r\uparrow) >= -v < \Psi^{\dagger}(r\downarrow)\Psi(r\downarrow) > \tag{2.1.38}$$

(the standard Hatree -Fock results for a point interaction), and

$$\triangle(r) =< \Psi(r\downarrow)\Psi(r\uparrow) >= -v < \Psi(r\uparrow)\Psi(r\downarrow) > \tag{2.1.39}$$

If we replace the $\Psi's$ by $\gamma's$ and if we use the mean values of eqn (2.1.30,2.1.31,2.1.31),we can put these conditions in to the explicit form

$$U(r) = -v\sum_{n}[|u_n(r)|^2 f_n + |v_n(r)|^2(1 - f_n)] \tag{2.1.40}$$

$$\triangle(r) = v\sum_{n} u_n v_n^*(1 - 2f_n) \tag{2.1.41}$$

these condtion assume that the potential U and $\triangle$ are self consistent.The density of particles is given by

$$n = 2 < \Psi^{\dagger}(r\uparrow)\Psi(r\uparrow) >= 2\sum_{n}[|u_n(r)|^2 f_n + |v_n(r)|^2(1-f_n)] \tag{2.1.42}$$

It is a combination of the contribution from hole and particle. $\triangle$ can be considered as pairing potential that couples the electron and holes .It is important to realize that the difference between $\triangle_k$ in the BCS theory and $\triangle(r)$ in BDG theory. The former is the energy gap to creat quasi particle excitation in state$\vec{k}$,while the later can not considered as energy gap, since it is a function of position.Throughout this work, we consider isotropic s-wave pairing. In this case, there is no Fock (exchange) interaction and the Hartree interaction simply shifts the energy levels. Therefore ,the Hartree-Fock potential U is neglected in this thesis.

Chapter 3

SUPERCONDUCTIVTY OF NANO STRUCTURES

3.1 INTRODUCTION

Increasing the critical temperature T_c of a superconductor has been a major challenge. On the one hand one can look for different materials that exhibit a higher T_c. Such a search has been very successful over the last 20 years. On the other hand micro structuring of a superconductor is a different and new road that is able to modify T_c (i.e. increase or decrease it) and may also give us further insight in the basic mechanism of superconductivity. In earlier works on micro structuring of a superconductor in the mesoscopic regime, enhancement of the critical current j_c was demonstrated to occur due to trapping of vortices. Also a large increase of the critical magnetic field H_c was realized through such mesoscopic structuring, which is mostly a consequence of surface superconductivity. But in both cases the zero-magnetic-field critical temperature was unaltered .In nano structures which are a few nano meter size , in one or more direction , exhibits quantum confinement which influence many physical properties such as superconductivity . Controlling of size and shape of the carrier

confinement favors the enhancement of superconductivity and also leads to oscillatory behavior of superconducting property. During the last decade nanowires have attracted much attention in the context of phase fluctuations of the order parameter (i.e, quantum phase slips) in the longitudnal direction. Blatt and Thompson calculated a remarkable sequence of peaks in the thickness dependence of the energy-gap parameter of single-crystalline superconducting nanofilms in the clean limit. They called these spikes shape resonances.

Recent advances in nanofabrication technology resulted in nanoscale structures like wires with width about 10 nm and films with thickness of a few monolayers . In particular, superconducting metallic nanowires or nanofilms are now attainable with electron mean free path being about the specimen width or thickness . To a great extent such nanoscale superconducting specimens can be considered as being in the clean limit. In this case nonmagnetic impurities can only influence the electron motion parallel to the wire or film. Arguments similar to the Anderson theorem [2] make it possible to expect that the longitudinal scattering of electrons on such nonmagnetic imperfections do not have a significant effect on the superconducting characteristics in the clean limit. Since the classical papers by Gorkov and Bogoliubov [2]it is known that the superconducting order parameter can be interpreted as the wave function describing the center of- mass motion of a Cooper pair. The Cooper-pair wave function is influenced by the surrounding electrons of the Fermi sea so that the single-fermion states with energies well below the Fermi level do not make any essential contribution to the order parameter. As a result, $\triangle(r)$ will depend on the density of the single-fermion states (per unit volume and per spin projection)situated in the Deybe "window " around the fermi level $\{E_F - \hbar w_D, E_F + \hbar w_D\}$

