THE EFFECT OF SCREENING ON THE THERMAL RESISTIVITY OF METALS

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CERTIFICATION

I certify that this research work was carried out by Mr. Adesakin Gbenga Elijah (PHY/05/7473) and has been approved as meeting the requirements of the Department of Physics, School of Sciences, Federal University of Technology, Akure, Nigeria for the award of Master of Technology (M. Tech) in Physics and to the best of my knowledge has not been submitted elsewhere for the award of a degree.

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Supervisor

13/11/08

Date

DEDICATION

Dedicated to God Almighty and to the Holy Spirit, my greatest teacher, who has been my source of inspiration. And in loving memory of my late father Chief Samuel Adesakin, may his gentle soul rest in perfect peace.

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ABSTRACT

A model for calculating electron-electron interaction, compressibility ratio, screening parameter and thermal resistivity of metals was proposed by using an interaction potential. A FOTRAN 90 computer programme was developed based on the model to calculate the properties of metals. The effect of screening on the compressibility ratio, and thermal resistivity of metals was studied. Results obtained revealed that the screened interaction potential in metals is effective within a distance of 1Å and depends directly on the electron concentration of the metals. The electron - electron interaction increases slightly with electron-gas parameter. The compressibility ratio decreases with an increase in the electron gas parameter, also the screening parameter increases with an increase in the electron gas parameter. The thermal resistivity increases with an increase in the electron gas parameter. It also increases with an increase in the screening parameter showing that the screening in metals affects the thermal resistivity of metals. The results obtained in the work revealed that thermal resistivity of metals increase with increase in temperature in agreement with theoretical predictions.

TABLE OF CONTENTS

LIST OF FIGURE

CHAPTER ONE

INTRODUCTION

Metals are of tremendous scientific, industrial and technological applications. Metals usually have crystalline structure and are good thermal and electrical conductors.

The physical properties of metals such as: electrical and electronic properties, magnetic properties and thermal properties make them functional materials. The physical properties of metals are as a result of their numbers of free electrons and how these free electrons are bound in metals.

Transport properties of metals are explained based on the free conduction theory. At room temperature and above, the transport properties of metals are dominated by the free or conduction electron. At low temperatures, the lattice or photon contribution comes into play.

As the electrons in the metals move as a result of thermal excitation of applied electric field, the electrons move and collide with one another. This collision gives rise to resistivity. Increase in temperature increases the rate of collision of the electrons.

Metals are good thermal conductors as a result of their free electrons. As these free electrons move into the metal to conduct heat, they collide with one another (electron-electron collision), they also collide with the phonons (electron-phonon collision), these collisions reduce the rate of thermal conductivity of the metals and gives rise to thermal resistivity.

Electron-electron interaction is manifest through screening. Screening accounts for and explains how electrons interact in metals. These are different screening theories that produce different screening parameters. But not all the screening parameters can produce values that are in good agreement with experimental values.

Considering the fact that screening affects how electrons behave in metals and the relevance of thermal resistivity in metals, it becomes necessary that the effect of screening on thermal

resistivity of metals should be studied to provide an insight on the physical properties of metals that give rise to screening affects the thermal resistivity of metals.

1.1 OBJECTIVE OF THE RESEARCH

The objective of this work is to

i. develop a model potential and screen the potential.

ii. use the screened potential to study electron-electron interaction in metals.

iii. calculate the Thomas Fermi screening parameters for metals.

iv. calculate the thermal resistivity of metals and study how electron-electron screening affects the thermal resistivity of metals. Compare the calculated thermal resistivity with available experimental values.

1.2 SIGNIFICANCE OF THE STUDY

The significance of the study are:

i. this study will provide a model that can be used to explain how electron-electron interaction affects the properties of metals.

ii. the study will provide a first hand data on the screening parameter of metals that are very important in computational condensed matter physics.

iii. the study will provide numerical values for the thermal resistivity of metals which can guide experimentalist and act as reference.

iv. this study will give the relationship between electron-electron screening and thermal resistivity of metals.

1.3 JUSTIFICATION FOR THE RESEARCH

The thermal resistivity of metals and alloys is a very important property that affects their industrial and technological applications. Electron-electron interaction is an important phenomenon that affects many properties of metals and alloys.

Considering the relevance of thermal resistivity to electron-electron interaction in explaining the properties of metals, the development of a model to explain and study electron-electron interaction in metals becomes a necessity. Also, calculation of thermal resistivity of metals and studying how screening in metals affects thermal resistivity becomes very relevant.

1.4 FREE-ELECTRON MODEL

At about 1900 the hypothesis of the free-electron gas was first used by Drude to explain both the optical properties and the high electrical and thermal conductivities of metals. He assumed that the valence electrons in a metal were able to move freely in the crystal and, at the temperature T of th crystal they behave like the particles of an ideal gas (hence the name "free electron model"). In the free-electron model, all electron-electron and electron-ion interactions are neglected.

In the following years Lorentz improved the model by assuming a Maxwell-Boltzman distribution for the electron velocity. The assumption of a Maxwell-Boltzmann gas, however, proved inconsistent with measurements of specific heat capacities of metals since such a gas of N electrons should give a contribution to the specific heat of 3NK/2. There was experimental proof (e.g measurements of the Hall Effect) that the electron concentration is of the order of the concentration of the atoms. According to this, the electronic contribution to the specific heat capacity of metals should be comparable to the Dulong-Petit value of the lattice heat, hence the total specific heat of a metal above the debye temperature θ should then be (3+3/2)NK. However,

metals also show a good agreement of their measured specific heat capacity with the Dulong-Petit value at 3NK. This indicates that the electron gas cannot be considered to be an ideal Maxwell-Boltzmann gas.

The basic assumption of Drude were qualitatively correct and were used in later theories. Experiments have shown that the metals are actually pure electronic conductors, without additional ion conduction, and electrolytic experiments showed that no mass transport occurs. The presence of alternating currents could be proved in metallic bodies which were rapidly moved to and fro. These currents are due to the inertia of the moving carriers. The specific charge of the carriers determined from these experiments were in perfect agreement within the limits of experimental errors with the values measured for free electrons in cathode rays. (Busch and Schade, 1976).

According to the free electron theory the nuclei and inner core electrons of a metal are fixed in their lattice sites in a crystal. The electrons are assumed not to interact with each other or with the nuclei at the lattice site. According to the free electron theory, electrons fill all the available energy levels up to the Fermi level which is the highest occupied energy level at absolute zero temperature. If the temperature of the crystal is raised to a temperature above absolute zero some of the electrons are not disturbed at all only a few of those electrons near the Fermi energy level are elevated to higher levels. This model is just an approximation and does not describe quantitatively any real system. The qualitative features, however, are similar to those present in a more complicated model. We have therefore attained the reason why the Debye theory for specific heats can provide reasonably good agreement with experiments, even though it ignores the motion of the electrons. Only those electrons with energies close to Fermi energy can contribute to the specific heat and their number is small in comparison with the number of atoms in the crystal.

The behaviour of an electron gas is often compared with that of molecules of water in the liquid state. Water is essentially incompressible, and in a large body of water the most violent

motion occurs only in the form of surface phenomena. The electron gas is likewise incompressible because of the pauli exclusion principle, and the surface of the system is often referred to as the "Fermi sea". That is the electrons near the Fermi energy are analogous to water molecules near the surface of the ocean. The same ideas and terminology are also used to describe nuclear matter; since protons and neutrons have spin half, they are fermions, and a heavy nucleus with many protons and neutrons similarly has its lowest energy states completely filled. (Semat and Albright 1972).

The electron gas is modeled by a system of large number of particles that are identical and non interacting contained in a box with impenetrable walls. The box is large and the number of particles is large and the properties of the system is independent of the shape of the box. Such a system can be described by a time independent schrodinger equation.

$$\nabla^2\phi(x,y,z)+\frac{2m}{\hbar^2}(E-V)\phi(x,y,z)=0 \qquad (1.1)$$

The behaviour of electron gas depends on

i. The number of particles that make up the gas

ii. the number of accessible state or level for each particle.

The weakness of free electron theory of metals is that:

i. It can not be used to classify metals into conductor, semiconductor and insulators.

ii It can not be used to explain some transport properties of metals. (Semat and Albright 1972).

1.5 SOMMERFIELD'S THEORY

According to Sommerfield the properties of the electron gas are determined by quantum-mechanical principles. Knowledge of the energy and momentum of the electrons can help to theoretically evaluate those properties of metals which depend on the valence electrons. In this

present case, this problem is reduced to a single-electron problem and the theory is based on the following assumptions:

i. The valence electrons move independently of one another in the potential of the metal ions and the other electrons.

ii. The potential in the interior of the metal is constant, i.e the electrons are not acted upon by forces provided that no external fields are applied. Therefore the electrons are called "free".

iii. A wave function is attributed to every electron which has been obtained as a solution of the time-independent schrodinger equation.

iv. The electron energy distribution is given by the Fermi-Dirac statistics.

The fourth assumption contains the Pauli exclusion principle according to which each eigenstate can be occupied by at most two electrons with opposite spins.

In this sense the N electrons are not perfectly independent from one another even if, according to assumption one and two, forces acting between the electrons among themselves and the electrons and the metal ions can be neglected.

By virtue of the De Broglie relation a wavelength of $\lambda = h/p$ is attributed to electron of momentum p. When we introduce the wave number $k = 2\pi/\lambda$,the de Broglie relation takes the form $p = \hbar K$

The motion of the electrons is considered as the propagation of particle waves, which for the stationary state is determined by the time-independent Schrodinger equation with suitable boundary conditions

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = O \qquad (1.2)$$

where ψ is the wave function, E is the total energy of the electron, V is the potential energy and m is its rest mass. The quantity ψ is also called the probability amplitude. The quantity $\psi\psi^* d^3r$ is the probability for an electron to be found in the volume elements d^3r. The probability for an electron to be anywhere in the system must be unity, this requirement is called the normalization condition which the wave function must satisfy.

$$\int \psi\psi^* d^3r = 1 \qquad (1.3)$$

Here ψ^* is the complex conjugate function of ψ. The integration is carried out over the total volume of the system considered.

As in the present case the potential energy is taken as constant ("free" electrons), and as it is defined to within an additive constant, we can put V = O in equation (1.2). when we can write.

$$\psi = C\exp(ik.r) \qquad (1.4)$$

where C is a normalizing constant, k is the wave vector and r is the position vector, we obtain from equation (1.2)

$$E(k) = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) \qquad (1.5)$$

This relation, $E(k)$ represents the dispersion relation for free electrons.

The boundary conditions supply us with a selection of a finite number of k values. Therefore, only certain energy values (eigen values) are allowed, and only certain definite functions (eigen-functions) are solutions to the schrodinger equation. The boundary conditions themselves are obtained from the homogeneity of the crystal (periodic boundary conditions). The spatial periodicity of the wave functions for cells of the size L^3, is

$$\psi(x,y,z) = \psi(x+L,y,z) = \psi(x,y+L,z) = \psi(x,y,z+L) \qquad (1.6)$$

Yields together with equation (1.4) the quantization condition for the K values:

$$K_x = n_x \frac{2\pi}{L}, k_y = n_y \frac{2\pi}{L}, K_z = n_z \frac{2\pi}{L} \tag{1.7}$$

or

$$k^2 = \left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) = \left(\frac{2\pi}{L}\right)^2 n^2 \tag{1.8}$$

where n_x, n_y, n_z are integers and from equation (1.5) we hence obtain the eigen values for traveling waves:

$$E_n = 2\pi^2 \frac{\hbar^2}{mL^2} n^2 \tag{1.9}$$

Using Z''_k to denote the k values from k = 0 to k = k(n), we get

$$Z''_k = \frac{L^3}{6\pi^2} k^3 \tag{1.10}$$

Where we equally have many energy values Z^0_E from E = o to E = E_n

$$Z''_k = \frac{L^3}{6\pi^2} \frac{(2mEn)^{3/2}}{\hbar^3} \tag{1.11}$$

The density of the energy eigenvalues D(E) i.e the number of energy value per unit energy interval can be obtained from this by differentiation with respect to E:

$$D(E)dE = \frac{dZ''_E}{dE} dE = \frac{L^3}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} dE \tag{1.12}$$

These quantization conditions yield the energy eigenvalues allowed for each individual's valence electron in the metal.

The application of the Pauli exclusion principle and the Fermi-Dirac statistics enables us to find out how many electrons have certain energy (the so-called energy distribution). According to the Pauli principle only two electrons (with anti parallel spins) can have the same momentum, the

same "state", which is defined by the set of the three quantum numbers n_x, n_y, and n_z according to equation (1.8).

The Fermi-Dirac statistics tell us about the occupation probabilities of the states of energy E. The energy distribution, that is, the number $N(E)dE$ of electrons with energies between E and $E+dE$, is given by the distribution function

$$N(E)dE = 2D(E)\,F(E)\,dE \tag{1.13}$$

with the Fermi-Dirac function

$$F(E) = \frac{1}{\exp\left(\frac{E-\varepsilon}{KT}\right)+1} \tag{1.14}$$

Where ε is the chemical potential of the Fermi-gas or the Fermi energy. From equation (1.12) and 1.14) we obtain for the distribution function (Busch and Schade 1976) for free electrons (fig1.1) as

$$N(E)dE = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{E^{1/2}dE}{\exp\left(\frac{E-\varepsilon}{KT}\right)+1} \tag{1.15}$$

1.6 PROPERTIES OF THE FERMI-DIRAC FUNCTION

The function F(E) depends only on an energy difference and is therefore independent of the choice of the origin of the energy scale; F(E) is also independent of the distribution of the quantum states D(E) and is generally valid for non-localized electrons. The function F(E) assumes only values between 0 and 1 as shown in Fig 1

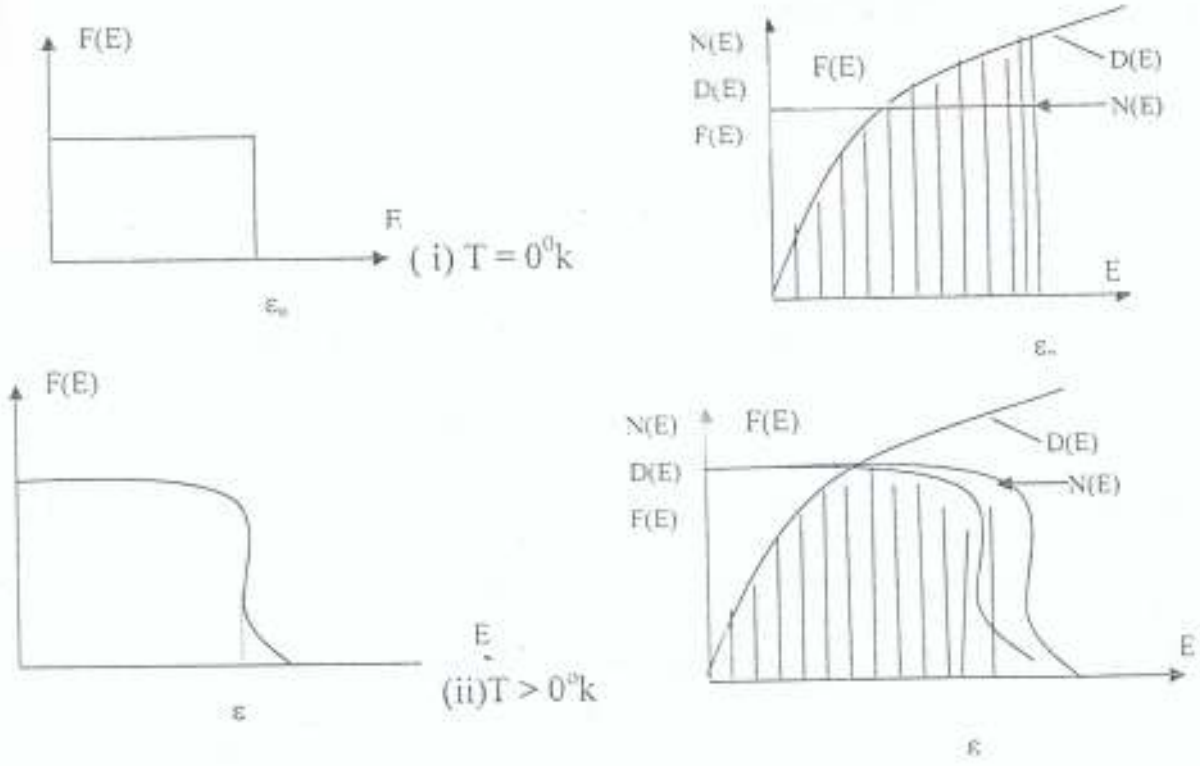


Fig 1.1 Fermi-Dirac function F(E), Distribution of equation of states D(E) and the distribution function N(E) for (i) $T = 0^{\circ}k$ and $T>0^{\circ}k$.

$$0 \le F(E) \le 1 \qquad (1.16)$$

In particular we have for

$$T = 0^{\circ} k \qquad E > \mathcal{E}_0 : \quad F(E) = 0$$

$$E \leq \mathcal{E}_0 : \quad F(E) = 1$$

$$T = 0^{\circ} k \qquad E >> \mathcal{E} : \quad F(E) \approx 0 \tag{1.17}$$

$$E << \mathcal{E} : \quad F(E) \approx 1$$

$$E = \mathcal{E} : \quad F(E) = \tfrac{1}{2}$$

The energy Εo is the Fermi energy. At T = 0°k all energy states are filled up to Εo with unit probability, for higher energies the occupation probability is equal to zero. For $T > 0^{\circ} k$ the occupation probability for states of the energy $E = \mathcal{E}$ is equal to half. The Fermi energy is a slightly temperature dependent energy parameter which is determined by the electron density.

The function F(E) has the following important properties

$$F(\varepsilon + \nabla E) = 1 - F(\varepsilon - \nabla E) \tag{1.18}$$

this is easily understood when we take into consideration (fig 1.1) that is

$$\frac{1}{\exp\left(\frac{\Delta E}{KT}\right) + 1} = 1 - \frac{1}{\exp\left(-\frac{\Delta E}{KT}\right) + 1} \tag{1.19}$$

and

$$\frac{1}{\exp\left(\frac{E-\varepsilon}{KT}\right)+1} = 1 - \frac{1}{\exp\left(-\frac{\varepsilon-E}{KT}\right)+1} \tag{1.20}$$

1.7 PROPERTIES OF THE ELECTRON GAS AT T = 0°K

At absolute zero all states are filled up to the Fermi energy E_o. This fact results from the Fermi-Dirac statistics. The value of this limiting energy depends on the total number N of valence electrons contained in the volume L^3, which occupy the allowed states in agreement with pauli's exclusion principle. From this we obtain an equation determining E_f

$$N = \int_0^{E_f} N(E)dE = 2\int_0^{E_f} D(E)F(E)dE \tag{1.21}$$

Using equation (1.12) and F(E) = 1 we obtain

$$E_f = \frac{\hbar^2}{2m}(3\pi^2 n_e)^{2/3} \tag{1.22}$$

where $n_e = N/L^3$ is the electron concentration.

The electron concentration in metals is of the order of the concentration of atoms. The calculation of E_f from equation (1.22) and (1.23) yields astonishingly high energy values even at absolute zero (of the order of several eV) for the valence electrons of highest energy.

$$n_e = n_{At} \tag{1.23}$$

The total energy of all valence electrons in the volume L^3 at absolute zero amounts to

$$U_0 = \int_0^{E_f} EN(E)dE \tag{1.24}$$

Substitution of equation (1.15) and (1.17) yields

$$U_0 = \frac{L^3}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_f^{5/2} \tag{1.25}$$

From this, using also equation (1.22), we obtain for the mean energy per electron

$$\overline{U}_0 = \frac{U_0}{N} = \frac{3}{5}E_F \tag{1.26}$$

In contrast to the classical Maxwell-Boltzmann gas whose particles have no energy at absolute zero, the electron gas has a considerable zero-point energy. It corresponds to a temperature of the order of 10^{40}K of a classical gas. This can be easily estimated by means of the following relations:

$$\overline{U}_o = \frac{3}{5} E_F = \frac{3}{2} KT_E \tag{1.27}$$

$$T_E = \frac{2}{5} \frac{E_F}{k} \tag{1.28}$$

where T_E is the degeneracy temperature.

In contrast to the ideal gas, the electron gas at absolute zero has high pressure Po (zero-point pressure). When we substitute the electron concentration n_e and the mean energy $\overline{U}_o$ in the general gas-kinetic relation for the pressure, we obtain the zero-point pressure of the electron gas as

$$P_o = \frac{2}{3} ne\overline{U}_o = \frac{2}{5} neE_F \tag{1.29}$$

This pressure is of the order of 10^5 atm. (Busch and Schade, 1976).

1.8 PROPERTIES OF THE ELECTRON GAS AT T > 0^OK

The following considerations are based on the assumption that the electron gas is in thermodynamic equilibrium with the metal ions in the lattice. If the temperature is raised, the mean energy of the electron gas is also raised via the interaction with the lattice vibrations (Phonon). The excitation energies transferred from the phonons to the electrons amount to about KT. As all states with energies $E < E_f$ are occupied, only the fastest electrons of energies $E = E_f$ can be excited to higher levels. Thus the curve of the Fermi-Dirac function is changed only near the Fermi energy, in an energy interval of the order of KT. The value of the Fermi energy is slightly temperature-dependent and is obtained from a normalization condition similar to equation (1.21), under the assumption of a temperature-independent electron concentration N/L^3 (Fig1.1):

$$N = \int_0^\infty N(E)dE = 2\int_0^\infty D(E)F(E)dE \tag{1.30}$$

Using equation (1.15) we obtain the equation for the determination of E_F

$$N = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{E^{1/2}dE}{\exp\left(\frac{E-E_F}{KT}\right)+1} \tag{1.31}$$

with the substitutions x = E/KT and $\alpha = E_F/KT$ we can rewrite this equation in the form

$$N = \frac{L^3}{2\pi^2}\left(\frac{2mKT}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{X^{1/2}dx}{\exp(x-\alpha)+1} \tag{1.32}$$

or

$$n_e = \frac{2}{\pi^{1/2}}n_0 F_{1/2}(\alpha) \tag{1.33}$$

with the "effective density of states"

$$n_0 = \frac{1}{4}\left(\frac{2mKT}{\pi\hbar^2}\right)^{3/2} \tag{1.34}$$

and the Fermi integral

$$F_{1/2}(\alpha) = \int_0^\infty \frac{X^{1/2}dx}{\exp(x-\alpha)+1} \tag{1.35}$$

the so-called effective density of states means essentially a critical electron concentration. In the Fermi statistics we often encounter integrals of the form

$$F(\alpha) = \int_0^\infty \frac{f(x)dx}{\exp(x-\alpha)+1} \tag{1.36}$$

These Fermi integrals in general cannot be solved analytically, but by means of series expansions they can be given approximately for certain ranges of $\alpha = E_F/KT$.

For $\alpha >> 1$ we can use Sommerfield's expansion

$$F(\alpha) \approx \int_0^{\alpha} f(x)dx + \frac{\pi^2}{6} f'(\alpha) + \frac{7\pi^4}{360} f'''(\alpha) + \qquad (1.37)$$

In particular for $f(x) = X^n$

$$F_n(\alpha) = \int_0^{\infty} \frac{X^n dx}{\exp(x-\alpha)+1} \approx \frac{\alpha^{n+1}}{n+1}\left[1 + \frac{\pi^2}{6}(n+1)n\alpha^{-2} + \ldots\ldots\right] \qquad (1.38)$$

This series converges rapidly for $\alpha >> 1$. (Busch and Schade, 1976)

1.9 DEGENERACY OF THE ELECTRON GAS

Deviations of the properties of the electron gas from those of an ideal gas are due to degeneracy. The presence of zero point energy and zero-point pressure are characteristic features of

degeneracy. The concept of electron gas degeneracy is in no way connected with the quantum-mechanical concept of degeneracy which means the existence of several states of the same energy.

The criterion for degeneracy is defined by the condition

$$E(T) \approx E_F >> KT \tag{1.39}$$

The electron gas is therefore degenerates as long as its temperature T is considerably below the degeneracy temperature T_E (equation 1.28)

$$T << T_E \tag{1.40}$$

The criterion in equation (1.39), together with equation (1.22) defines a critical electron concentration n_{crit}: for concentrations given by

$$n_e >> n_{crit} = \frac{1}{3\pi^2}\left(\frac{2mk}{\hbar^2}\right)^{3/2} T^{3/2} \tag{1.41}$$

Comparison with equation (1.34) shows that n_{crit} is approximately equal to the effective density of states:

$$n_{crit} = \frac{4}{3\pi^{1/2}} n_a \tag{1.42}$$

At T = 300°K the critical density $n_{crit} \approx 10^{19}\,cm^{-3}$; the electron concentration in monovalent metals, however, if $n_e = 10^{22} cm^{-3}$. Thus the electron gas of metals is highly degenerate, the degeneracy would disappear only at temperatures considerably above the melting point of the metals. (Busch and Schade 1976).

1.10 SPECIFIC HEAT OF THE ELECTRON GAS

Only the fastest electrons and thus only a small fraction of all electrons can take up thermal energy because of the pauli principle. For this reason the specific heat of the degenerate electron gas is much smaller than that of a classical gas.

The specific heat Cv is obtained from the temperature dependence of the energy U(T) of the electron gas in the volume L^3.

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{V=L^3} \tag{1.43}$$

The total energy U(T) is obtained in analogy to equation (1.24) from

$$U(T) = \int_0^\infty EN(E)dE \tag{1.44}$$

Substitution of equation (1.15) yields

$$U(T) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{E^{3/2}dE}{\exp\left(\frac{E-E_F}{KT}\right)+1} \tag{1.45}$$

with the substitutions $x = E/KT$ and $\alpha = E_F/KT$ we have

$$U(T) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} (KT)^{5/2} F_{3/2}(\alpha) \tag{1.46}$$

where

$$F_{3/2}(\alpha) = \int_0^\infty \frac{X^{3/2}dx}{\exp(x-\alpha)+1} \tag{1.47}$$

According to equation (1.38) in the case of degeneracy ($\alpha = \varepsilon/KT >> 1$) we have

$$F_{3/2}(\alpha) \approx \frac{2}{5}\alpha^{3/2}\left[1+\frac{5}{8}\left(\frac{\pi}{\alpha}\right)^2+\ldots\ldots\ldots\ldots\right] \tag{1.48}$$

When we again replace ε by E_F in the correction term, we obtain with equations (1.46) and (1.48) for the electron gas energy

$$U(T)=\frac{L^3}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{KT}{E_F}\right)^2+\ldots\ldots\ldots\ldots\right] \tag{1.49}$$

Repeated application of the binomial expansion on equation

$$n_e=\frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon^{3/2}\left[1+\frac{\pi^2}{8}\left(\frac{KT}{E}\right)^2+\ldots\ldots\ldots\ldots\right] \tag{1.50}$$

enable us to obtain

$$\varepsilon(T)=E_F\left[1+\frac{\pi^2}{12}\left(\frac{KT}{E_F}\right)^2\right] \tag{1.51}$$

while the substitution of $\varepsilon(T)$ from equation (1.51) yields

$$U(T)=\frac{L^3}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}E_F^{5/2}\left[1+\frac{5\pi^2}{12}\left(\frac{KT}{E_F}\right)^2+\ldots\ldots\ldots\ldots\right] \tag{1.52}$$

and using equation (1.25) and (1.26) we find

$$U(T)=\frac{3}{5}NE_0\left[1+\frac{5\pi^2}{12}\left(\frac{KT}{E_F}\right)^2+\ldots\ldots\ldots\ldots\right] \tag{1.53}$$

the temperature dependence of the mean energy per electron equation (1.26) is given by

$$U(T)=\frac{U(T)}{N}=\frac{3}{5}E_0\left[1+\frac{5\pi^2}{12}\left(\frac{KT}{E_0}\right)^2+\ldots\ldots\ldots\ldots\right] \tag{1.54}$$

from equation (1.53) we obtain

$$C_V = \frac{\pi^2}{2}\frac{NK^2}{E_o}T = \gamma T \qquad (1.55)$$

for the specific heat of the electron gas, where

$$\gamma = \frac{\pi^2}{2}\frac{NK^2}{E_F} \qquad (1.56)$$

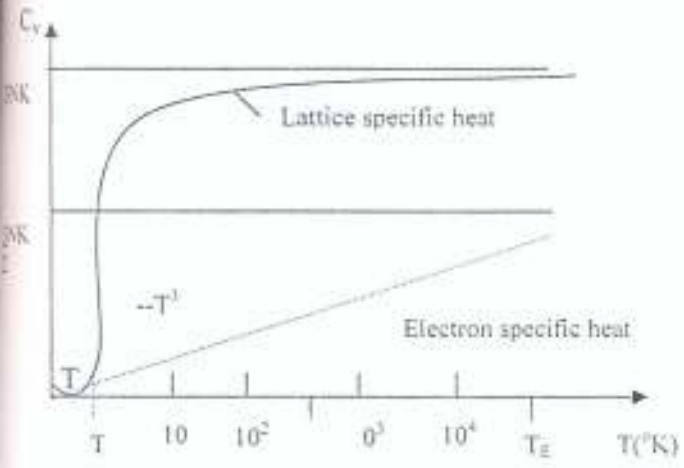


Fig 1.2 Lattice specific heat and specific heat of the electron gas as functions of temperature.

Introducing the degeneracy temperature T_E in equation (1.28) into equation (1.55) we get

$$C_V = \frac{\pi^2}{5}NK\frac{T}{T_E} \qquad (1.57)$$

Unlike the classical gas, the electron gas has a temperature dependent specific heat, which is directly proportional to the temperature. From equation (1.57) we see immediately that the C_v value for temperatures above the Debye temperature θ_D (θ_D is of the order of 100°K) is only about 1% of theDulong-petit value NK of the Lattice specific heat. Only at very low temperatures do the

electrons contribute noticeably to the specific heat of metals: as T→ 0°k the electron contribution of the lattice vibrations drops as T^3. When we equate these two contributions we obtain the temperature T* below which the specific heat of the electron gas is predominant (fig 1.2):

$$\frac{12}{5}\pi^4 NK\left(\frac{T^*}{\theta}\right)^3 = \frac{\pi^2}{5}NK\frac{T^*}{T_E} \tag{1.58}$$

for copper, for instance with $\theta = 310^0K$ and $T_E \approx 3 \times 10^{40}k$ we find $T^* \approx 3^0K$.

The total specific heat of metals at $T << \theta$ is therefore

$$C_{v\,total} = YT + \beta T^3 \tag{1.59}$$

or

$$\frac{C_{v\,total}}{T} = Y + \beta T^2 \tag{1.60}$$

where $\beta = \frac{12}{5}\pi^4 \frac{NK}{\theta^3}$ (1.61)

In particular, the energy eigenvalue density D(E) is changed when one assumes that the electrons move in a periodic rather than a constant potential. The value of Y is in other words directly related to the eigenvalue density at the point $E=E_F$ as a combination of equation (1.12), (1.22) and (1.56) shows

$$Y = \frac{2}{3}\pi^2 K^2 D(\varepsilon_u) \tag{1.62}$$

This relation can be obtained quite generally without the restriction of the free electron model. A measurement of the specific heat in the low-temperature range can thus yield information on the eigen value density at the Fermi energy ε_F. (Busch and Schade, 1976).

1.11 LIMITS OF SOMMERFIELD'S FREE-ELECTRON MODEL

The free-electron model and the application of Fermi Dirac statistics have proved very successful in improving our physical comprehension especially of the monovalent metals. It is an astonishing fact that, in spite of the neglect of the strong electrostatic forces between the positive ions and the electrons, Sommerfield's model may explain satisfactorily the following properties of metals:

i. The specific heat of the electron gas.

ii. Thermionic emission.

iii. Field emission.

iv. The wiedemann-Franz law.

v. The diamagnetism and paramagnetism of the electron gas.

The theoretical calculation of galvanomagnetic effects, such as the magnetoresistance and the Hall effect, may deviate considerably from the experimental results. Thus, for example, the magnet-resistance measured for tungsten is higher by a factor of 1012 than that calculated on the basis of the free electron model similarly, the positive Hall coefficients of some metals (e.g Zn, Cd) cannot be explained by this model. (Busch and Schade 1976).

1.12 THERMAL RESISTIVITY OF METALS

Thermal resisitivy of metals is the reciprocal of the thermal conductivity of metals. Thermal resistivity is one of the phenomenon that arises as a result of transport process. In metals, thermal conduction is due to electrons and phonons. The free electrons contributes immensely to the thermal conduction at high temperatures. Thermal resistivity is brought out by electron-electron,

electron-phonon, electron-impurity scattering. These hinder thermal conductivity. The electron-electron scattering contribution to the thermal resistivity is proportional to temperature.

Accurate values of thermal resistivity due to electron-electron scattering can be obtained from the simultaneous measurement of electrical resistivity and thermal resistivity at high temperatures. This method has been used to measure the thermal resitivity due to electron-electron scattering for noble metals and alkaline metals. (Macdonald and Geldart, 1976).

The electron-electron scattering of the thermal resistivity is one of the main causes for the deviation of the Lorentz function from the wiedemann-franz law above Debye temperature (Lundmark, 1990). In the measurement of the thermal resistivity, the temperature dependence of the thermal resistivity is measured and the contribution from electron-electron scattering is extracted.

Thermal resisitivity is given by (Kukkonen and Wilkins, 1979) as

$$W = \left(\frac{3}{C_v V_F^2}\right)\left(\frac{2\pi^2}{3K\tau_u}\right) \tag{1.63}$$

where C_V is the specific heat capacity, V_F is the Fermi velocity, τ_u and K are related to angular averages of the scattering rate. Specifically, the relaxation time for a quasi-Particle at the Fermi surface is $2\tau_u/\pi^2$ where $\frac{1}{\tau_u}$ is proportional to an angular average of the scattering rate and it is (Kukkonen and Wilkins, 1979)

$$\frac{1}{\tau_u} = \frac{M^3 (K_B T)^2}{8\pi^3 \hbar^6} \left\langle W(K_1, K_2, K_1 + q, K_2 - q) \right\rangle \tag{1.64}$$

where m is mass of an electron, K_B is Boltzmann constant T is temperature and $\hbar$ is normalized planck's constant. An exact method for obtaining the thermal resistivity due to electron-electron scattering can be obtained once the quasi-particle scattering rate is known. In the

calculation of the thermal resisivity of metals, the metallic systems are modeled by a uniform electron gas with the electron mass modified to take account of band structure effects and the electron-electron interaction is modified to take account of the screening of this interaction by the core electrons. A simple approximation for the scattering function based on the Landau Fermi-liquid theory was used in comparing predicted values for thermal resistivity with experiment in the alkali metals, and it was found that the approximate scattering function is sufficiently accurate when the thermal resistivity of low-density alkali metals is much higher than the simple metals of groups 1B, 2B, 3A and 4A. [MacDonald and Geldart (1979)]

CHAPTER TWO

LITERATURE REVIEW

2.1 THERMAL RESISTIVITY OF METALS

Bar-Sagi (1976) calculated the thermal resisitivity of super-conductors based on bound density of states. He used a pair potential. The results of the calculated thermal conductivity was good agreement with experimental values.

Iwamoto (1999) calculated the effects of screening on the thermal resistivity of metals due to electron-electron scattering based on the approximate correlation energy. He used the static screening potential with the screening length determined by the compressibility which is derived from the Monte-carlo values for the correlation energy. The result obtained was compared with other theories and experimental values and it was found that the thermal resistivity of metals depends quite sensitively on the screening length.

Kukkonen and smith (1973) calculated the validity of the Born approximation as applied to electron-electron scattering in metals based on the exact solutions of the Boltzman equation. They used the knowledge of inter electronic potential, and found that for the screened coulomb interaction $V = \frac{\exp-(k_s r)}{r}$. Theory found that:

i. The Born approximation over estimates the scattering cross section and the electron-electron contribution to the thermal resistivity by about a factor of 2.

ii. The scattering cross section and the thermal resistivity are sensitive functions of the screening wave vector Ks.

iii. Neither the Thomas-Fermi nor the Bohm-pines screening wave vector yields a thermal resitivity that agrees with recent experiments on metals.

They concluded that the knowledge of the approximate interelectronic potential is considerably more important for calculating the transport coefficients than the use of the Born approximation instead of the exact partial wave method. Kukkonen and Wilkins (1979) calculated the interaction between two electron quasiparticles in terms of the dielectric and vertex functions of the uniform electron gas. The effective interaction and its contribution to the thermal resistivity was used, and the result obtained is consistent with experimental values.

Kus (1976) succeeded in calculating the electronic and thermal resitivity of metals using the forms of energy dependence of the trial function. In his calculation, realistic forms for the electron-phonon matrix elements were used and the effect of Umklapp processes was included. It was found that the electrical and thermal resistivities of metals in both the dilute and concentrated regions deviated significantly from Mathiecssen's rule and this result was in good agreement with experimental values.