, where w_D is the Debye frequency. Quantum confinement of electron in the clean nano wires and nano films results in a splitting of the band of single-electron states in a series of subbands that shifts in energy with changing wire or film thickness.This shift leads to quantum-size oscillations in the mean density of single-electron states. When the bottom of such a subband passes through the Fermi surface, the density of states increases abruptly and a size-dependent superconductivity resonance comes into play . So, any superconducting property $(T_c, \triangle)$ exhibits quantum- size oscillations. The resonant enhancements and , quantum-size oscillations are substantial in the nanoscale regime and decay with increasing wire/film thickness. Thus, following Blatt and Thompson articles [7] the enhancement of superconductivity due to the passage of subbands through the Fermi surface can be called a shape(size) superconducting resonance.In agreement with these expectations, photoelectron spectroscopy has demonstrated clear signatures of the formation of such QWS's in thin crystalline metallic films.

3.2 Bogoliubov-de Gennes equation

A direct consequence of quantum confinement is a nonuniform spatial distribution of the superconducting order parameter $\triangle = \triangle(r)$. It is well known that, the Bogoliubov-de Gennes (BdG) equations are a very powerful formalism which is able to describe a position-dependent parameter(in our case the order parameters). In the absence of a magnetic field $\triangle(r)$ can be chosen as a real quantity, and the BdG equations read as

$$\begin{pmatrix} H_e & \triangle(r) \\ \triangle(r) & -H_e \end{pmatrix} \begin{pmatrix} u_n(r) \\ v_n(r) \end{pmatrix} = E_n \begin{pmatrix} u_n(r) \\ v_n(r) \end{pmatrix} \tag{3.2.1}$$

where E_n is the quasi particle energy ,and $u_i, and v_i$ are the particle and hole like wave functions respectively .The single electron hamilitonian is given by

$$H_e = \frac{-\hbar^2}{2m}\nabla^2 + U_0(r) - \mu \tag{3.2.2}$$

with μ the chemical potential and m the electrn band mass(set to the free electron mass for isotropic case). To study quantum-size effects, a crystalline nano film and nano wire in the clean limit in the confinement direction are considered i.e ($\ell_e \geq$ the thickness or width) .The periodic lattice potential is taken into consideration by introducing the electron band mass i.e, the parabolic band (PB) approximation.The order parameter (pairing potential) is related to the eigenfunctions $u_i(r)$ and $v_i(r)$ through

$$\triangle(r) = v\sum_n u_n(r)v_n^*(r)(1-2f_n) \tag{3.2.3}$$

with v the coupling constant and $f_n = f(E_n)$

$$f_n = \frac{1}{e^{\beta E_n}+1} \tag{3.2.4}$$

is the fermi function ($\beta = \frac{1}{k_B T}$ with T the temperature and k_B the Boltzmann constant .The sum in eqn(3.2.3)is over all positive energies E_n , but in addition it is limited to the Debye window of the single-electron energies $|\xi_n| < \hbar w_D$, where w_D is the Debye frequency. The BdG equations(3.2.1) should be solved together with the self-consistency relations(3.2.3)for a given chemical potential which is determined by

$$n_e = \frac{2}{V}\int dr^3 \sum_n [|u_n(r)|^2 f_n + |v_n(r)|^2(1-f_n)] \tag{3.2.5}$$

where n_e is the mean electron density and V is the volume of the wire / film .The sum in eqn (3.2.5)is over states with positive E_n .

3.3 NANO FILMS

we use the periodic boundary condition in the plane of the film in this case $\triangle(r) = \triangle(z)$,then the eigen wave functions are

$$u_n(r) = \frac{e^{ik_y y}}{\sqrt{L_y}} \frac{e^{ik_x x}}{\sqrt{L_x}} \widetilde{u}_n(z) \tag{3.3.1}$$

$$v_n(r) = \frac{e^{ik_y y}}{\sqrt{L_y}} \frac{e^{ik_x x}}{\sqrt{L_x}} \widetilde{u}_n(z) \tag{3.3.2}$$

where $n = (k_x, k_y, j)$ with k_x and k_y the free electron wave vector in (x,y) direction and j the quantum number related to the electron motion in the z direction normal to the film. Due to the electron confinement in the z direction

$$\tilde{u_n}(z) = \tilde{u_n}(0) = 0, \tilde{v_n}(z) = \tilde{v_n}(0) = 0 \tag{3.3.3}$$

The eigen functions $\tilde{u_n}$,$\tilde{v_n}$ and $\triangle(z)$ can be expanded in the quantum well state given by

$$\Phi_\ell(z) = \sqrt{\frac{2}{L_z}} \sin(\frac{\Pi(\ell+1)}{L_z})z \tag{3.3.4}$$

the BdG equation takes the form given below

$$E_n \widetilde{u}_n^\ell = [\frac{\hbar^2}{2m}(\frac{\pi^2(\ell+1)^2}{L_z^2} + k_x^2 + k_y^2) - \mu]\widetilde{u}_n^\ell + \sum_{\ell'} \triangle_{\ell\ell'} \widetilde{v}_n^{\ell'}) \tag{3.3.5}$$

$$E_n \widetilde{v}_n^\ell = [\frac{\hbar^2}{2m}(\frac{\pi^2(\ell+1)^2}{L_z^2} + k_x^2 + k_y^2) - \mu]\widetilde{v}_n^\ell + \sum_{\ell'} \triangle_{\ell\ell'} \widetilde{u}_n^{\ell'}) \tag{3.3.6}$$

with

$$\triangle_{\ell\ell'} = \int dz \Phi_\ell^*(z) \triangle(z) \Phi_\ell(z) \tag{3.3.7}$$

Note that $\triangle(z)$ is expressed in terms of $\widetilde{u}_n(z)$ and $\widetilde{v}_n(z)$ by means of eqn (3.2.3) where $u_n(r)$ and $u_n(r)$ are replaced by $\widetilde{u}_n(z)$ and $\widetilde{v}_n(z)$. equations(3.3.7 and 3.3.8) were solved numerically by converting these equations in to matrix form and using iterations until full self-consistency was reached. At the first iteration the bulk values for pair potentials $\triangle(z) = \triangle_{bulk}$ is taken. At each iteration step the eigenvalues E_n and corresponding eigenvectors $(\widetilde{u}_n^0, ...\widetilde{u}_n^\ell, \widetilde{v}_n^0, ...\widetilde{v}_n^\ell)$ were calculated by transforming the governing matrix to a diagonal form and then new values of $\triangle(z)$ were found through eqn (3.2.3).The thickness-dependent superconducting temperature T_c was found as the point above which $\triangle(z) = 0$ is the only solution of eqns (3.3.7 and 3.3.8).

3.4 NANO WIRES

Introducing the cylindrical coordinates ρ ,θ, z, we can write $\triangle(r) = \triangle(\rho)$, and the periodical boundary conditions are implied in the longitudinal (z) direction, the eigen wave functions are

$$u_n(r) = \frac{e^{ik_z z}}{\sqrt{L_z}} \frac{e^{im\theta}}{\sqrt{2\pi}} \widetilde{u}_n(\rho) \tag{3.4.1}$$

$$u_n(r) = \frac{e^{ik_z z}}{\sqrt{L_z}} \frac{e^{im\theta}}{\sqrt{2\pi}} \widetilde{u}_n(\rho) \tag{3.4.2}$$

where n =(j,m,k) with j the quantum number associated with the ρ coordinate, m the azimuthal quantum number, and k the wave vector in the z direction. Substituting eqns (3.4.1 and 3.4.2) into eqn (3.2.1) ,the BdG equations takes the form given below

$$E_n \tilde{u}_n(\rho) = [\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial^2 \rho} + \frac{\partial}{\partial \rho}\frac{1}{\rho} - \frac{m^2}{\rho^2} - k^2) - \mu]\tilde{u}_n(\rho)$$

$$+\triangle(\rho)\tilde{u}_n(\rho) \tag{3.4.3}$$

$$E_n\tilde{v}_n(\rho) = [\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial^2\rho} + \frac{\partial}{\partial\rho}\frac{1}{\rho} - \frac{m^2}{\rho^2} - k^2) - \mu]\tilde{v}_n(\rho) + \triangle(\rho)\tilde{u}_n(\rho) \tag{3.4.4}$$