Lundmark (1990) succeeded in calculating the umklapp scattering contribution to the electron-electron scattering and the thermal resistivity in metals. He used an isotropic Fermi-liquid model where we have corrected for the anisotropic scattering in terms of a fractional Umklapp scattering functions, which is calculated using a pseudopotential band structure model. The results he obtained was in good agreement with the experimental values.

Lundmark (1998) calculated the exchange and correlation contribution to the electron-electron scattering of the thermal resitivity in metals. He used a Fermi liquid model in which the electron-electron interaction is given by self energy derivatives. The results of the calculated exchange and correlation contribution to the electron-electron scatterings were in good agreement with experimental values.

MacDonald and Geldert (1979) succeeded in calculating the electron-electron scattering and the thermal resistivity of metals. They used a modelled uniform electron gas with a modified mass

and electron-electron interaction to account approximately for the crystalline effects. They also found that the electron-electron contribution to the thermal resistivity are in good agreement with the experimental values.

Pecheur and Toussaint (1972) calculated the phonon limited thermal resistivity of metals based on their symmetry directions. They used the Mannari-ziman-Baym theory. The results obtained was found to be in good agreement with the experimental values.

2.2 ELECTRON-ELECTRON INTERACTION AND THERMAL RESISTIVITY OF METALS

Electron-electron interaction play an important role in the transport processes in metals. Experimentally, one measure the transport coefficients and singles out the information about the electron-electron correlations among other effects. As for thermal resistivity for example both the electrons and phonons contributes as carriers of heat. Their heat transport may be impeded by electron-phonon, electron-impurity and electron-electron scattering as well as phonon-phonon scattering. In this case, one measures the temperature dependence of the thermal resistivity and extracts the contribution from electron-electron scattering. Such an analysis for different metals gives rise to valuable information about the interelectron potential, where many body effects modify the bare coulomb interaction significantly.

Theoretically, many schemes have been proposed to take into account the many body effects in calculating the thermal resitivity. To obtain the effects of electron-electron scattering on the thermal resistivity of metals we use the screened coulomb interaction with the effective potential composed of bare coulomb potential divided by the dielectric function, where we use the static long-wavelength limit of the dielectric function. Then the effective potential is characterized by the screening length which is the only density dependent parameter in the theory. It is sufficient to

require that the static long wavelength limit of the dielectric function satisfy the compressibility sum rule in order to determine this screening length uniquely.

The basic assumption in the present theoretical scheme is that the screening of the bare electron-electron interaction is approximately described with the use of the static long-wavelength limit of the dielectric function. The advantage of the present one-parameter theory is its simplicity. This is also a natural extension of theories with the screened coulomb interaction such as the Thomas Fermi, Bohn-pines and Hubbard approximations. Thermal resistivity of metals depends on the compressibility quite sensitively.

It is assumed that the electron-electron interaction potential is of the screened coulomb form

$$V(r) = e^2 \frac{\exp(-q_s r)}{r} \qquad (2.1)$$

were, e is the electronic charge, q_s is the screening length and r is the distance.

To determine the screening wave number q_s, we regard equation (2.1) as a bare coulomb potential which is screened by a static dielectric function in Fourier space

$$V(q) = \frac{4\pi e^2}{\varepsilon(q,0)q^2} \qquad (2.2)$$

Where

$$\varepsilon(q,o) = 1 + \frac{q_s^2}{q^2}$$

If the static dielectric function is approximated by its long-wavelength limit, then, the screening length q_s may be uniquely determined by the compressibility sum rule

$$\lim_{q\to 0} \varepsilon(q,o) = 1 + (q_s/q)^2 (k/k_o) \qquad (2.3)$$

where

$$q_{FT} = \left(\frac{6\pi ne^2}{E_f} \right)^{1/2} \qquad (2.4)$$

is the Fermi-Thomas screening length, n is the electronic density and E_F is the Fermi energy. The ratio k/k_o is the compressibility normalized by its free Fermi gas value. The screening length may be expressed in terms of the spin-parallel and spin-anti-parallel screening wave numbers ($q_{\uparrow\uparrow} and q_{\uparrow\downarrow}$) Iwamoto (1998) as

$$q_s = q_{FT} / [1 + (1/2)\{(q_{FT}/q_{\uparrow\uparrow})^2 + (q_{FT}/q_{\uparrow\downarrow})^2\}]^{1/2} \qquad (2.5)$$

2.3 FERMI LIQUID

A Fermi liquid is a generic term for a quantum mechanical liquid of fermions that arises under certain physical conditions:

(i) when the temperature is sufficiently low

(ii) when the system is translationally invariant

Under these conditions, the interaction between the particles of the many body system does not need to be small (i.e electrons in a metal).

The Fermi liquid is qualitatively analogous to the non-interacting Fermi gas, in the following sense. The system's dynamics and thermo-dynamics at low excitation energies and temperatures may be described by substituting the non-interacting fermions with quasiparticles, each of which carries the same spin, charge and momentum as the original particles. Physically these may be thought of as being particles whose motion is disturbed by the surrounding particles and which themselves perturb the particles in their vicinity.

Each many particle excited state of the interacting system may be described by listing all occupied momentum states just as in the non-interacting system. As a consequence, quantities such as the heat capacity of the Fermi liquid behave qualitatively in the same way as in the Fermi gas (e.g the heat capacity rises linearly with temperature).

However, the following differences to the non-interacting Fermi gas arises:

(i) The energy of a many particle states is not simply a sum of the single-particle energy of all occupied states.

(ii) Specific heat, compressibility, spin-susceptibility and other quantities show the same qualitative behaviour (e.g dependence on temperature) as in the Fermi gas, but the magnitude is (sometimes strongly) changed.

(iii) In addition to the mean-field interactions, some weak interactions between quasiparticles remain which lead to scattering of quasiparticles off each other.

(iv) Green's function and momentum distribution of quasiparticles behave as for the fermions in the Fermi gas.

(v) The structure of the "bare" particles (as opposed to quasiparticle) Green's function is similar to that in the Fermi gas (where for a given momentum, the Greens functions in frequency space is a delta peak at the respective single-particle energy).

(vi) The distribution of particles (as opposed to quasiparticles) over momentum states at zero temperature still show a discontinuous jump at the Fermi surface (as in the Fermi gas), but it does not drop from one to zero the step is only of size Z.

(vii) In a metal the resistance at low temperature is dominated by electron-electron scattering in combination with umklapp scattering (Wikipedia, 2006).

.4 FERMI LIQUID THEORY

The basic idea of the theory is to compare the excited states of the quantum liquid with those f a free Fermi gas. In order to do this, it is assumed that there exists a one-to-one correspondence etween the states of the Fermi gas and the states of the liquid. It assume that Fermi liquid can be btained by switching on the interaction between the particles of the Fermi gas infinitely slowly, in his way every state of the liquid corresponds to a state of the Fermi gas. Therefore the liquid

corresponds to a state of the Fermi gas. Therefore the liquid obtained in this way is called a Fermi liquid

The only way to know if a given system is a Fermi liquid is to measure the properties of the system experimentally and see if the results are consistent with the predictions of the Landau's theory. (Peter, 2002)

Fermi liquid can be defined as an interacting system whose spectrum of elementary excitations is similar to that of a free Fermi gas. this based on the assumption that there exists a one-to-one correspondence between the states of the free Fermi gas and those of the interacting system. If one takes a state of the Fermi gas and adiabatically turns on the interaction between the particles a state of interacting system is obtained.

The elementary excitations of the interacting Fermi liquid correspond to particle and hole excitations of the free Fermi gas. Such an excitation can be created by adding a particle with momentum P to the ideal distribution and turn on the interaction between the particles. As the interaction is increased it is observed that the density of the particles in the neighbour hood is changing, for an electron gas, the surrounding electrons are pushed away cloud of positive charge density in this region is obtained, because of the one-to-one correspondence, the states of the interacting system can be classified by the distribution function of the Fermi gas which is referred to as the quasiparticle distribution functions. As the particles of a Fermi gas, quasiparticles obey the exclusion principle. Since quasipaticle excitations can be generated only if their momentum lies outside the Fermi surface, the quasiparticle distribution is bounded by the Fermi surface. (Peter, 2002).

The only Fermi liquid found in nature is liquid helium below 0.1°K. But the theory can also be applied to conduction electron in metals and semi-metals.

In the absence of excitations above the Fermi energy, the total energy E of a fermion system is given by the ground state energy Eg. Labeling the excited states by momentum P as in the ideal gas, E is expressed as

$$E = Eg + \sum_{p} \varepsilon(p) n_{p} \qquad (2.6)$$

where n_p is the distribution function of quasiparticles in the excited state with momentum, *P*. $\varepsilon(p)$ is energy which depends on momentum the entropy S of the system is

$$S = -K \sum_{p} [n_p \ln n_p + (1 - n_p) \ln(1 - n_p)] \qquad (2.7)$$

where K is the Boltzmann constant

In equilibrium, the distribution functions is determined by temperature and is determined by the condition that the free energy is minimum. (Akira, 1991).

2.5 QUASIPARTICLES

Quasiparticle is the simplest elementary excitations of the Fermi liquid theory. A method of creating such an excitations is to start with the ground state of the non-interacting fermion system; this state is always filled up to a limiting maximum or Fermi momentum $P_F = \hbar K_F$ at 0 K.

Consider a non interacting Fermi gas, the probability of finding a particle with momentum p and spin σ in the equilibrium state is given by the Fermi-Dirac distribution function.

$$n_{p\sigma} = \frac{1}{\exp(\varepsilon_{p\sigma} - \mu)/k_B + 1} \qquad (2.8)$$

Where $\varepsilon_{p\sigma}$ the quasiparticle energy, T is the temperature, K_B is the Boltzmann constant, μ is the chemical potential, and $n_{p\sigma}$ is the Fermi-Dirac distribution function. The quasiparticle energy is given by

$$\varepsilon_{p\sigma} = \frac{p^2}{2m} \tag{2.9}$$

where p is the momentum and m is the electron mass

Excited states of the system are obtained by creating particles outside the Fermi surface or holes inside the Fermi surface. The elementary excitations of the interacting Fermi liquid correspond to particles and hole excitations of the free Fermi gas, such an excitation is obtained by adding a particle with electron gas the surrounding electrons are pushed away and we get a cloud of positive charge density in this region. We consider our particle together with this cloud as an independent entity which is called quasiparticle.

The damping of the quasiparticle is due to collisions. For zero temperature it is easy to see that the lifetime of quasiparticles varies as the inverse square of the energy separation from the Fermi surface. Generally the quasiparticle lifetime is given by

$$\frac{1}{\tau_{p\sigma}} \propto \frac{(\pi K_B T)^2 + (\varepsilon_{p\sigma} - \mu)^2}{1 + \exp(\varepsilon_{p\sigma} - \mu)/K_B T} \tag{2.10}$$

where $\tau_{p\sigma}$ is the quasiparticle lifetime, K_B is the Boltzmann constant, $\varepsilon_{p\sigma}$ is the quasiparticle energy,

T is the temperature, μ is the chemical potential.

If we add a quasiparticle with momentum p and spin σ to an unoccupied quasiparticle state,

then the total energy of the system will increase by an amount which we call quasiparticle energy.

This means that the quasiparticle energy, $\varepsilon_{p\sigma}$ is defined as the variation of E with respect to Fermi-

Dirac distribution function $n_{p\sigma}$ and the change in energy is

$$\delta E = \sum_{p\sigma} \varepsilon_{p\sigma} \delta n \tag{2.11}$$

where

$$\delta n_{p\sigma} = n_{p\sigma} - n^{\circ}{}_{p\sigma} \tag{2.12}$$

is the departure from the groundstate distribution $n^0_{p\sigma}$

The interaction energy of two quasiparticles is defined as $F_{p\sigma p'\sigma'}$ the energy of a quasiparticle ($p\sigma$) changes due to the presence of another quasiparticle ($p'\sigma'$). A variation of the distribution function produces a variation of $\varepsilon_{p\sigma}$ given by

$$\delta\Sigma_{p\sigma} = \sum_{p'\sigma'} f_{p\sigma,p'\sigma'}\,\delta n_{p'\sigma'} \tag{2.13}$$

therefore $f_{p\sigma,\,p'\sigma'}$ is a second variation of the total energy

$$f_{p\sigma,p'\sigma'} = \frac{\delta^2 E}{\delta n_{p\sigma}, \delta n_{p'\sigma'}} \tag{2.14}$$

The quasiparticle energy can be written as

$$\varepsilon_{p\sigma} = \varepsilon_{p\sigma} + \sum_{p\sigma} f_{p\sigma,p'\sigma'}\delta n_{p'\sigma'} + \ldots\ldots\ldots\ldots \tag{2.15}$$

where $\varepsilon^0_{p\sigma}$ is the quasiparticle energy if there are no other quasiparticles. The energy of the whole system is thus.

$$E = E_o + \sum_{p\sigma} \varepsilon_{p\sigma} \delta n_{p\sigma} + \frac{1}{2} \sum_{p\sigma p'\sigma'} f_{p\sigma p'\sigma'} \delta n_{p'\sigma'} + \ldots\ldots\ldots \quad (2.16)$$

where E_o is the groundstate energy without any excitations. (Peter, 2002).

26 THE INTERACTIONS

There are three basic screened coulomb interactions in a metal:

i. The effective interaction between two external 'test' charges, e.g the screened ion-ion interaction used to calculate phonon frequencies in simple metals.

ii. The interaction between an electron and a test charge which is needed to calculate the scattering of an electron by an ionized impurity.

iii. The effective interaction between two electrons.

Effective interaction is defined as the Born approximation of the total scattering amplitude. Simple calculations of the effective interaction takes into account the coulomb interaction between the charge under consideration e.g test charge or electron and the screening electrons, but neglect the interaction of the screening electrons with each other. In this approximation, all the three effective interaction are identical and in Thomas-Femi theory, the effective interaction is

$$U_{TF} = \frac{4\pi e^2}{q^2 + q_{TF}^2} \quad (2.17)$$

where q_{TF} if is the magnitude of screening wave vector, e is the electronic charge, q is the coulomb charge in a more sophisticated approach, the Lindhard or the random-phase approximation yields

the effective interaction that is the bare coulomb interaction, $V(q) = 4\pi e^2/q^2$ screened by the Lindhard dielectron function, $\varepsilon_L(q)$.

When electron-electron interactions are included, these three effective interactions differ, the test-charge-test-charge interaction, $U_{tt(q)}$ is modified because the screening electrons now avoid each other due to the pauli exclusion principle (exchange) and due to their mutual coulomb repulsion (correlation). This interaction may be formally written

$$U_{tt}(q) = \frac{V(q)}{\varepsilon(q)} \qquad (2.18)$$

where V(q) is the coulomb potential interaction and $\varepsilon(q)$ is the dielectric function of the electron gas. The electron-test-charge interaction $U_{et}(q)$ differs from $U_{tt}(q)$ because the electron under consideration is indistinguishable from the screening electrons and therefore it has an exchange as well as a direct coulomb interaction with them. (kukkonen and Wilkins, 1979)

The effective electron-electron interaction $U_{ee}(q)$ may become complicated if both electrons under consideration may exchange with the screening electrons. Furthermore, if they have parallel spins they may exchange with each other as well. Because of these complications, there is no simple formal result for $U_{ee}(q)$ and the problem must be addressed through the Bethe-salpeter equation. (Kukkonen and Wilkins, 1979).

The effective interaction between an electron on the Fermi surface (/K/ = K_F) and a test charge is given by

$$U_{et}(q) = Z(K_F)\Lambda(K_F,q)U_{tt}(q) \qquad (2.19)$$

where Z (K_F) is the quasiparticle renormalization factor of the uniform electron gas, $\Lambda(K_F,q)$ is the vertex functions $U_{et}(q)$ is the electron-test charge interaction and U_{tt} is the test charge-test charge interaction

The electron-electron interaction is

$$U_{ee} = [Z(K_F)\Lambda(K_F,q)]^2 \frac{V(q)}{\varepsilon(q)} \qquad (2.20)$$

where V(q) is the coulomb potential and ε(q) is the dielectric function and

$$V_{(q)} = \frac{4\pi e^2}{q^2} \qquad (2.21)$$

The interaction in equation (2.20) is appropriate for electrons with opposite spins. The vertex function takes into account the pauli exclusion principle. The interaction between two electrons with parallel spins is gives as

$$U_{\sigma\uparrow\sigma\uparrow}(q) = U_{\sigma\uparrow\sigma\downarrow}(q) - U_{\sigma\uparrow\sigma\downarrow}(k_2 - k_1 - q) \qquad (2.22)$$

where k_1 and k_2 are the initial moments of the two electrons under consideration (Kukkonen and Wilkins, (1979).

Equation (2.20) and (2.22) are a reasonable first approximation to the effective electron-electron interaction.

With these results, the formal expressions for all three interactions in a metal can be written in terms of the dielectric and vertex functions of the electron gas. Unfortunately, these functions are not precisely known. These functions could be calculated independently but several existing dielectric functions are used to extract the vertex function from ε(q) by the constrain on the model interaction.

In the constraints on the model interaction, the static dielectric function is defined in terms of the proper polarization Π(q) as

$$\varepsilon(q) = 1 + V(q)\Pi(q) \qquad (2.23)$$

there exists an exact relation between the proper polarization and the compressibility k which is given by

$$\frac{\Pi(q=0)}{\Pi^{\circ}(q=0)} = \frac{k}{k_o} \qquad (2.24)$$

where $\Pi^{\circ}(q)$ is the polarization k_o is the compressibility of a system of noninteracting electrons an k is the compressibility of the electron gas alone. (2.24) is know as the compressibility sun rul Another identity that yields exact results is

$$\Lambda(K_F, q=0) = \frac{1}{(m*/m)Z(K_F)} \frac{K}{K_u} \tag{2.25}$$

where m* is the effective mass of the electron and m is the mass of electron. [Kukkonen and Wilkins 1979]

2.7 COMPRESSIBILITY

The compressibility is determined by the second derivative of the total energy with respect to the volume.

$$K = \left(V \frac{\partial^2 E}{\partial V^2} \right)^{-1} \tag{2.26}$$

where k is the compressibility, E is the total energy and V is the volume.

There are many different calculations of ground-state energy of the electrons gas and their internal agreement is quite good. Since the compressibility is determined by the most recent calculations also agree quite well with each other, it is commonly accepted that they yield something close to the true compressibility.