Due to the elecron confinement in the transvere direction , we should put

$$\tilde{u_n}(\rho) = \tilde{u_n}(0) = 0, \tilde{v_n}(\rho) = \tilde{v_n}(0) = 0 \tag{3.4.5}$$

Then, $\tilde{u_n}(r)$ and $\tilde{v_n}(r)$ functions are expanded in terms of the Bessel functions as follows

$$\tilde{u}_n(\rho) = \sum_j \Phi_{jm}(\rho)u^n_{jm} \tag{3.4.6}$$

$$\tilde{v}_n(\rho) = \sum_j \Phi_{jm}(\rho)v^n_{jm} \tag{3.4.7}$$

where the orthonormal bessel fuction is given by

$$\Phi_{jm}(\rho) = \frac{\sqrt{2}}{RJ_{m+1}(\alpha_{mj})}J_m(\frac{\alpha_{mj}}{R}) \tag{3.4.8}$$

where J_m is the m^{th} order and α_{mj} its j^{th} zero .Using eqn (3.4.8)in eqn (3.4.3and 3.4.4) , the BDG will be written as

$$E_n\tilde{u}^n_{jm} = [\frac{\hbar^2}{2m}(\frac{\alpha^2_{jm}}{R^2} + k^2 - \mu]\tilde{u}^n_{jm} + \sum_{j'} \triangle_{mjj'}\tilde{v}^n_{jm} \tag{3.4.9}$$

$$E_n\tilde{v}^n_{jm} = [\frac{\hbar^2}{2m}(\frac{\alpha^2_{jm}}{R^2} + k^2 - \mu]\tilde{v}^n_{jm} + \sum_{j'} \triangle_{mjj'}\tilde{u}^n_{jm} \tag{3.4.10}$$

where

$$\triangle_{mjj'} = \int_0^R \Phi_{jm}(\rho)\triangle(\rho)\Phi_{jm}(\rho)d\rho \tag{3.4.11}$$

In the BdG equation ,states with the energy range$[\hbar w_D, \hbar w_D]$ are included.There fore j varies from 1 to N_ℓ (the maximam number of j) for a given m,defined by

$$|\frac{\hbar^2}{2m}\frac{\alpha_{jm}^2}{R^2} - \mu| < \hbar w_D \tag{3.4.12}$$

And eqns (3.4.9 and 3.4.10) are reduced $2N_jX2N_j$ matrix for the expansion coefficent for each angular momemtum m. Using iteration procedure until self-consistent solution is obtained ,we can find the values $\triangle(\rho)$ and T_c at a given radius. To obtain the correct quantum-size oscillations in the physical properties of nano-superconductors when studied within the parabolic band approximation (based on the band mass m_e) , one should use the effective Fermi level rather than the true one . The effective Fermi level is determined by the band structure in the presence of quantum confinement and, so, it depends on the interplay between the crystal and confinement directions.

Chapter 4

4.1 Results and Discussion

We have used the following parameters $\mu_{bulk} = 0.93ev$, N(0)v=0.39 , where $N(0) = \frac{mk_F}{2\pi^2\hbar^2}$ is the bulk density of state at the fermi surface, and $\frac{\hbar w_D}{k_B} = 96K$ .Fig (4.2) represents the numerical solution of the self consistent Bogoliubovde Gennes equation for $\frac{T_c}{T_{bulk}}$ for pb nano film taking $L_x = L_y = 800nm$ to cosinder the bulk limit , where the L_z varies ,and fig (4.1) represents the numerical value of the self consistent Bogoliubovde Gennes equation for $\frac{T_c}{T_{bulk}}$ of Pb nano wire ,where $L = 800nm$ and R varies.As it is shown in the figures the superconducting temperature increases at a resonant point above its bulk value T_cbulk and, then, decreases slightly below T_cbulk ,and the resonance of T_c for Pb nano wire is greater than that of nano film. It is also shown,quantum-size oscillations are washed out with increasing thickness.

4.2 Conclusion

To conclude, quantum confinement is the major effect governing the superconducting properties of a clean nanoscale specimen. Based on a numerical solution of the Bogoliubovde Gennes equations, we investigated how the superconducting properties of

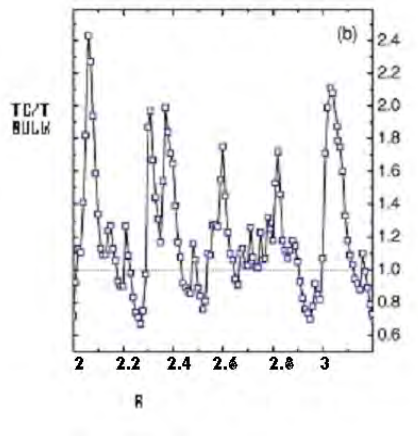

Figure 4.1: Oscillation of transition temperature for Pb nano wire

a nanoscale specimen depend on the confining geometry. We investigated the width-dependence of superconducting resonances responsible for the remarkable quantum-size oscillations of the superconducting properties typical for nanoscale superconductivity and first calculated by Blatt and Thompson [8]for a thin superconducting slab Recently, such oscillations were observed in experiments with Pb(111)[5].We believe that the nontrivial interplay of the quantum-size and quantum-shape effects can be a possible avenue towards an optimal design of future nanostructured superconducting devices.