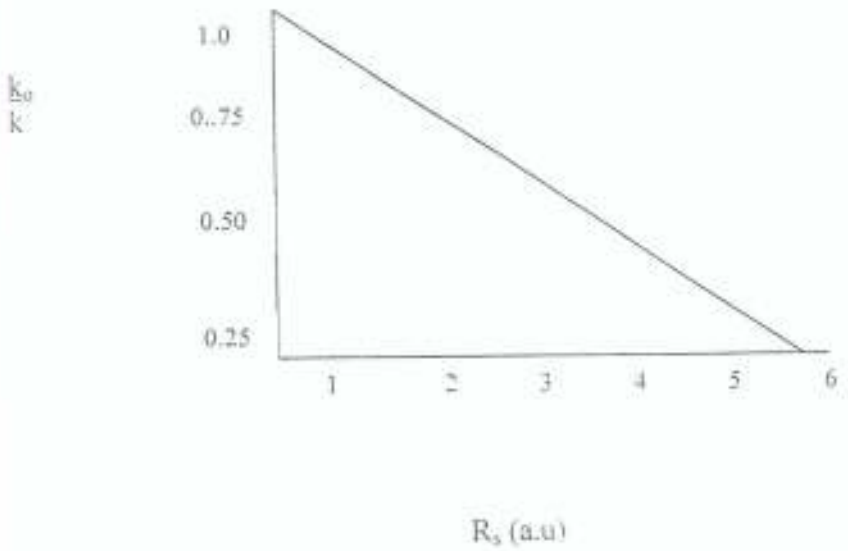


Fig 2.1; Ratio of the noninteracting electron compressibility k_o to the compressibility of interacting electron gas k as a function of r_s.

We note that the compressibility ratio becomes negative for the electron gas parameter for dimensionless coupling constant $r_s > 5.18$. This is due to a divergence in compressibility k. the divergence occurs at $r_s = 6.03$ in Hartree-Fock theory. (Kukkonen and Wilkins 1979).

2.8 COMPRESSIBILITY RULE

The compressibility sum rule expresses the self-consistency condition that the static response of the system to the long-wavelength perturbation (the static long-wavelength limit of the dielectric function) be equal to the compressibility. Here, one may utilize the accurate density dependent ground state energy obtained via the monte Carlo method to calculate the compressibility via thermodynamic relations. The basic assumption in the present theoretical scheme is that the screening of the bare electron-electron interaction is approximately described with the use of the static long-wavelength limit of the dielectric function (Iwamoto, (1999).

Requiring that the compressibility obtained from the ground-state energy is identical to that obtained from an appropriate q = 0 limit of the dielectric function is called the compressibility sum rule. The constraint imposed by the compressibility sum rule turns out to be extremely important but it also presents an immediate problem when it is applied to real metals because the compressibility of the uniform electron gas become negative. To generalize the effective interaction the effects of core polarization is included by finding the dielectric and vertex functions of the combined system of the electron gas and the polarizable background. The most important consequence of including core polarization is to modify the compressibility sum rule so that in addition to reducing the strength of the effective interaction. (Kukkonen and Wilkins, (1979).

2.9 LANDAU THEORY OF A FERMI LIQUID

In the Landau theory, it is postulated that an assembly of interacting fermions may be described by a set of quasiparticles (whose interactions are weak relative to those of the real particles), and where the number of quasi-particles are equal to the number of real fermions present. Each quantum level available to the quasi particles is associated with a definite momentum p and spin σ. The density of states in a momentum interval dp is

$$d\tau = \frac{2}{(2\pi\hbar)^3} dp \qquad (2.27)$$

where the factor of 2 appears because each momentum state is associated with two spin states, $d\tau$ is the density of state and $\hbar$ is the normalized Planck's constant. (Brooker and Sykes, 1970).

Landau tried to described fermion systems in terms of quasiparticles that are more or less free. His basic idea is that if the interaction is switched on adiabatically, the energy states may still be specified in terms of the free-particle states. However, the states depend on many other particles in the system, and therefore can be a function of the distribution function of quasiparticles (Isihara, 1991).

The energy of a particle of momentum p and spin σ is $E(p, \sigma)$. The interaction of the quasi-particles is taken into account by saying that the energy $E(p,\sigma)$ of a particle changes by an amount $f(p,\sigma : p',\sigma')\delta n(p',\sigma')\frac{1}{2}d\tau'$ when the occupation probability of $\frac{1}{2}d\tau'$ quantum states of spin σ' around p' is changed by $\delta n(p',\sigma')$. It turns out that the functions f need be known only at the Fermi surface, where it is a function only of the angle χ between the vectors p, p'(and of the two spins). Assuming the spin-dependent part of the interaction to be due entirely to exchange, Landau expressed the interaction in terms of dimensionless functions $F(\chi), Z(\chi)$ where

$$f(p,\sigma : p',\sigma') = f(p,p') + \sigma.\sigma'\Sigma(p,p') \tag{2.28}$$

and

$$F(\chi) = \left[\frac{\partial \tau}{\partial E} f(p,p')\right] p = p' = P_F \tag{2.29}$$

$$Z(\chi) = \left[\frac{\partial \tau}{\partial E}\Sigma(p,p')\right] p = p' = P_F \tag{2.30}$$

The functions $F(\chi), Z(\chi)$ are expanded in spherical harmonics to give

$$F(\chi) = F_o + F_1\cos\chi + F_2 P_2(\cos\chi) + \ldots\ldots\ldots\ldots \tag{2.31}$$

$$Z(\chi) = Z_o + Z_1 \cos\chi + Z_2 P_2(\cos\chi) + \ldots\ldots\ldots \quad (2.32)$$

The parameter F_o, F_1 and Z_o in the equation (2.31) and (2.32) can be obtained from the velocity of sound, the specific heat, and the magnetic susceptibility of the liquid. Hone has shown that one additional parameter usually chosen to be Z_1, can be obtained from the requirement that the forward scattering amplitude for fermions of parallel spin must be zero. Higher parameters cannot be found very easily and they are usually ignored, though an attempt has been made to evaluate F_2. The parameters in the equation (2.31) are dependent on the density of the liquid but in the first instance they are independent of temperature.

The quasi-particles obey a Fermi distribution with a Fermi energy μ, and a Fermi momentum P_F given by

$$P = \frac{MP_F^3}{3\pi^2\hbar^3} \quad (2.33)$$

where m is the mass of a fermion $\hbar$ is the normalised planck's constant and p is the density of the liquid. The velocity of quasi-particles on the Fermi surface is

$$V_F = \left[\frac{\partial E}{\partial P}\right]_{P=P_f} = \frac{P_f}{M^*} \quad (2.34)$$

where M* is the effective mass of an electron (Brooker and Sykes, 1970)

2.9.1 Fundamental assumption of Fermi liquid theory

The first fundamental assumption in the Fermi liquid theory is that there is a one-to-one correspondence between the quasi-particles and the low-lying excited states of the Fermi liquid.

The second fundamental assumption in the Fermi liquid theory is that as we turn on particle interactions, the excitation energy spectrum Ep of the quasiparticle has the same form as that of the non-interacting particle system. (Animalu, 1977).

2.9.2 APPLICATIONS OF LANDAU THEORY OF FERMI LIQUID

The main advantage of the Fermi liquid theory is that it enables us to investigate the effect of particle interaction on macroscopic properties of the quasi-particle model.

Landau also applied the concept of local energy to the study of the dynamical properties of the Fermi liquid (Animalu 1977).

2.10 SCREENING

Screening is the reduction of electric field at large distance from the positive charges (Inkson, 1984). According to Wilkes, (1973) screening is the cancellation of the attraction of the ionic positive charge by the electrons due to the heaping up of electron density in low potential regions. Screening is the most important manifestation of electron-electron interactions and in determining the behaviour of any charge carrying disturbance in a metal. When an electron moves through a periodic potential, there are interactions which are strong and are of long range being the coulomb's force between the charges and the exchange force associated with the anti-symmetry of the wave functions (Ziman, 1969). Screening is brought about by the coulomb and exchange potentials and is effective when the electrons are close to each other. When they are far apart from each other, screening becomes negligible. Screening affects the interaction of two electrons with each other as the interacting electrons can be considered as external charges by other electrons. Screening is a many-body problem (a problem in which all the electrons are mutually interacting, which arises from the Hartree self-consistent field (Wilkes 1973 and Mahan, 1990). Screening characteristically reduces the importance of electron-electron interactions.

Screening charge is the mobile charge attracted by impurity electric field, which has its own istribution in space. The screened potential is obtained from its charge sum with impurity charge. he screening charge is from the unbound conduction electrons of the metal; or semiconductor. As e screening charge moves through the crystal, they spend a little more time near the impurity otential if it is attractive than they do elsewhere in the solid (Mahan, 1990). If the impurity otential is repulsive for electrons, they tend to spend less time near the impurity, so the average harge is depleted near the impurity. If the screening charge is positive, it signifies a reduction in he average electron density, which is negatively charge. Dielectric screening is produced by a redistribution of the electron gas (Ziman, 1969).

The most important behaviour of an electron gas is described by the wave vector of the dielectric function for zero frequency $\varepsilon(k,o)$ which can be used to estimate the potentials that occur in metals and give rise to energy-band structure (Kittel, 1976 and Harrison, 1980).

If a positive charge of charge density $\rho(r)$ is super imposed in an electron gas of concentration $n_o e$, where e is electronic charge, the positive charge will give rise to an electrostatic potential $\phi(r)$. If $V(r)$ is the electrostatic potential established as a result of the movement of the charge density, then the total $u(r)$ is given (Inkson, 1984) as

$$u(r) = \phi(r) + V(r) \tag{2.35}$$

the electrostatic potential is found from the poisson's equation

$$\nabla^2\phi = 4\pi\rho(r) \tag{2.36}$$

with E = - $\nabla\phi$ being the electrostatic field. The positive and negative charge density distribution are related to the total charge density distribution by

$$\rho(r) = \rho_{ext}(r) + \rho_{ind}(r) \tag{2.37}$$

But $\rho(r) = e^2U(r)N(E_F)$ by sommerfeld model (Inkson, 1984) where $N(E_F)$ is the density of states at the Fermi energy. This shows that the potential at any point raises the energy of each electron state by $eU(r)$ (Inkson, 1984).

$$\nabla^2\varphi_{(r)} = 4\pi e^2U(r)N(E_F) \tag{2.38}$$

but $\varphi(r) = U(r) - V(r)$

$$\nabla^2[U(r) - V(r)] = 4\pi e^2U(r)N(E_F) \tag{2.39}$$

$$\nabla^2U(r) - 4\pi e^2U(r)N(E_F) = \nabla^2V(r) \tag{2.40}$$

$$(\nabla^2 - \lambda_s^2)U(r) = \nabla^2V(r) \tag{2.41}$$

where $\lambda_s^2 = 4\pi e^2 N(E_F).\lambda_s^{-1}$ is the screening length or screening parameter. This is the distance within which the potential is reduced to about one third of its unscreened value, and is a rough measure of the effective range of the field due to the charge (Stanley, 1963).

2.11 THOMAS-FERMI SCREENING THEORY

The schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_i(r) - eU(r)\Psi_i(r) = E_i\Psi_i(r) \tag{2.42}$$

is solved to obtain the total charge in the presence of the total potential

$$U(r) = \phi(r) + V(r) \tag{2.43}$$

The energy versus wave vector of an electron at the position r in the presence of the potential is of the form

$$E(k) = \frac{\hbar^2 k^2}{2m} - eU(r) \tag{2.44}$$

The electrochemical potential μ of the electron gas must be constant in equilibrium, independent of position. In a region where there is no electrostatic potential, the chemical potential is related to the electronic concentration, n_o (Kittel, 1976) by

$$\mu = E_F^{\ o} = \frac{\hbar^2}{2m}(3\pi^2 n_o)^{2/3} \tag{2.45}$$

At absolute zero, in a region where the electrostatic potential is U(r), the electrostatic potential is constant and is given (Kittel, 1976) as

$$\mu = E_F(r) - eU(r) \tag{2.46}$$

$$\therefore \quad \frac{\hbar^2}{2m}(3\pi^2 n_o)^{2/3} = \frac{\hbar^2}{2m}(3\pi^2 n(r)^{2/3} - eU(r) \tag{2.47}$$

$$\frac{\hbar^2}{2m}[3\pi^2 n(r)]^{2/3} - \frac{\hbar^2}{2m}[3\pi^2 n_o]^{2/3} = eU_{(r)} \tag{2.48}$$

If equation (2.48) is expanded by a Taylor's series expansion (that is $F(x) = \sum_{n=0}^{\infty} \frac{(x-a)^n}{n} f^n(a)$) of

E_f then equation (2.48) can be written (Kittel, 1976) as

$$\frac{dE_f}{dn_o}[n(r) - n_o] = eU(r) \tag{2.49}$$

from equation (2.45)

$$\frac{dE_f}{dn_o} = \frac{\hbar^2}{2m}(3\pi^2)^{2/3}\frac{d}{dn_o}n_o^{2/3}$$

$$\therefore \frac{dE_f}{dn_o} = \frac{3}{2}\frac{\hbar^2}{2m}(3\pi^2)^{2/3} n_o^{-1/3} = \frac{2E_f}{3n_o} \tag{2.50}$$

Hence equation (2.49) becomes

$$\frac{2E_f}{3n_o}[n(r) - n_o] = eU(r) \tag{2.51}$$

$$\therefore n(r) - n_o = \frac{3n_o eU(r)}{2E_f} \tag{2.52}$$

But $n(r)$-n_0 is the induced charge density ρ_{ind}. The Fourier component of this equation

(Kittel, 1976) is

$$\rho_{ind}(k) = -\frac{3n_o e^2}{2E_f} U(k) \tag{2.53}$$

where k is the wave vector. But according to Kittel (1976).

$$K^2 U(k) = 4\pi\rho(k)$$
$$\therefore \rho_{ind}(k) = -\frac{6\pi n_o e^2}{E_f K^2}\rho(k) \tag{2.54}$$

The zero frequency dielectric function of an electron gas is defined (Kittel, 1976 Harrison, 1980, and Mahan, 1990) as

$$\varepsilon(o,k) = 1 - \frac{\rho_{ind}}{\rho(k)} \tag{2.55}$$

where ρ(k) is the external charge density and $\varepsilon(o,k)$ is the static dielectric function

using equation (2.54) in (2.55) gives

$$\varepsilon(o,k) = 1 - \frac{(-)6\pi n_o e^2}{E_f K^2 \rho(k)}\rho(k) \tag{2.56}$$

$$\therefore \varepsilon(o,k) = 1 + \frac{\lambda_s^2}{K^2} \qquad (2.57)$$

where $\lambda_s^2 = 6\pi n_e e^2 / E_f = 4\pi e^2 N(E_f)$

Equation (2.57) is called the Thomas Fermi dielectric function and λ_s^{-1} is the Thomas-Fermi screening length measured in Amstrong units. The screening length is the distance within which the effect of screening can be felt (Inkson, 1984). But the screening parameter is given (Ashcroft and Mermin, 1976) as

$$\lambda_s = \frac{2.95}{\sqrt{r_s}} A^{a-1} \qquad (2.58)$$

where r_s is the electron gas parameter or radius of the Wigner-Seitz cell measured in atomic units (a.u). The screening parameter is of the order of the Fermi wave vector showing that disturbances are screened in a distance, which is similar to inter particle spacing. In copper for example, the Thomas-fermi screening Length is 0.55Å(Kittel, 1976). This shows that the electrons are highly effective in shielding external charges (Ashcroft and Mermin, 1976).

2.12 HARTREE DIELECTRIC FUNCTION

The Hartree dielectric function concerns the effect of electron screening on the "bare" interaction between a valence electron and the ions in the crystals (Animalu, 1977). Consider the screening of bare electron-ion potential V_b by the dielectric constant of the valence electron gas. The effective (screened) potentials is the sum of the bare electron-ion potential V_b and the screening potential, V_{sc}. that is

$$V(r) = V_b(r) + V_{sc} \qquad (2.59)$$

The screening potential is related to the electron density by the poisson's equation and the electron density, $\rho(r)$ is obtained quantum mechanically from the electron wave function (Animalu, 1977). The electron wave function ϕ_k is determined by the solution of the schrodinger's equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\phi_k(r) = E_k\phi_k(r) \qquad (2.60)$$

In order to calculate V(r) in equation (2.59) equation (2.60) which involves $V(r)$ is solved self-consistently using the fact that $V(r)$ is a weak potential which implies that the wave function can be solved by perturbation theory (Animalu, 1977). The wave function perturbed by the screened potential can be written to the first order terms of the free electron eigenfunction as (Wilkes, 1973).

$$\phi(k) = \sum_q A_q \psi(k+q) \qquad (2.61)$$

where q is a continuous variable replacing the reciprocal lattice vector, the free electron wave function is

$$\psi(k+q) = e^{i(k+q)r} \qquad (2.62)$$

the electron density is

$$\rho(k) = \phi(k)\phi^*(k) = \sum_q A_q \psi(k+q) \sum_q A^*_q \psi^*(k+q) \tag{2.63}$$

$$\rho(k) = \phi(k)\phi^*(k) = \psi(k)^*\psi(k) \sum_q A_q \psi(k+q)\psi^*(k) + A^*_q \psi^*(k+q)\psi(k) \tag{2.64}$$

Writing $\psi_{(k)}$ in full reduces this to

$$\rho(k) = 1 + \sum_q A_q e^{i(k+q)r} - e^{ikr} + A^*_q e^{-i(k+q)r} e^{ikr} \tag{2.65}$$

$$\therefore \rho(k) = 1 + \sum_q A_q e^{iqr} + A^*_q e^{-iqr} \tag{2.66}$$

In each sum, one terms is much larger than others, this is the one for q = 0. In multiplying the sums, all terms are smaller than the first except those containing $A_0\psi(k)$ or $A^*_0\psi^*(k)$ or both. From first order perturbation theory (Wilkes, 1973).

$$A_q = \frac{V_q}{E_k - E_{k+q}} \tag{2.67}$$

where

$$V_q = \frac{1}{\Omega_0} \int V(r) e^{iqr} dr \tag{2.68}$$

Ω_0 is the atomic volume, V(r) is the screened potential, Vq is the three dimensional fourier transform of the screened potential.

$$\therefore A^*_q = \frac{V^*_q}{E_k - E_{k+q}} \tag{2.69}$$

where

$$V_q^* = \frac{1}{\Omega_o}\int V(r)e^{iq.r}dr \tag{2.70}$$

since the potential is an even function, $V(r) = V(-r)$ and $V_q^* = V_{-q} = V_q$

$$\therefore A_q^* = \frac{V_q}{E_k - E_{k+q}}$$

$$\rho(k) = 1 + \sum_q \frac{V_q e^{iq.r}}{E_k - E_{k+q}} + \frac{V_q e^{iq.r}}{E_k - E_{k+q}} \tag{2.71}$$

$$\therefore \rho(k) = 1 + \sum_q \frac{2V_q e^{iq.r}}{E_k - E_{k+q}}$$

The unity in equation (2.71) shows that constant electron density arises for each state which balances the positive charge of all the ions. The electron charge density in real space $\rho(r)$ is obtained from the relation (Wilkes, 1973 and Animalu, 1977)

$$\rho(r) = \frac{2}{(2\pi)^3}\int_{k_f} \rho(k)d^3k \tag{2.72}$$

$$\rho(r) = \frac{2}{(2\pi)^3}\int_{k_f} 1 + \sum_q \frac{2V_q e^{iq.r}}{E_k - E_{k+q}} d^3k \tag{2.73}$$

where k_f is Fermi wave vector and the integral is over all directions of k. Recall that

$$E_k = \frac{\hbar^2 k^2}{2m} \text{ and } E_{k+q} = \frac{\hbar^2 (k+q)^2}{2m} \tag{2.74}$$

$$\therefore \rho(r) = \frac{2}{(2\pi)^3} \int_{-kf}^{kf} 1 + \sum_{q} \frac{2V_q e^{iq.r}}{\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 (k+q)^2}{2m}} d^3k \qquad (2.75)$$

$$\rho(r) = \sum_{q} \left(\frac{8mV_q e^{iq.r}}{\hbar^2 (2\pi)^3} \int_{-kf}^{kf} (|k|^2 - |k+q|^2)^{-1} d^3k \right)$$

or

$$\rho(r) = \sum_{q} e^{iq.r} \rho_e(q)$$

where

$$\rho_e(q) = \frac{8mV_q}{(2\pi)^3 \hbar^2} \int_{-kf}^{kf} (|k|^2 - |k+q|^2)^{-1} d^3k \qquad (2.76)$$

Equation (2.76) contains a volume integral over the Fermi surface.

Wilkes, (1973) evaluated the integral in equation (2.76) and obtained

$$\rho_e(q) = \frac{mVq}{\hbar^2 \pi^2} \left[\frac{k_f}{2} + \frac{(k^2{}_f - q^2/_4)}{2q} \ln \left| \frac{2k_f + q}{2k_f - q} \right| \right] \qquad (2.77)$$

This is the Fourier component of the screening charge. It depends on the Fourier component of the screened potential, Vq. Since the screening charge depends on the screened potential, it is a self-consistent problem.

The screening or repulsive potential, V_{sc} produced by the screening charge of the valence electrons is obtained from the electrostatic poison's equation (Animalu, 1977).

$$\nabla^2 V_{sc}(r) = -4\pi e^2 \delta\rho(r) \qquad (2.78)$$

where $\delta\rho(r)$ is the change in electronic charge density above or below its mean value in the crystal.

using Fourier transforming the screened potential gives (Wilkes, 1973)

$$V_{sc}(q) = -\frac{4\pi e^2}{q^2}\rho_e(q) \tag{2.79}$$

$$\therefore V_{sc}(q) = -\left(\frac{4\pi me^2}{\pi^2\hbar^2q^2}\right)V_q\left(\frac{k_f}{2} + \frac{k_f^{\,2} - q^2/_4}{2q}\right)\ln\left|\frac{2k_f + q}{2k_f - q}\right| \tag{2.80}$$

which can be written as $V_{sc}(q) = V_qX$ (2.81)

where

$$X = -\frac{4\pi me^2}{\pi\ \hbar^2q^2}\left(\frac{k_f}{2} + \frac{k_f^{\,2} - q^2/_4}{2q}\right)\ln\left|\frac{2k_f + q}{2k_f - q}\right|$$

But the sum of the bare electron-ion potential and the screening potential gives the screened potential.

$$\therefore V_q(q) = V_b(q) + V_{sc}(q)$$

But $V_{sc}(q) = V_qX$

$$\therefore V_q(q) = V_b(q) + V_qX$$
$$\therefore V_q(q) - V_qX = V_b(q)$$

$$\therefore V_q(q) = \frac{V_b(q)}{1 - X} \tag{2.82}$$

Hence

$$V_q(q) = \frac{V_b(q)}{\left[1 + \frac{4me^2}{\pi\hbar^2q^2}\left(\frac{k_f}{2} + \frac{k_f^{\,2} - q^2/_4}{2q}\right)\ln\left|\frac{2k_f + q}{2k_f - q}\right|\right]} \tag{2.83}$$

this can be written in terms of the dielectric function, $\varepsilon_H(q)$ as

$$V_s(q) = \frac{V_b(q)}{\varepsilon_H(q)}$$

Where

$$\varepsilon_H(q) = 1 + \frac{4me^2}{\pi\hbar^2 q^2}\left(\frac{k_f}{2} + \frac{k_f^2 - q^2/4}{2q}\right)\ln\left|\frac{2k_f + q}{2k_f - q}\right|$$

$\varepsilon_H(q)$ is called the Hartree dielectric constant of the electron gas and q is the reciprocal lattice vector. As q tends to zero, the Hartree dielectric constant tends to the Thomas-Fermi limit (Animalu, 1977). The Hartree dielectric constant for free electron gas is a time-independent dielectric function since it was computed from time independent potential (Harrison, 1980). Small q components of the potential are well screened while large q components are weakly screened. The Hartree dielectric constant is well behaved in the intermediate region.

2.13 LINDHARD DIELECTRIC FUNCTION

The Lindhard dielectric function is commonly called the random phase approximation (RPA) dielectric function. It is a model for a static $\varepsilon(q)$ or dynamic $\varepsilon(q,w)$ dielectric function. The

Lindhard dielectric function predicts correctly a number of solid properties such as plasmons (Mahan, 1990).

Consider free electron-gas subjected to a time-dependent perturbation such that the potential seen by an electron at a point, r and time, t is given (Ziman, 1969)as

$$\delta U(r,t) = U\exp(iqr)\exp(iwt)\exp(\propto t) \tag{2.85}$$

where W is the frequency of oscillation, q is the reciprocal Lattice-vector and $\propto$ is a time constant parameter. If the above potential acts on a state defined as

$$|K) = \exp i\left(\frac{k.r + E(k)}{\hbar}\right)T \tag{2.86}$$

where E(k) is the energy. This mixes with other states so that the wave function becomes

$$\psi_k(r,t) = |k\rangle a_{k+q}(t)|k+q\rangle \tag{2.87}$$

where a_{k+q} is given by the first order perturbation theory (Ziman, 1969) as

$$a_{k+q} = \frac{\langle k+q|\delta U|k\rangle}{E_k - E_{k+q} + \hbar w - i\hbar\alpha} \tag{2.88}$$

the change in charge density (Ziman, 1996) is

$$\delta p = e\left[\sum_k |\psi_k(r,t)|^2 - 1\right] = e\sum_k \left[a_{k-q}(t)e^{iq.r}a^*_{k+q}e^{-iq.r}\right] \tag{2.89}$$

But

$$a^*_{k+q} = \frac{\langle k+q|\delta U^*|k\rangle}{E_k - E_{k+q} + \hbar w - i\hbar\propto}$$

$$\delta P = e\Sigma\left[\frac{U}{E_k - E_{k+q} + \hbar w - i\hbar\alpha} + \frac{U}{E_k - E_{k+q} - \hbar w + i\hbar\alpha}\right]e^{iqr}e^{iwt}e^{\alpha t} + \text{complex conjugate} \tag{2.90}$$

In equation (2.90), the summation is over all states whether occupied or not. The charge density obtained above gives rise to a potential field $\delta\phi(r,t)$ acting on the electrons through the coulomb's interactions by poisson's equation

$$\nabla^2(\delta\phi) = -4\pi e\delta\rho \tag{2.91}$$

Assuming that the potential field has the same space and time variation as the charge density, then

$$\delta\phi(r,t) = \phi e^{iq.r}e^{iwt} + \text{complex conjugate} \tag{2.92}$$

Combining equation (2.90), (2.91) and (2.92) gives (Ziman, 1969)

$$\begin{aligned} -q^2\phi &= -\left[4\pi e^2 U\sum_k \frac{f^n(k)-f^0(k+q)}{E(k)-E(k+q)+\hbar w-i\hbar\alpha}\right] \\ \therefore \phi &= \left[\frac{4\pi e^2}{q^2}\sum_k \frac{f^n(k)-f^0(k+q)}{E(k)-E(k+q)+\hbar w-i\hbar\alpha}\right]U \end{aligned} \tag{2.93}$$

This is the potential that arises as a result of the charge distribution created by the original potential δU. To achieve self-consistency, we assume that the perturbation δU should have already contained $\delta\phi$.

$$\therefore \delta U(r,t) = \delta V(r,t) + \delta\phi(r,t) \tag{2.94}$$

where $\delta V(r,t)$ is the actual potential that was applied to the system and is of the form

$$\delta V = Ve^{iq.r}e^{iwt}e^{\alpha t} + \text{Complex conjugate}$$

$$\therefore U = V + \left[\frac{4\pi e^2}{q^2}\sum_k \frac{f^0(k)-f^0(k+q)}{E(k)-E(k+q)+\hbar w-i\hbar\alpha}\right] \tag{2.95}$$

or

$$U = \frac{V}{\varepsilon(q,w)} \tag{2.96}$$

where

$$\varepsilon(q,w) = 1 + \frac{4\pi e^2}{q^2} \sum_k \frac{f^0(k) - f^0(k+q)}{E(k+q) - E(k) - \hbar w + i\hbar\alpha} \tag{2.97}$$

The sign in the denorminator has been changed for convenience. ε(q,w) is the Lindhard's dielectric function. Equation (2.96) is the Lindhard formula for the Hartree dielectric function of a free electron gas. It is evaluated with α approaching zero. It is an exact expression for the dielectric function in the Hartree approximation (Harrison, 1980).

The dielectric function obtained above using quantum mechanical treatment is appropriate for approximating the screening of any weak potential in the free electron gas. The situation is slightly more complicated when a non-local pseudopotential is to be screened (Harrison, 1980).

The static Hartree dielectric function has a logarithmic singularity when $q = 2k_F$. The function is continuous but its first derivative becomes infinite logarithmically at this point. This is a weak singularity but becomes important in many properties of metals. It gives rise to a similar singularity in the dispersion curve (frequency versus wave number) for lattice vibrations in crystals. This is known as the Kohn effect or the kohn anomalies in the lattice vibration spectrum. The kohn effect arises as a result of the potential set up by a phonon due to the motion of the ions. The electrons moves to screen this field and the ions interact with one another through the screened field which will be inversely proportional to the dielectric function. This modifies the forces between the ions and the lattice frequency of this mode of vibration will depend on the dielectric function. The singularity in dielectric function will be reflected in the phonon frequency.

The same effect is likely to be observed in any other system of waves propagated in the solid for example, spin waves interacting with the conduction electrons. This is a general method for investigating the Fermi surface of metals although in practice the detection of the effect may not be feasible (Ziman, 1969).

When the reciprocal lattice vector, q is small of the order of the Fermi wave vector, k_f at the zero frequency limit, the static dielectric function is obtained from equation (2.97) by rationalizing the denorminator and letting α approach zero. The static dielectric function is given (Ziman, 1969 and Harrison, 1980) as

$$\varepsilon(q,o) = 1 + \frac{4\pi e^2 n}{q^2 \frac{2}{3} E_f} \left[1 + \frac{4k_f^2 - q^2}{8k_f} \ln \left| \frac{2k_f + q}{2k_f - q} \right| \right] \qquad (2.98)$$

setting $X = \frac{q}{2k_f}$ and evaluating equation (2.98) can be written (Ziman, 1969, Harrison, 1980, and Bowen et al, 1994) as

$$\varepsilon(q,o) = 1 + \frac{\lambda_s}{2q^2} \left[1 + \frac{1}{2x}(1 - x^2) \ln \left| \frac{1+x}{1-x} \right| \right] \qquad (2.99)$$

where $1/\lambda_s$ is the Thomas-Fermi screening length, when the reciprocal lattice vector is small compared to the Fermi wave vector, the Lindhard dielectric function reduces to the Thomas-Fermi dielectric function. That is in the limit of slowly varying disturbances, Lindhard theory reduces to the Thomas-Fermi theory.

Hubbard introduced a correction factor into the lindhard dielectric function to account for the existence of exchange and correlation hole around the electron. The effect of the correlation factor is to reduce electron-electron interactions in dielectric screening (Mahan, 1990). The correlation factor is expressed in terms of the local field correction G(p). With the introduction of the correction factor, the Lindhard dielectric function is expressed (Bowen et al, 1994) as

$$\varepsilon(q,o) = 1 - \frac{\chi}{1 + G(p)\chi} \tag{2.100}$$

where

$$\chi = 1 + \frac{\lambda_s^2}{2q^2}\left[1 + \frac{1}{2x}(1-x^2)\ln\left|\frac{1+x}{1-x}\right|\right] \tag{2.101}$$

and

$$G(p) = \frac{1}{2}\frac{q^2}{q^2 + k_f^2} \tag{2.102}$$

The dielectric function in equation (2.100) describes how the potential is affected by the screening charge from the conduction electrons in metals as a results of the exchange and correlation hole around each electron. According to Mahan (1990), when one electron is participating in the dielectric screening, others are likely to be found near by. This should have the same effect on the nature of the dielectric screening.

A knowledge of the dielectric screening can also be used to predict some properties of metals such as the pair distribution function, screening charge, compressibility and correlation energy (Mahan, 1990).

Since screening affects some properties of metals and can be used to explain and predict some properties of metals, hence there is a need to investigate its effect on the thermal resistivity of metals.

2.14 FREQUENCY-DEPENDENT LINDHARD SCREENING

If the external charge density has time dependence $e^{-i\omega t}$, then the induced potential and charge density will also have such a time dependence, and the dielectric constant will depend on frequency as well as on wave vector. In the limiting case, where collisions can be ignored, the Lindhard argument can be straight-forwardly generalized by using time-dependent rather than stationary perturbation theory. One finds that the static result of Thomas-Fermi theory must be generalized to be

$$\chi(q) = -e^2 \int \frac{dk}{4\pi^3} \frac{f_{k-\frac{1}{2}q} - f_{k+\frac{1}{2}q}}{\hbar^2 k.q/m} \tag{2.103}$$

where F_k denotes the equilibrium Fermi function for a free electron with energy $\hbar^2 k^2/2m$ .q is the charge and m is the mass of electron

$$\therefore f_k = \frac{1}{\exp[\beta(\hbar^2 k^2/2m - \mu)] + 1} \tag{2.104}$$

when q in equation (2.103) is small compared to K_f the numerator of the integrand can be expanded about its value at q = o

$$f_{k\pm\frac{1}{2}q} = f_k \pm \frac{\hbar^2 k}{2m}.q\frac{\partial}{\partial\mu} f_k + O(q)^2 \tag{2.104}$$

where μ is the Fermi energy.

The static result in equation (2.103) can be modified by adding the quantity $\hbar w$ to the denominator of the integrands. This more general form is of considerable importance in the theory of Lattice vibrations in metals, as well as in the theory of superconductivity. Here we note that when q approaches zero at fixed w, the Lindhard dielectric constant

$$\varepsilon(q,w) = 1 + \frac{4\pi e^2}{q^2} \int \frac{dk}{4\pi^3} \frac{f_{k-1/2q} - f_{k+1/2q}}{\hbar^2 k.q/m + \hbar w} \tag{2.105}$$

reduces to the Drude result

$$\varepsilon(w) = 1 - \frac{w_p^2}{w^2} \tag{2.106}$$

where w_p is known as plasma frequency, given by

$$W_p^2 = \frac{4\pi ne^2}{M} \tag{2.107}$$

where n is the number of electron, e is the electronic charge and m is the mass of electron.

Which we derived under the assumption of a spatially uniform disturbance. [Ziman, 969, Harrison, 1980 and Bowen et al, 1994]

2.15 FERMI SURFACE

In metals, there are many states whose energy is equal to Fermi energy. Since the energy of each state is a continuous function of the wave vector k, this relation $E_j(k) = E_F$ describes a continuous surface in k-space, which separates the region of occupied from the region of unoccupied states. This region of separation is called the Fermi surface.

The Fermi surface is the surface of constant energy E_F in k-space which separates the filled and unfilled orbital at absolute zero. Based on the free electron approximation, all such surfaces are

spheres. If there volume V conduction electrons per cell, the volume of this sphere must be sufficient to contain VN states.

$$VN = \left(\frac{2N\Omega}{(2\pi)^3}\right)\left(\frac{4\pi}{3}\right)K_F^3 \qquad (2.108)$$

where K_F is the electron wave vector at the Fermi, surface N is the number of states, V is the volume and Ω is the atomic volume for face centre cubic fcc.

$$K_F = \left(\frac{3\pi^2 V}{\Omega}\right)^{1/3} = 1.24\left(\frac{2\pi}{a}\right) \qquad (2.109)$$

where a is the lattice constant

This gives us the radius of the Fermi surface containing V electrons, where

$$\Omega = \frac{1}{4}a^3 \qquad (2.110)$$

is the atomic volume appropriate for fcc, a is the lattice constant. The Fermi surface have portion in the second and higher zones. (Busch and Schade 1976)

2.16 TRANSPORT EQUATION AND DYNAMIC PROPERTIES

The transport equation explain how Landau applied the concept of local energy to the study of the dynamical properties of the Fermi liquid. To set up the transport equation for the flow of

quasi-particles, Landau considered $\varepsilon_p(r,t)$ as the classical Hamiltonian of the system that depends on

the time t through the distribution function $n_{p\sigma}(r,t)$, like

$$\varepsilon_p(r,t) = \varepsilon_p + \sum_{p\sigma} f_{\sigma\sigma'}(P,P')\delta n_{p'\sigma'}(r,t) \qquad (2.111)$$

where ε_p is the excitation energy, $f_{\sigma\sigma'}(P,P')$ is the interaction between two quasi-particle and $n_{p'\sigma'}(r,t)$ is the distribution function.

This assumption can be justified for systems with short-range forces. The Boltzmann equation.

$$\frac{\partial n_{p\sigma}}{\partial t} + \nabla_r n_{p\sigma} \cdot \nabla_p \varepsilon_p - \nabla_p n_{p\sigma} \cdot \nabla_r \varepsilon_p = I(n_{p\sigma}) \qquad (2.112)$$

where $I(n_{p\sigma})$ is the collision integral. This does however, involve the distribution $n_{p\sigma}$ over all momentum space including where it makes no sense. To resolve this apparent difficulty, we linearize the equation by writing

$$n_{p\sigma}(r,t) = n^o{}_{p\sigma} + \delta n_{p\sigma}(r,t) = \bar{n}^o{}_{p\sigma} + \delta \bar{n}_{p\sigma}(r,t) \qquad (2.113)$$

where $n^o p\sigma$ and $\bar{n}^o p\sigma$ are independent both of r and t.

$$\frac{\partial}{\partial t}\delta n_{p\sigma} + \nabla_r \delta \bar{n}_{p\sigma} \cdot \nabla_p \varepsilon_p = I(\delta n_{p\sigma}) \qquad (2.114)$$

The first term in equation (2.114) measures the departure from actual equilibrium, where the second term (called the diffusion term) measure departure from local equilibrium.

The above result enables us to compute the current carried by the quasi-particle. In absence of collisions, the current J, is given by the conservation equation.

$$\frac{\partial \rho}{\partial t} + divJ = 0 \tag{2.115}$$

where the charge density fluctuation is

$$\delta\rho = \sum_{p\sigma} \delta n_{p\sigma} \tag{2.116}$$

setting $I(\delta n_{p\sigma}) = 0$ in equation (2.114) we obtain

$$\frac{\partial P}{\partial t} + \nabla_r \sum_{p\sigma} \delta \vec{n}_{p\sigma} \nabla_p \varepsilon_p = 0 \tag{2.117}$$

where

$$J = \sum_{p\sigma} \delta \vec{n}_{p\sigma} V_p \tag{2.118}$$

we have

$$V_p = \frac{\partial \varepsilon_p}{\partial p} = \frac{P_F}{M^*} \tag{2.119}$$

where V_p is the velocity of quasi-particle. M^* is the effective mass P_F is the Fermi momentum and ε_p is the excitation energy. Here $J \neq \sum_{p\sigma} \delta n_p V_p$ as would have been expected by forming a wave packet, but is given in terms of the departure from local equilibrium. This can be interpreted physically by rewritting equation (2.118) in the form

$$J = \sum_{p\sigma} J_p \delta n_{p\sigma} \qquad (2.120)$$

where j_p is the current due to the back flow of quasiparticles and μ is the Fermi energy or chemical potential, and $f_{\sigma\sigma'}(P,P')$ is the interaction between two quasiparticles.

The formation of wave packet fails to give the correct value for the current because a wave packet created from a superposition of quasi-particle states does not represent a single quasi-particle but a collective excitation of the system.

There is an important sum rule that expresses this physical fact clearly for a translationally invariant system. The sum rule establishes a relation between the effective mass M* appearing in the definition of the velocity of a quasi-particle (as obtained by forming a wave packet) and the interaction, $f_{\sigma\sigma'}(P,P')$ between quasi-particles that gave rise to the backflow current in equation (2.121). In a translationally invariant system, and in absence of any periodic potential, the total current is a constant of the motion and of the form in equation (2.120) but with $j_p = p/m$. (This is a consequence of Galilean invariance) By comparing this with equation (2.121) we find an identity that takes the form (for an isotropic system)

$$\frac{1}{m} = \frac{1}{m^*} + \frac{\Omega P_F}{8\pi^3\hbar^3} \sum_{\sigma'} \int_{-1}^{+1} f_{\sigma\sigma'}(\cos\theta)\cos\theta\, d(\cos\theta) \qquad (2.122)$$

Equation (2.122) is useful in the determination of the interaction between two quasiparticle and does not apply to a real metal in which some periodic potential is present.

Most Macroscopic dynamical properties of the interacting electron gas, in particular, those dependent on the response to external fields are consequences of the transport equation (2.111), if the classical Hamiltonian in the later is generalized to include the potential energy due to the external field. The most important consequences of the Fermi liquid theory, which is central in the

theory of elementary excitations of the valence electron gas in a metal are concerned with the spontaneous oscillations of the Fermi liquid in the absence of any external field. The driving force is provided by the fluctuations in the distribution function

$$\delta n_p(r,t) \sim \delta n_p \exp[i(qr - wt)] \qquad (2.123)$$

Which creates a self-consistent field. This is analogous to the plasma oscillations arising from density fluctuation, δρ, in Bohm and Pines theory, by virtue of the relation (2.116) between δρ and $\delta n_{p\sigma}$. These Oscillations correspond to the elementary excitations of the Fermi liquid and have two characters, namely, particle-like excitations and collective modes. The excitation energy $\hbar w_q$ is determined from equation (2.114) and (2.123) by

$$qV_p \delta \bar{n}_{p\sigma} - w_q \delta n_p = 0 \qquad (2.124)$$

or

$$(qV_p - w_q)\delta n_{p\sigma} + qV_p \delta(\varepsilon_p - \mu) \sum_{p'\sigma'} f_{\sigma\sigma'}(P, P') \delta n_{p'\sigma'} = 0 \qquad (2.125)$$

where w_q is the angular frequency, q is the charge and $n_{p\sigma}$ is the distribution of the quasi-particles.

The particle-like excitations correspond to continuous spectrum, while the collective excitations correspond to discrete spectrum in the solutions of this equation. The change-over from one type of excitations to another depends on the strength of the quasi-particle interactions. (Animalu, 1977).

2.17 CONCEPT OF ELEMENTARY EXCITATIONS

There are two ideas behind the concept of elementary excitations.

i. The idea that the total binding energy of the ground state is not a very important physical quantity, and does not have much to do with the behaviour of a physical system. What is important physically is the behaviour of the lower excited state relative to the ground state which are likely to be excited at relatively low temperature or by weak external fields. Here, we think immediately of a metal or semiconductor in which all the behaviour is determined by the low excited state which we speak of as having a few moving charge carriers, or of the elastic or thermal properties of a solid determined by the presence of a small number of Lattice waves, which is call phonons. Thus our interest is often focused on the set of low-lying excited states of a system as the physically most fundamental property of it. (Anderson, 2000).

ii. The low-lying states are of a particular simple character, and can be treated with much greater mathematical rigor and physical understanding than other states. Because, in spite of the minimizing effects the many-body corrections to the wave function and energy of the true ground state ψ_g are very great in particular the energy of the true ground state and the single particle approximation ψ_{HF} have little or nothing to do with each other because the energy of the true ground state differs in the coordinates of each of the N particles.

To know about the group properties of the ground state in an insulator for instance, the electronic wave function has the fall symmetry of the translation group. $T\psi_g = \psi_g$

For simplicity, consider the excited states of the system with precisely one added particle in Hartree-fock approximation, the lowest such state of a given crystal momentum k would be the state in which the extra electron is in the lowest empty band in the state of momentum k.

$$\psi_k = (C_k^n)^+ \psi_{HF} \tag{2.126}$$

This is of course nothing like an eigenstate. We can however compare the lowest eigenstate ψ_k of momentum k and one extra electron to the true ground eigenstate ψ_g. There will be an operator q^+_k which represents the relationship between these two states:

$$\psi_k = q_k^+ \psi_g \tag{2.127}$$

The most important thing about the operator q^+_k is that it inevitably represents only a very small displacement of the entire system. In these simple case, we see that out of the $N \approx 10^{23}$ electrons only those of momentum k are disturbed to a finite amount. In more complicated cases, it may be that every electron is displaced as in a plasma oscillation but only by an infinitesimal amount.

Thus, as far as almost all the electron are concerned the lowest eigenstate ψ_k is the same nearly as the energy of the true ground state ψ_g. For example, consider a wave packet made up from momentums near a central value k_o.

$$\psi_{packet} k_o, r_o = \int \exp\left[-ik.r_o - \frac{1}{2}\left(\frac{k-k_o}{\Delta k}\right)^2 \right] \psi_k dk \tag{2.128}$$

The resulting disturbance in the wave function will be localized to the region near r_o of size $1/\Delta k$. If the wave function were truly Hartree-Fock, this would necessarily be so.

$$(\psi_{packet})_{HF} = \int \exp -ik.r_o \exp\left[-\frac{1}{2}\left(\frac{k-k_o}{\Delta k}\right)^2\right] C_k^+ \psi_{H-F}\, dk$$

$$= \int dr \left(\int e^{-ik(ro-r)} \exp\left[-\frac{1}{2}\left(\frac{k-k_o}{\Delta k}\right)^2\right] dk \right) \psi^*_{(r)} \psi_{HF} \qquad (2.129)$$

$$= \left(\int dr f_{packet}{}^{(r)} \psi^*_{(r)} \right) \psi_{HF}$$

where

$$f_{packet}(r) \propto e^{(k_o(r-r_o)} \exp\left[-\left(\frac{\Delta k}{2}\right)^2 (r-r_o)^2\right] \qquad (2.130)$$

In the more general case, the formation of a packet will result in a disturbance of the true ground state ψ_g which is localized. The operator

$$q^+_{packet}(r_o, k_o) = \int dk \exp\left[-ik.r_o - \frac{1}{2}\left(\frac{k-k_o}{\Delta k}\right)^2\right] q^+_k \qquad (2.131)$$

is an operation which creates only a localized disturbance.

Forming a wave function which has two of these wave packets present (Anderson, 2000).

$$\psi(k_o, r_o : k_o^1, r_o^1) = q^+(k_0, r_0) q^+(k_o^1, r_o^1) \psi_g \qquad (2.132)$$

where $k_o \neq k_o^1, r_o \neq r_o^1$ we can expect that the two packets will not interfere with each other very much, for most of the possible values of r_o and r_o^1. thus if the excited state ψ_k has excitation energy $E_k = (\psi_k/x/\psi_k) - E_g$, we can expect that the excited state containing two such excitations has the sum

of the two energies, to order 1/N (that being the order of the actual overlap of the two wave functions)

$$E(k_a, k_a^{1}) = E_{k_a} + E_{k_a^{1}} + 0(\frac{1}{N}) \qquad (2.133)$$

This is the fundamental thought behind the concept of elementary excitations: that in a very large system two such excitations will not interfere, whether they be simple quasiparticles such as phonons, excitations, or something even more complicated. Thus, when the number of excitations present is sufficiently small, the properties of the system and particularly the energy, will be a linear superpositions of the properties of noninteracting elementary excitations. Another consequence in this case is that two operators $q_{k's}$ which are not interacting will have the true fermion anticommutation rules. It is not easy to show but it is true that we can always take the operators as having fermion commutation rules in general. (Anderson, 2000).

A preliminary definition we can make of an elementary excitation is that, an elementary excitation of momentum k is that operator which creates the lowest excited state of a particular type of momentum k from the ground state. From the above reasoning, we expect these excitations to interact only weakly in order 1/N, so that the system can contain relatively large number of them, and thus be in a state of very high degree of excitation in terms of absolute number n of excitations, and still we can treat the excitations as an approximately noninteracting gas of independent particles. It is important to realize that the above idea of packet formation is not confined to the particular type of excited state discussed, but may be applied to lowest eigenstates chosen in such a way as to represent single phonons, spin waves, etc.

Another way of saying it is that the concept of elementary excitations is a way of linearizing the equations of the system about the true ground state rather than about some independent particle approximation.

The approximate independence gives a common approach to the calculation and the understanding of thermal and transport properties. Treating the elementary excitations as to a zeroth approximation, a gas of none interacting Bose or Fermi particles as the case my be, and then the statistical mechanics and transport theory is not more difficult than they are for a perfect none interacting gas. (Anderson, 2000).

CHAPTER THREE

RESEARCH METHODOLOGY

In this chapter, a description of how the research was carried out is explained.

3.1 ELECTRON-ELECTRON INTERACTION

In metals, there are three basic screened coulomb interactions. These are (i) the effective interaction between two external "test" charges (ii) the interaction between an electron and a test charge (iii) the effective interaction between two electrons.

Consider an electron-electron interaction. The interaction potential between the two electrons is

$$V(q) = \frac{4\pi e^2}{q^2} \tag{3.1}$$

As a result of the screening, the electrons avoid each other due to the Pauli principle and due to their mutual coulombs repulsion. This interaction can be written as

$$U_{int} = \frac{V(q)}{\varepsilon(q)} \tag{3.2}$$

where $\varepsilon(q)$ is dielectric constant. The dielectric constant is expressed as

$$\varepsilon(q)=1+\frac{\lambda_s^2}{q^2} \tag{3.3}$$

where λ_s is the inverse Thomas Fermi screening length.

$$U_{int}(q)=\frac{\frac{4\pi e^2}{q^2}}{1+\frac{\lambda_s^2}{q^2}}$$

$$U_{int}(q)=\frac{4\pi e^2}{q^2+\lambda_s^2} \tag{3.4}$$

Fourier transforming we have

$$U_{int}(r)=\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} V(k)\exp(ikr)dk \tag{3.5}$$

$$U_{int}(r)=\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{4\pi e^2}{k^2+\lambda_s^2}\exp(ikr)dk$$

$$U_{int}(r)=\exp\frac{(-\lambda_s r)}{r} \tag{3.6}$$

The effective interaction between an electron on the Fermi surface ($K=K_F$) and a test charge is given as (Kukkonen and Wilkin, 1979)

$$U_{int}=Z(K_F)\Lambda(K_F,r)U_{int}(r) \tag{3.7}$$

where $Z(K_F)$ is the vertex function $Z(K_F)$ is the quasiparticle renormalization factor.

Since the two electrons exchange with the screening electrons independently, each electron acquires a vertex correction and the approximated effective interaction between electrons with opposite spins is

$$U_{sc} = [Z(K_F)\Lambda(K_F, q)]^2 U_{sc}(r) \tag{3.8}$$

since Thomas Fermi interactions is used in this work. both $Z(K_F)$ and)$\Lambda(K_F,q)$ are considered to be unity.

The compressibility is the derivative of the total energy with respect to volume

$$K = \left(V \frac{\partial^2 E}{\partial V^2} \right)^{-1} \tag{3.9}$$

The ratio of the compressibility of a system of non-interacting electrons to the compressibility of the electron gas K is given by Kukkonen and Wilkins (1979) as

$$\frac{K_{sc}}{k} = 1 - \frac{\alpha r_s}{\pi}\left[1 + \frac{0.0335\pi\alpha r_s}{2} + \frac{0.02\pi\alpha r_s^2}{3}\left(\frac{0.1 + 2r_s}{(0.1 + r_s)^3}\right)\right] \tag{3.10}$$

in the low wavelength limit (small q) the effective interaction is determined by the compressibility

$$Uee = \frac{4\pi}{\lambda_{TF}^2}[k / K_o] \tag{3.11}$$

where λ_{TF} is Thomas Fermi screening parameter.

3.2 THERMAL RESISTIVITY MODEL

The thermal resistivity of metals is given by

$$W = \left(\frac{3}{C_v V_F^2}\right)\left(\frac{2\pi^2}{3k\tau_a}\right) \tag{3.12}$$

where Cv is the specific heat capacity, V_F is the Fermi velocity, τ_a and k are related to angular averages of the scattering rate. The relaxation time for quasiparticle at the Fermi surface is $2\tau_a/\pi^2$ where $1/\tau_a$ is proportional to an angular average of the scattering rate (Kukkonen and Wilkins, 1979).

$$\frac{1}{\tau_a} = \frac{M^3(K_B T)^2}{8\pi^4\hbar^6}\left\langle W(k_1, K_2, k_1+q, k_2-q)\right\rangle \tag{3.13}$$

k depends weakly on another average of the scattering rate. The scattering rate is the rate for the scattering of two quasiparticle from the state K_1 and K_2 both on the Fermi surface to states K_1+q and K_2-q, also on the Fermi surface.

The total scattering rate is related to the centre of mass scattering and is given (Kukkonen and Wilkins, 1979) as

$$W(k_1, K_2, k_1+q, k_2-q) = \frac{2\pi}{\hbar}\left(\frac{2\pi\hbar^2}{\mu}\right)\left(\frac{\sigma(\theta)}{2}\right) \tag{3.14}$$

where μ is reduced mass, $\hbar$ is normalized planck's constant $\sigma(\theta)$ is the centre of mass scattering angle.

Hence

$$\frac{1}{\tau_n} = \frac{2(K_B T)^2}{\pi\hbar(e^2/a_n)}\frac{1}{a_n^2}\left\langle \frac{\sigma(\theta',\phi)}{Cos\frac{1}{2}\theta'} \right\rangle \tag{3.15}$$

where (Kukkonen and Smith, 1973)

$$\left\langle \frac{\sigma(\theta',\varphi)}{Cos\frac{1}{2}\theta'} \right\rangle = \frac{a_n^2}{4\pi}\int_{\cdot} \frac{dE}{2E_F}\frac{\sum(E)}{\left[1-(\quad/2E_F)\right]^{1/2}} \tag{3.16}$$

and

$$\sum(E) = \sigma_n + \frac{a\sigma_1}{2} + \frac{55\sigma_3}{32} + \left(\frac{10\pi}{2E_F\mu}\right) Sin\delta_n Sin\delta_2 \cos(\delta_n - \delta_2) \tag{3.17}$$

Kukkonen and Smith (1973) used a screened coulomb potential and calculated the scattering phase shifts for l =0, 1 and 2 to get the scattering cross section. They used the exact solution of the Boltzmann transports equation to derive the following interpolation formula for the thermal resisitivty as (Iwamoto, 1999)

$$W = 1.10x10^{-8}\left(r_s^{5.04}/A^{3.06}\right) TCmK/W \tag{3.18}$$

where r_s is electron gas parameter and

$$A = \lambda_s / r_s^{1/2} K_F \tag{3.19}$$

K_F is Fermi wave vector and T is absolute temperature. Hence

$$\frac{W}{T} = 1.10x10^{-4}\left(r_s^{5.04}/A^{3.06}\right) CmK/W \qquad (3.20)$$

A FOTRAN 90 computer programme was developed to calculate the Thomas Fermi screening parameter, the electron-electron interaction parameter and thermal resistivity of 44 elemental metals based on the equations given above.

CHAPTER FOUR

RESULTS AND DISCUSSION

In this chapter the result obtained from the model and equations given in chapter three are obtained. The parameters were calculated based on the FORTRAN 90 computer programme developed based on the equations given in chapter three.

4.1 SCREENED INTERACTION POTENTIAL

Figures 4.1, 4.2, 4.3, 4.4 and 4.5 shows the variation of screened interaction potential with distance for alkaline, earth-alkaline, group three and transition metals. As shown in the figures the interaction for $r > 1\,\mathring{A}$, the screened interaction potential is nearly the same for all the metals in a group. But for $r < 1\,\mathring{A}$, the screened interaction potential is different for different metals in a group. For group one, two and three metals, at any point, the screened interaction potential increase down the group. This suggests that the higher the electron density concentration the higher the screened electron interaction potential. Figures 4.1, 4.2 and 4.3 reveals that the alkaline metals have the highest screened interaction potential showing that the higher the electronic concentration, the higher the screened interaction potential. The screened interaction potential of transition metals shown in figures 4.4 and 4.5 do not follow any particular trend just as their electron density concentration do not follow a particular trend. Of all the metals investigated, caesium has the highest screened interaction potential of 29.95ev at $r = 0.5\,\mathring{A}$. These show that screened interaction potential depends on the density of valence electrons present in metals.

Figure 4.6 shows the variation of electron-electron interaction with electron density parameter for different metals calculated using equation (3.11), figure 4.6 reveals that as r_s increases, the electron-electron interaction increase. There is an exponential increase in the electron-electron interaction for $4 \leq r_s \leq 5.5$. In this density region, we have the alkaline metals.

The results obtained for the electron-electron interaction calculated using the compressibility sum rule is in perfect agreement with the screened interaction potential obtained in figure 4.1. the electron-electron interaction potential calculated using the compressibility sum rule for ceasium (Cs) has negative value of the compressibility ratio which result from the divergence of the compressibility at $r_s = 6.03$ (Kukkonen and Wilkins, 1979).

4.2 COMPRESSIBILITY RATIO

Figure 4.7 shows the variation of compressibility ratio with electron gas parameter for different metals calculated using equation (3.10). Figure 4.7 reveals that the compressibility ratio decreases with an increase in the electron gas parameter. As shown in figure 4.7, the compressibility ratio decreases with an increase in the electron gas parameter. This seems to suggest that electrons in metals in the high density limit have lower polarizability and higher compressibility while electrons in metals in the low-density limit have high polarizability and low compressibility.

The trend exhibited by the compressibility ratio suggests that the higher the number of valence electrons the smaller is the compressibility ratio. The compressibility ratio obtained in this work is in perfect agreement with the theoretical prediction of Kukkonen and Wilkins, (1979).

4.3 SCREENING PARAMETER

The screening parameter is the distance within which the screening effect can be felt. Figure 4.8 shows the variation of the screening parameter with electron density parameter for metals. As revealed in the figure, as the electron density parameter increase the screening parameter (length) increases with increase in electron density parameter. Figure 4.8 reveals that metals in the high-density limit has low screening parameter. In the high-density limit, we have the transition and

noble metals. The Alkaline metals in the low-density limit ($r_s > 4\overset{\circ}{A}$) have high screening parameters. This may be due to the high number of valence electrons in these metals.

Figure 4.9 show the compressibility ratio as a function of screening parameter. As revealed by figure 4.9, the compressibility ratio decreases with increase in the screening parameter. This suggests that metals with high screening parameters like the alkaline metals has small compressibility ratio. Also, this seems to suggest that screening has an inverse effect on the compressibility ratio.

4.4 THERMAL RESISTIVITY

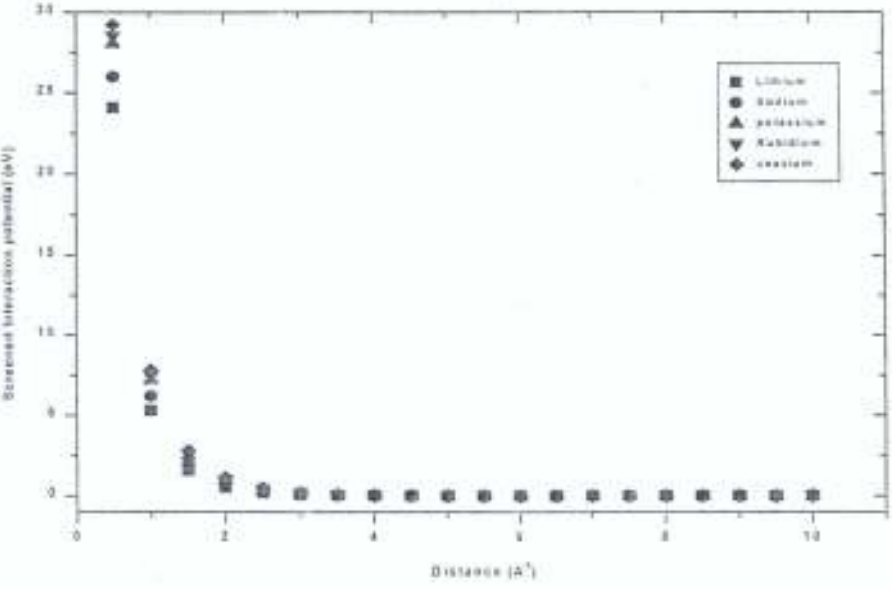
The variation of thermal resistivity with electron density parameter r_s is shown in figure 4.10. As revealed by figure 4.10, for the transition metals and inner transition metals in the high-density limit, $r_s \leq 2.75$ a.u the calculated thermal resistivity of metals in the region is small and does not increase so much as we move from one metal to another. But for $3 \leq r_s \leq 5.8$ a.u the thermal resistivity of metals in this density region increase as we move from one metal to another and they have relatively high values compared to metals in the high-density region. This may be due to the large number of valence electrons found in metals in the low-density region. Furthermore, the results show in figure 4.10 indicates that the thermal resistivity of metals is highly affected by the valence electrons in the metals. Thus thermal resistivity of metals arises or has a great contribution from the valence electrons in the metals.

Figure 4.11 shows the variation of thermal resistivity with screening parameter for metals. Figure 4.11 exhibits the same trend as figure 4.10. Figure 4.11 shows that the thermal resistivity increases slowly with screening parameter till when the screening parameter is 0.55 $\overset{\circ}{A}$. But when the screening parameter is above 0.57 $\overset{\circ}{A}$, the thermal resistivity increases exponentially with the screening parameter. Figure 4.11 seems to suggest that the screening between the electrons affects

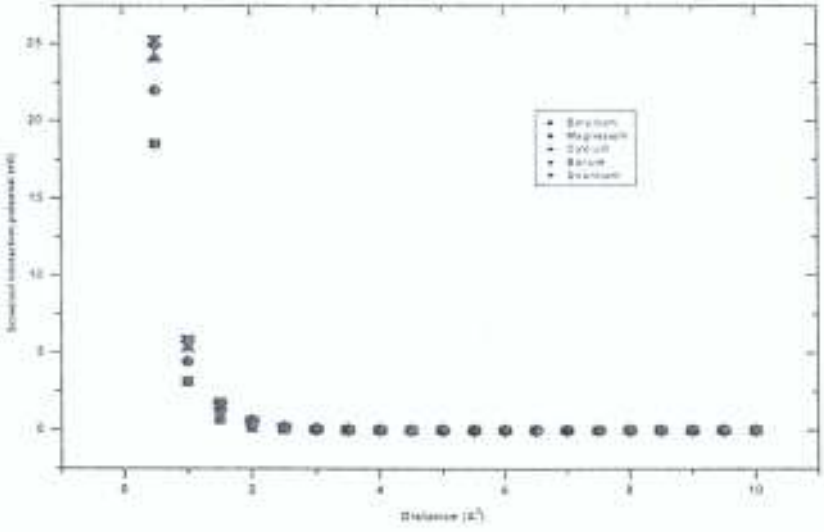
the thermal resistivity of the metals as metals with small screening parameter have small thermal resistivity and metals with high screening parameter has high thermal resistivity.

Figures 4.12, 4.13, 4.14 and 4.15 respectively shows the variation of thermal resistivity with temperature for alkaline, alkaline-earth, group three metals and transition metals respectively. The figures shows that thermal resistivity of the metals increases with an increase in temperature. This may be due to the fact that increase in temperature causes an increase in electron-electron interaction which causes an increase in the thermal resitivity of the metals. Comparing figures 4.12, 4.13 and 4.14 one can observed that at any given temperature, the thermal resistivity of alkaline metals is the highest followed by the alkaline-earth metals and least is the group three metals. This trend may be due to the high electronic concentration of the metals as the electronic concentration of the metals exhibits the same trend. Figures 4.12, 4.13 and 4.14 reveals that for a group of metals, the thermal resistivity increases down the group, just as the number of electrons in metals increases down the group.

In figure 4.15, the thermal resistivities of transition metals does not exhibit any trend unlike what is observed in figures 4.12, 4.13 and 4.14, this may be due to the fact that the transition metals are not found in the same group and their electronic concentration varies as we move from one metal to another.



4.1: Variation of Screened Interaction Potential with Distance for Alkaline Metals



4.2: Variation of Screened Interaction Potential with Distance for Alkaline-Earth Metals

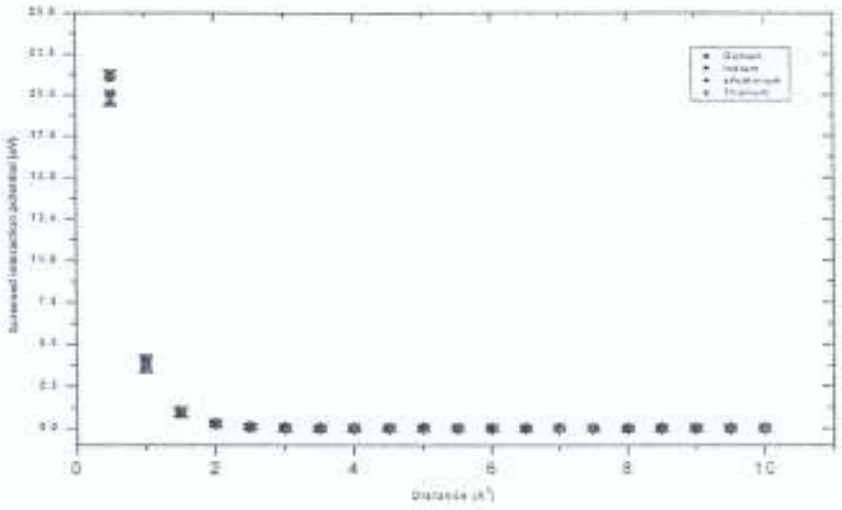


Fig. 4.3: Variation of Screened Interaction Potential with Distance for Group Three Metals

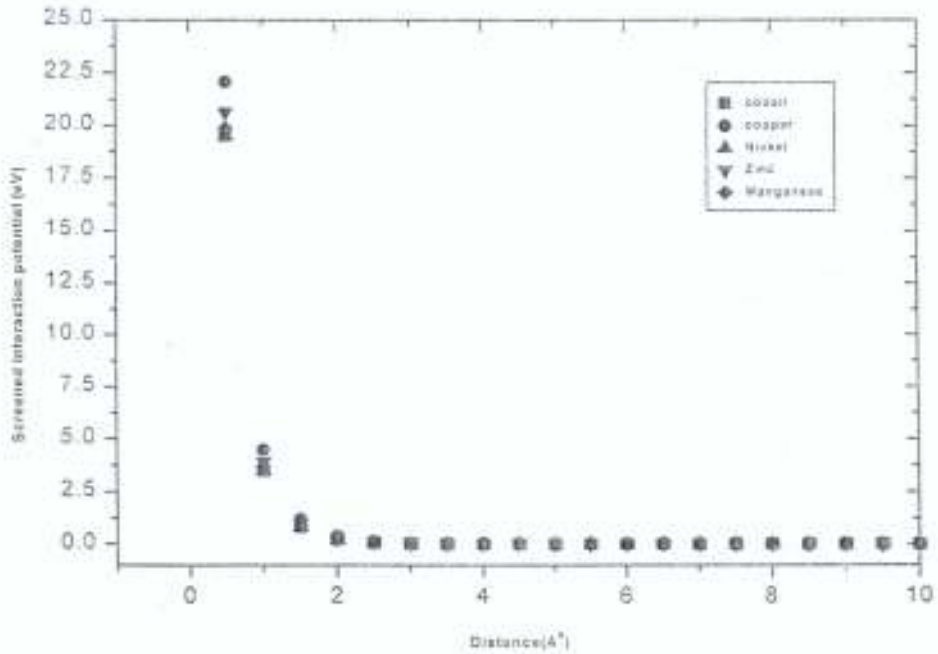
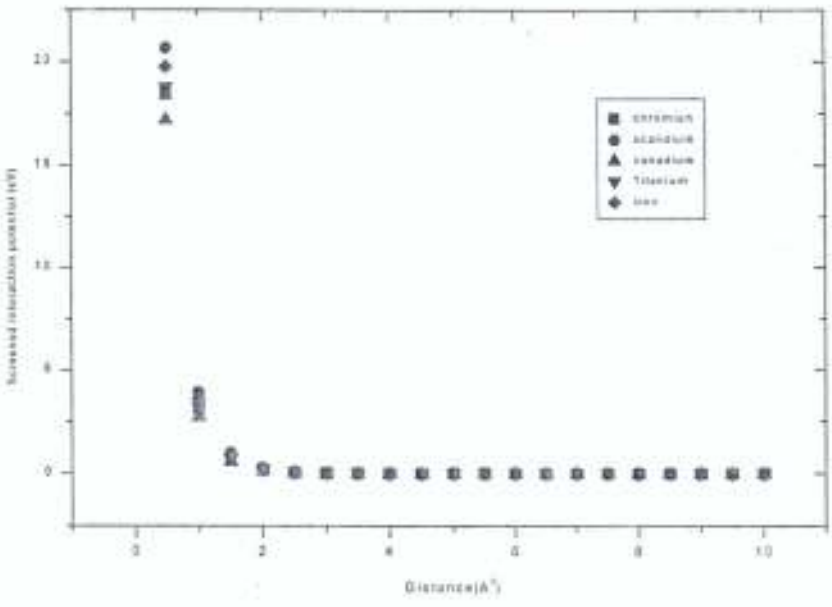
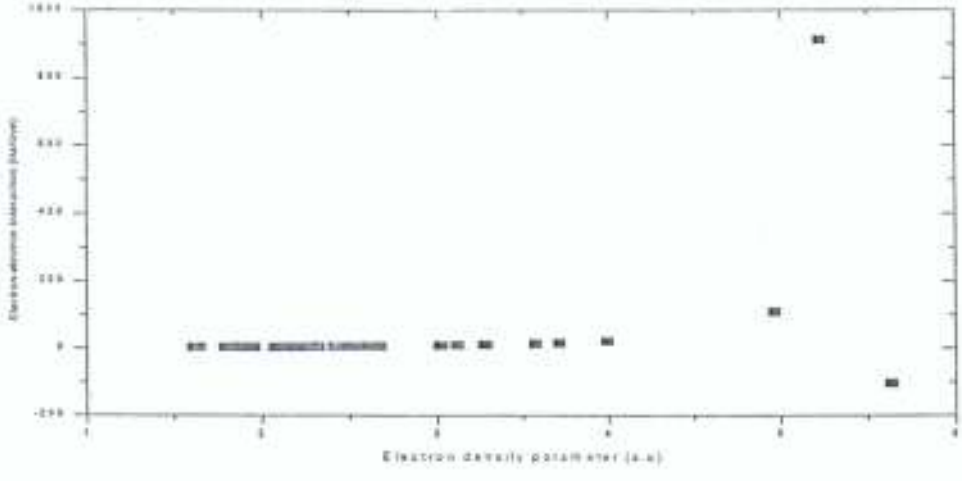


Fig. 4.4: Variation of Screened Interaction Potential with Distance for Transition Metals



ig. 4.5: Variation of Screened Interaction Potential with Distance for Transition Metals



ig. 4.6: Variation of Electron-electron interaction with Electron Density Parameter

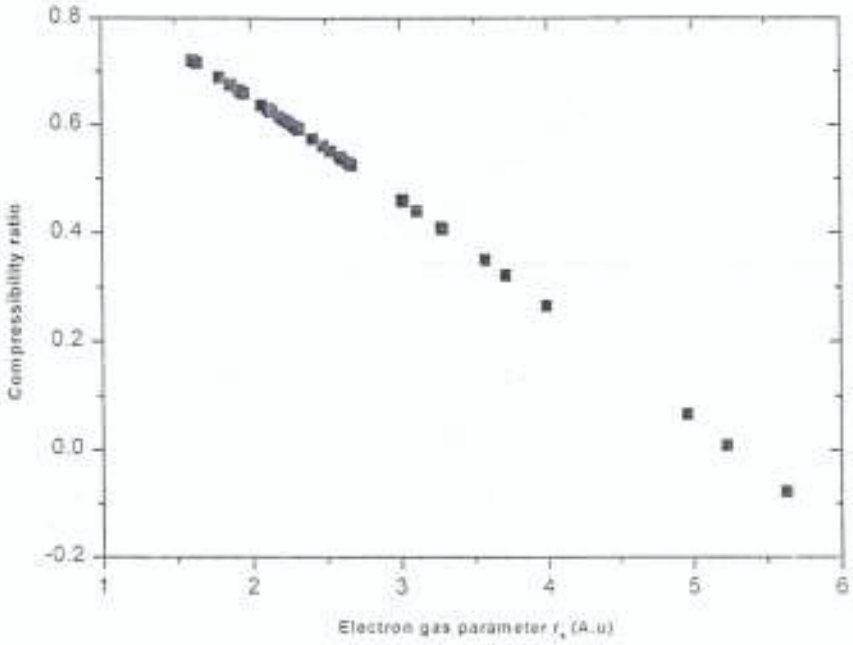


Fig. 4.7: Variation of Compressibility Ratio with Electron Gas Parameter

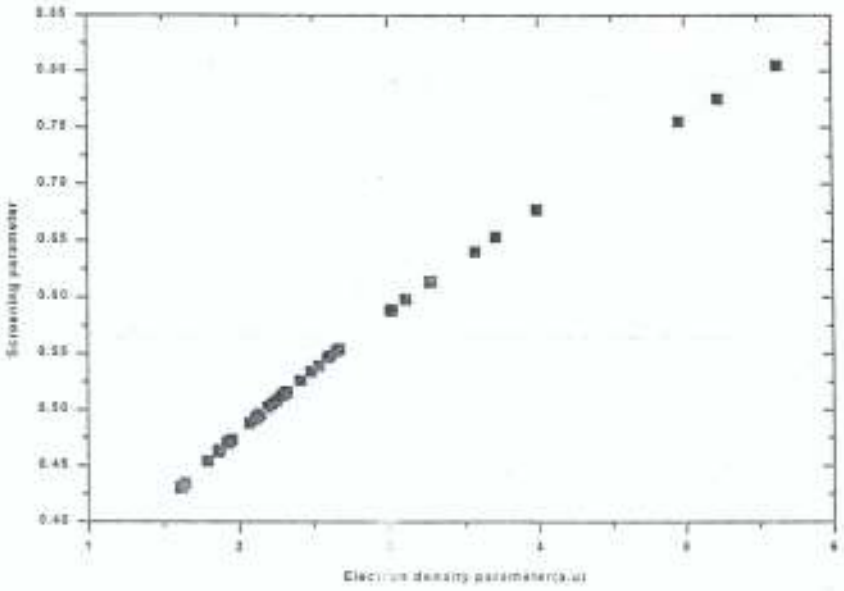


Fig. 4.8: Variation of Screening Parameter with Electron Density Parameter

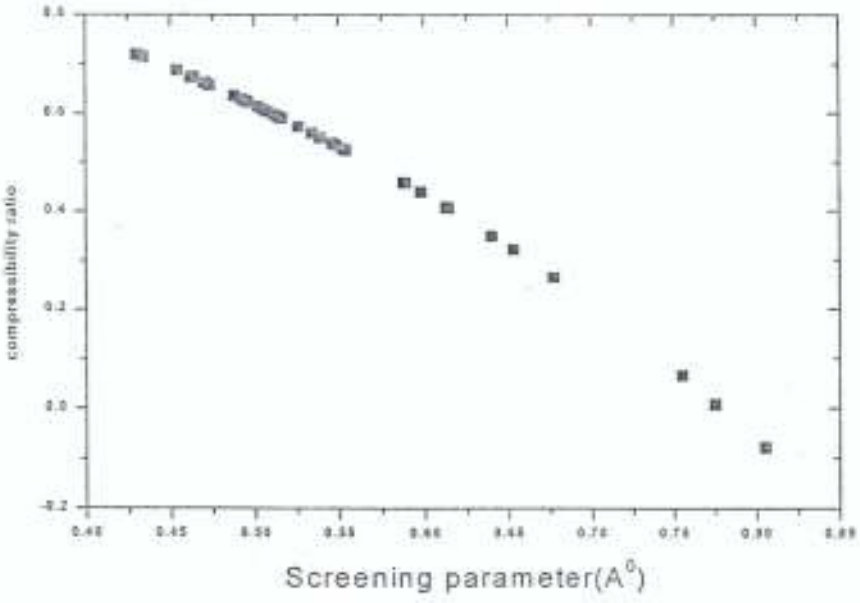


Fig. 4.9: Variation of Compressibility Ratio as a function of Screening Parameter

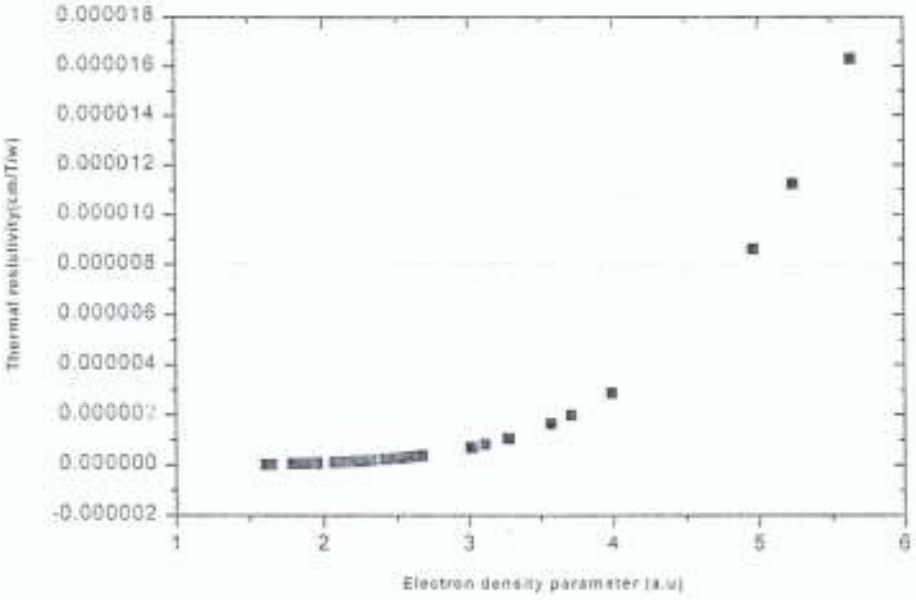


Fig. 4.10: Variation of Thermal Resistivity with Electron Density Parameter

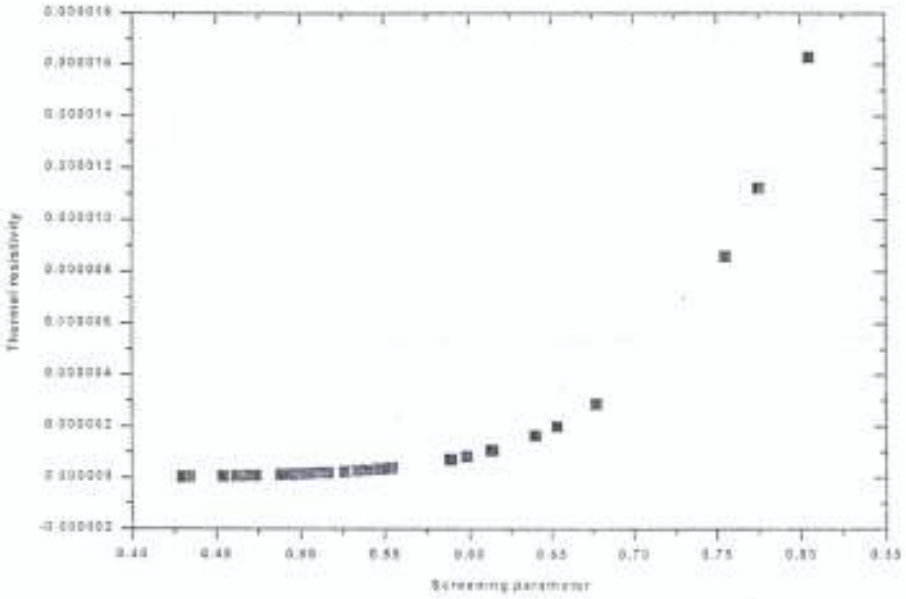


Fig. 4.11: Variation of Thermal Resistivity with Screening Parameter

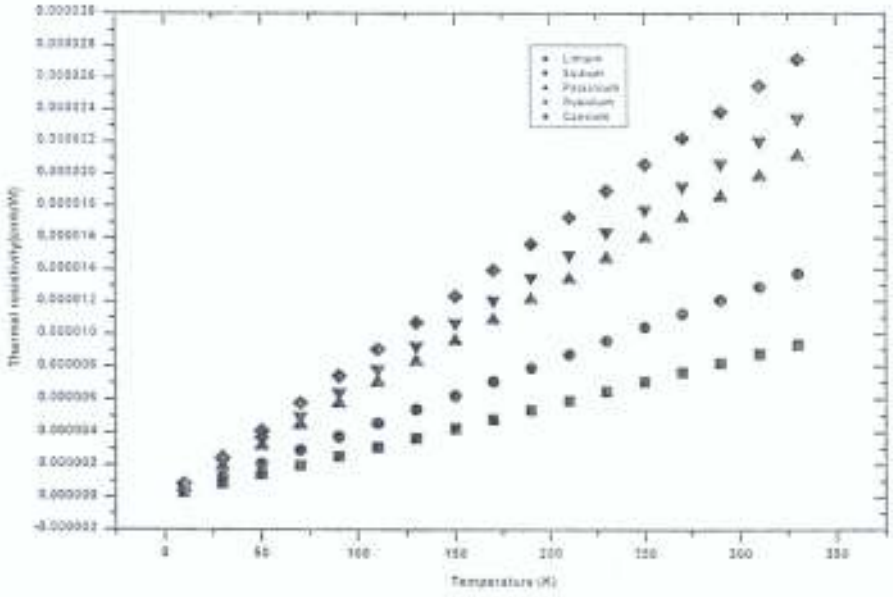


Fig. 4.12: Variation of Thermal Resistivity with Temperature for Alkaline Metals

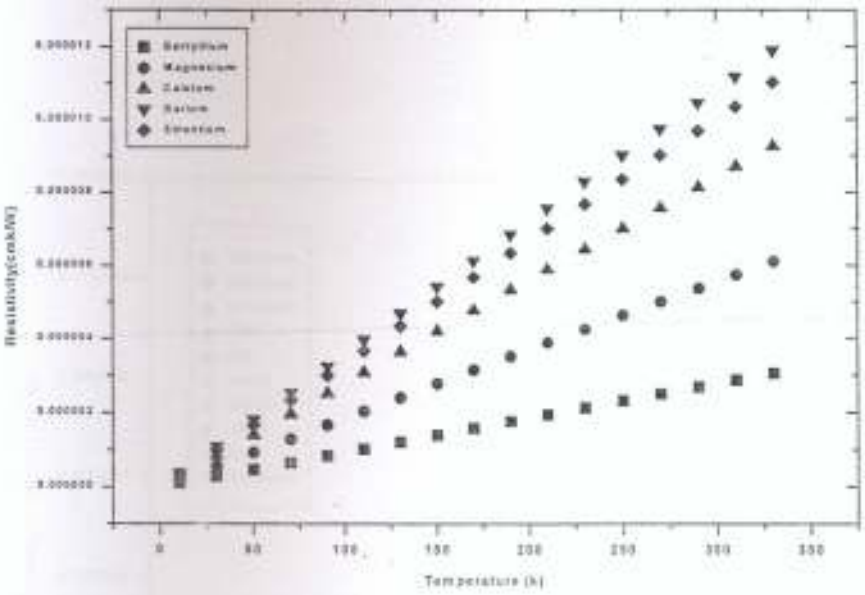


Fig. 4.13: Variation of Thermal Resistivity with Temperature for Alkaline-Earth Metals

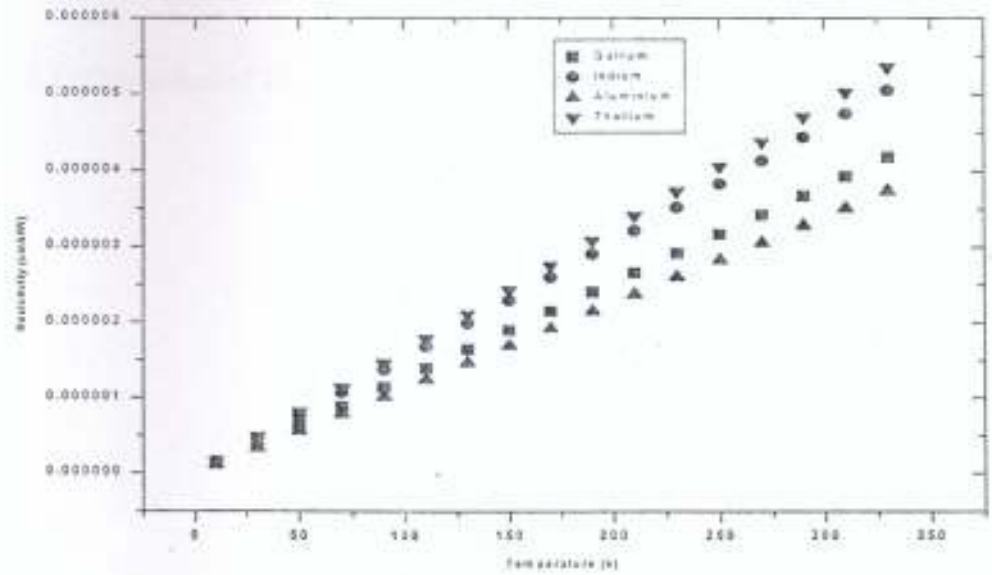


Fig. 4.14: Variation of Thermal Resistivity with Temperature for Group Three Metals

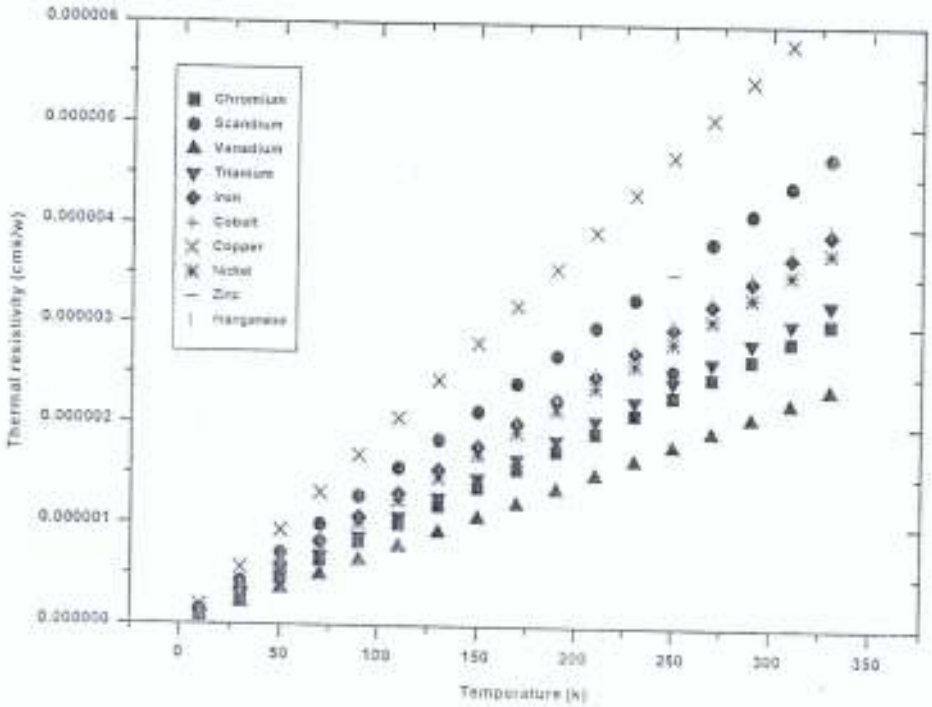


Fig. 4.15: Variation of Thermal Resistivity with Temperature for Transition Metals

CHAPTER FIVE

CONCLUSION AND RECOMMENDATION

5.1 SUMMARY OF THE WORK

In this work, a model for calculating screened electron-electron interaction potential for metals was developed. Also, the compressibility ratio and electron-electron interaction was calculated. Also the free electron screening parameter was calculated

The thermal resistivity of metals, its temperature variation and the effect of electron screening on thermal resistivity of alkaline, earth-alkaline transition and inner-transition metals were investigated. Also the effect of screening on the compressibility ratio was studied.

5.2 CONCLUSION

Thermal resistivity of metals can be explained based on free electrons as the thermal resistivity of metals depends directly on the number of free electrons in a metal.

Electron-electron interaction in metals is effective in small distances from the electron. The electron-electron interaction is more pronounced in alkali metals because of the presence of high valence electrons. Thermal resistivity is affected directly by screening parameter while there is indirectly relationship between compressibility ratio and screening. Down groups one, two and three in the periodic table, thermal resistivity increases while this trend is absent in transition metals.

5.3 APPLICATION OF RESULTS

The results obtained in this study will be very useful to experimentalist as it will act as guide in determining the thermal resistivity of metals. The results will also be very useful in the study of transport properties of solids.

The results will be very useful in further development of theories or models for explaining thermal resistivity and transport properties of solids.

5.4 RECOMMENDATION

Having investigated the effect of screening on thermal resistivity of metals, I wish to make the following recommendations

i. Ab initio method should be used to calculate the thermal resistivity of metals and the result obtained compared with the ones obtained in this work.

ii. The effect of thermal resistivity on other transport properties of metals should be investigated.

iii. Thermal resistivity and compressibility of liquid metals should be calculated and the results obtained compared with the one obtained in this work

REFERENCE

Akira Ishara. (1991).Condensed Matter Physics.Oxford University Press, New York. PP 46-65

Anderson P.W., (2000). Concepts in solids (Lectures in the theoty of solids). World scientific publishing co. pte. Singapore.

Animalu, A. O. E, (1977). Intermediate quantum mechanics of crystalline solids. Eaglewood clif.

Ashcroft, N.W and Mermin, D. N., (1976). Solid state Physics. Holt, Rinehart and Winston, New York.

Bar-Sagi, J.(1976). Calculation of Thermal Conductivity produced by the proximityeffect. Physical Review, Tel Aviv University, Isreal.

Bowen, C. Sugiyama, G. and Alder, B.J. (1994). Static dielectric response of the electron gas. Physical Review B, 50(20): 14838-14840.

Sykes, J. and Brooker, G. A.(1970). The transport coefficients of a Fermi liquid. Oxford, England.

Busch, H., and Schade, H. (1976). Lectures on solid state physics. Zurich, Switzerland.

Harrison, W. A. (1980). Electronic structure and properties of solids. The physics of chemical bonds, W. H. Freeman and company, San Francisco. pp 250-314.

Inkson, J. C. (1984). Many-body theory of solids. Plenum press, New York. pp1-23.

Iwamoto, N., (1999). Effects of screening on the thermal resistivity of metals due to electron-electron scattering. Physical Review B, 59(15): 9687-9690.

Kittel, C. (1976). Introducdtion to Solid State Physics, 5th edition, John Willey, New York.

Kohn, W. (1999). Nobel Lecture: Electronic structure of wave functions and density functional Reviews of Modern Physics 71(5): 1253-1263.

Kukkonen, C. A., and Smith, H. (1973). Validity of the Born approximation as applied to Electron-Electron scattering in metals: Implications for thermal conductivity. Physical Review B, 8(10): 4601-4606.

Kukkonen, C. A., and Wilkins, J. W (1979). Electron-electron scattering in simple metals. Physical Review B, 19(12): 6075-6093.

Lundmark, L. (1990). The Umklapp scattering contribution to the electron-electron scattering part of the thermal resistivity in alkali metals. Condense Matter 2:9309-9322.

Lundmark, L. (1998). The exchange and correlation contribution to the electro-electron scattering part of the thermal resistivity in alkali metals. Condense Matter 8:1021-1040.

MacDonald, A. H., and Geldert, D.J.W. (1979). Electron-Electron scattering and the thermal resistivity of simple metals. Metal phys. 10:677-692.

Mahan, G.D. (1990). Many Particle Physics 2nd edition, Plenum Press, New York.pp419-483.

Peter, T., (2002). Fermi liquid theory, Physical Review B. pp1-11.

Pecheur P. and G. Toussaint, (1972). Thermal-Resistivity Anisotropy of Zinc and Cadmium. Physical Review B, France.

Semat, H., and Albright, J.R., (1972). Introduction to atomic and nuclear physics. Norwich, Great Britain.

Stanley, R. (1963). The wave mechanics of electrons in metals, first edition. Amsterdam, North Holland, pp270-274

Wilkes, P. (1973). Solid State theory in metallurgy. Cambridge University Press. pp233-251.

Ziman, J. M. (1969). Principles of the theory of solids. Cambridge University Press, New York, pp30-110