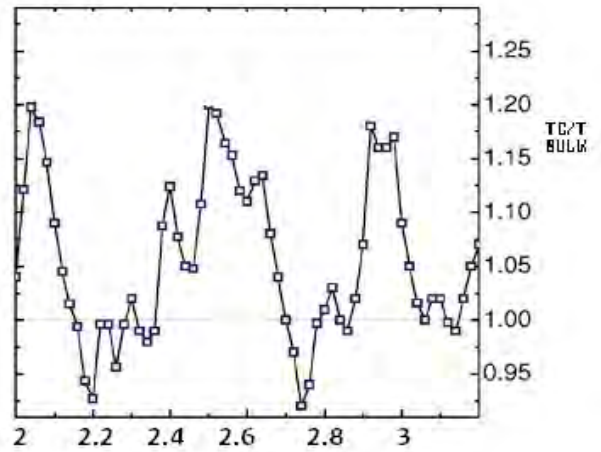

Figure 4.2: Oscillation of transition temperature for Pb nano film

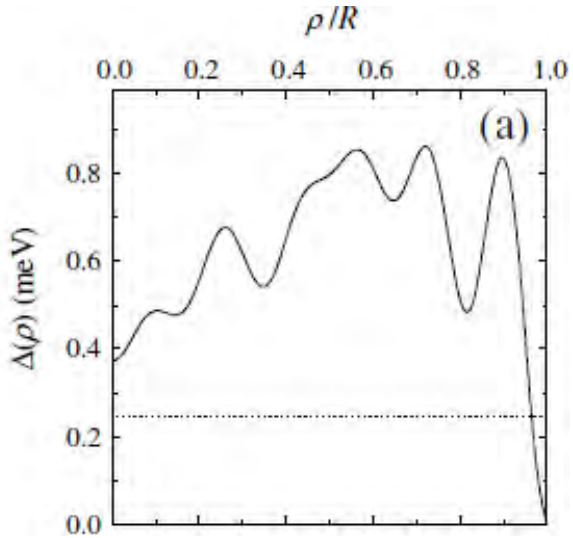

Figure 4.3: Oscillation of parameter for Pb nano wire

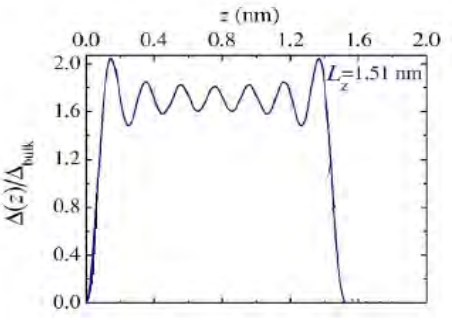

Figure 4.4: Oscillation order paramter for Pb nano film

Bibliography

[1] G.Rickazen, *T*heory of superconductivty, intersciencepublishers , New york, (1966).

[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev, **108**, 1175 (1957)

[3] Michael Tinkham, *I*ntroduction to Superconductivity, Dover publication, INC, Minneola, New York,2^{nd} edition.

[4] Introduction: Phenomenon of Superconductivity Alexey Ustinov Physikalisches Institut University of Erlangen ustinov@physik.uni-erlangen.de

[5] Yang Guo, Yan-Feng Zhang, Xin-Yu Bao, Tie-Zhu Han,Zhe Tang, Li-Xin Zhang, Wen-Guang Zhu,1 E. G. Wang, Qian Niu,Z. Q. Qiu, Jin-Feng Jia, Zhong-Xian Zhao, Qi-Kun Xue, Science , **306**, 1915(2004).

[6] Yan-Feng Zhang, Jin-Feng Jia, Tie-Zhu Han, Zhe Tang, Quan-Tong Shen, Yang Guo, Z. Q. Qiu, and Qi-Kun Xue1,Phys. Rev, **95**, 096802(2006).

[7] B.G.Orr,H.M.Jaeger,and A.M.Goldman , Phys. Rev Letter, **53**, 2046(1984).

[8] JohnM.Blatt and ColinJ.Thompson, Phys. Rev Letter, **10**, 332(1963).

[9] http://www.springer.com/978-3-540-44376-6

[10] J. S. Blakmore, *S*olid State Physics, Cambridge University Press, London, 2^{nd} Edition, (1974).

[11] C. Kittle, *Introduction to solid state physics*, John Wieley and Sons Inc, New York, 6^{th} edition, (1998).

[12] Yuri. M. Galperin, *I*ntroduction to Modern Solid State Phyiscs, Blidern, Oslo.

[13] Shigeji Fujita and Slavador Godoy, *Q*uantum Statistical Theory of Superconductivity, Plenum Press, New York and London, (1996).

[14] J. R. Hook and H. E. Hall, *S*olid State Physics, John Wieley and Sons Inc, New York, revised reprinting 2^{nd} edition (1987).

[15] L. N. Cooper, Phys. Rev, **104**, 1189 (1956).

[16] H. Frohlich, Phys. Rev, **79**, 845(1950).

[17] C. Kittle, *Q*uantum Theory of Solid State, John Wieley and Sons Inc, New York, revised reprinting 2^{nd} edition, (1987).

[18] Taylor and Heinonen, *A* Quantum Approach to Condenced Matter Physics, John Wieley and Sons Inc, New York.

[19] Joseph Callway, *Q*uantum Theory of Solid State, Academic Press, USA.

[20] N. W. Ashcroft/ Mermin, *S*olid State physics, Holt, Rinehart and Wiston, New York, (1976). .

[21] C. M. Wei, and M. Y. Chou, Phys. Rev B, **66**, 233408 (1957).

[22] Xin-Yu Bao,Yan-Feng Zhang,Yupeng Wang, Jin-Feng Jia, Qi-Kun Xue, X. C. Xie, and Zhong-Xian Zhao, Phys. Rev Letter, **95**, 0247005(2006)

[23] T. Ishiguro, K. Yamaji and G. Salito, *O*rganic Superconductors , Springer, 2^{nd} edition, (1997).

Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

Name: Fikreselassie Teklay Brhane

Signature:

Place and time of submission: Addis Ababa University, June 2009

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

Name: Proffessor Singh.P

Signature: