ON THE EFFECT OF THE ENERGY SPECTRUM ON THE CONDUCTION IN SOLIDS

THESIS

Submitted to

Ain Shams University

in Partial Fulfilment of the Requirements for the Degree

Of

MASTER OF SCIENCE

By

Essayed Mohamed Abd El Rahman

Department of Applied Mathematics

Faculty of Science

Ain Shams University

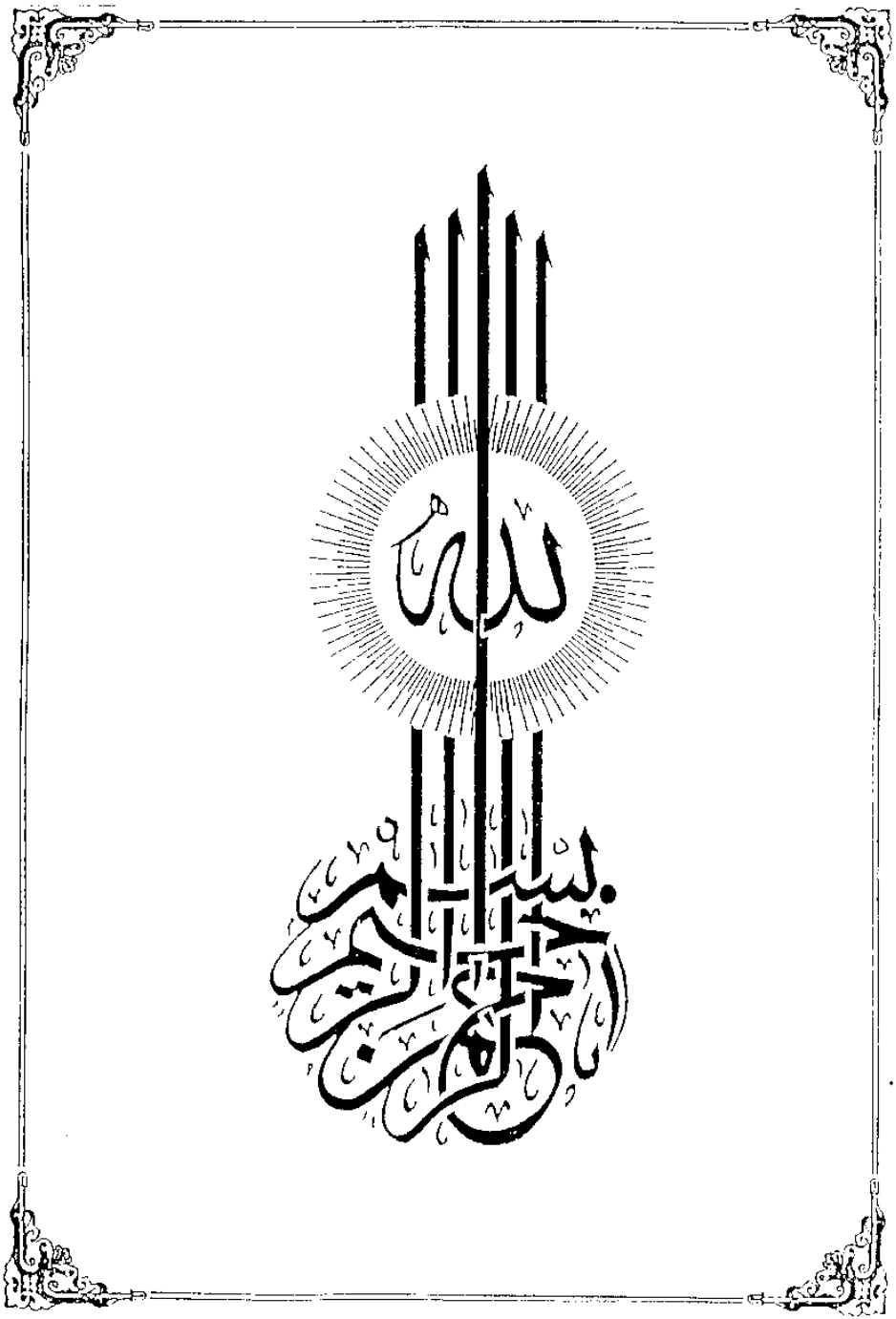
Cairo

1977

ACKNOWLEDGEMENT
==========

I wish to express my thanks to Professor Dr. I.I. Hanna, Head of Applied Mathematics Department for his helpful guidance, useful criticism under his supervision, and encouragement throughout this work.

---oooOooo---



ON THE EFFECT OF THE ENERGY SPECTRUM ON

THE CONDUCTION IN SOLIDS

Thesis Advisor

Prof. Dr. I. I. HANNA

Approved

I. I. Hanna

I. I. Hanna

Prof. Dr. I. I. HANNA

Head of Applied Maths. Dept.

S U M M A R Y

The scattering of electrons by optical modes of phonons is considered for when the energy of phonons is assumed to diverge from the usual assumption $h\nu_o$, the frequency ν_{op} assumed to follow a dispersion law

$$\nu_{op} = \nu_o' - Aq^2$$

In chapter one we give a short survey of all existing theories and the usual approximations used to solve the Boltzmann equations for electrons.

In chapter two we set up the Boltzmann equation for the distribution function of the electrons assumed to be scattered by phonons only. The results obtained, assuming the above relation is completely different than what is obtained before. The result of this consideration led to the split of transport equation into two different forms, each is valid for a range of energy compared with $h\nu_o$, ν_o being the maximum frequency in the optical branch of phonon dispersion relation.

Chapter three is devoted for the solution of the Boltzmann equations in the two different ranges of electron energy spectrum and the relevant expression for the electric and thermal current densities are obtained. The corresponding

electric " σ" and thermal "K " conductivities are calculated and a proper formula for the thermoelectric power $\mathcal{S}$ is deduced. The results so- obtained for σ and $\mathcal{S}$ are compared with their corresponding values σ_0 and $\mathcal{S}_0$ deduced assuming $\nu_q = \nu_0$.

In chapter four we construct the Boltzmann equations in the presence of a magnetic field and solve them in a way similar to that of chapter three. The results of σ and K when compared with those obtained before are altered in a ratio similar to that of chapter three.

We conclude that more studies of the effect of the phonon energy spectrum on the electron conductivities, particularly in the optic range, are necessary, to reveal the exact role of the phonon-electron scattering in the conduction theory of semi-conductors.

M. Sc. COURSES

STUDIED BY THE AUTHOR (1974-1975)

1. Solid State Physics. (3 hours per week).

2. The Theory of Propagation of Electromagnetic Waves (3 hours per week).

3. An Advanced Course in Hydrodynamics (3 hours per week).

J. Hamm

CONTENTS

INTRODUCTION

CHAPTER ONE

CHAPTER ONE

INTRODUCTION

The solid with which we shall be concerned is that material which have a crystalline structure. Such a structure is described interms of a single periodic lattice, but with a group of atoms attached to each lattice point.

Solids are usually divided, according to its conductivity either electrical or thermal, into two distinct categories. Those of high conductivity and known as metals and those of no conductivity and classified under the term insulators. Conductivity of metals is attributed to the charge or energy carries which are the free electrons. A third type of solids is termed semi-conductors and lie, according to its conductivity, midway between metals and insulators. Essentially they are insulators, but owe its conductivity to the presence of metallic impurity atoms which help in transforming the solid from the second category to its position close to the first category. The more these metallic impurities are present, the more we get closer to metallic solids. Such a property gave semiconductors an important character and has been applied intensively.

Now a days, transport properties in different types of solids are understood if we accept the band theory* of solids based upon the early work of "Kornig" and "Penny" (1925) and its extension to semi-conductors given by "Wilson" (1936). According to this theory if we put different values of electronic energy "E" varying from - ∞ to + ∞ in Shrodinger wave equation we find that eigenfunctions arise only for certain ranges of "E", which is the so-called energy bands and that these intervales are separated from each other by intervals in which no eigen-functions are possible. Within each allowed energy interval, the independent eigen-functions can be specified by the wave vector $\underline{K}$. But since the number of allowed $\underline{K}$ - values is very large, it is possible to treat $\underline{K}$ as a continuous variable. Thus within each band of energy $E_n(\underline{K})$, n denoting the energy band, $E_n(\underline{K})$ may be regarded as a continuous function of $\underline{K}$ which is periodic in $\underline{K}$ and has maximum and

- - - - - - - - - - - -

* For detailed discussions of the band theory see Wilson (1953) and or Ziman (1972).

minimum values either within or on the boundary of the first zone. The calculations of the form of the energy bands in actual solids are extremely complicated, but the simplest way in which this can be done is by taking the dependence of the energy on $\underline{k}$ to be expressed in the form of "Taylor expansion". The so-obtained expression in the simplest possible case, where the second order derivative tensor reduces to a scalar, has the form.

$$E_{\underline{k}} = E_0 + \frac{\hbar^2}{2m^*} \underline{k}^2 \qquad (1\text{-}1)$$

where E_0 is the minimum energy in the band, and m^* is the effective mass.

The same effect is produced by considering the periodicity in $V(\underline{r})$ produced by the static (at rest) ions at the lattice points. The same energy spectrum is produced with allowed bands and forbidden gaps. The same calculations (Patterson, 1970 , p. 111) has proved that the periodic nature of the solid, particularly when we are concerned with low concentrations of electrons (as in the case of semi-conductors) may be taken into account by using an effective electronic mass m^* rather than an actual mass m . This is the quasi-free electron model, which we shall adopt for our present purpose of studying the transport effects in semi-conductors.

Atoms (ions) cited at the lattice points are subject to mutually interacting forces which hold the solid together. In the presence of a temperature gradient, these atoms are set into vibrational motion about its positions of equilibrium. The motion of each atom (ion) affects the motion of all other atoms (ions), and we are then concerned, not with individual vibrations of the atoms (ions) but with the collective vibrations of the whole assembly. These collective vibrations take the form of displacement waves spreading throughout the whole volume of the solid. The regular form of the space lattice is reflected on the normal modes of vibrations, each normal mode gives rise to a simple harmonic motion which is also periodic in the same space and consequently has the same effect on atoms in corresponding positions.

Each normal mode is characterized by three parameters the wave vector $\underline{q}$ whose magnitude defines the wavelength " λ " of the wave through the relation

$$\lambda = 2\pi / |\underline{q}| \qquad (1\text{-}2)$$

and whose direction specifies the direction of propagation; the frequency w of the vibration and finally a unit vector ϵ indicating the direction of the displacement of the atoms (ions).

The set of values of $\underline{q}$ bear a one-to-one correspondance with the set of $\underline{K}$ values which are used to define the wave-vector of the conduction electron (see 1-1). Thus $\underline{q}$ is restricted to a set of values equal to the number of unit cells in the crystal and distributed uniformly in the first Brillouin Zone (see Fig. 1-1). But the results obtained for values of $\underline{K}$ outside the Brillouin zone can be shown to possess the same property as same $\underline{K}$ value within the zone. To each value of the wave vector $\underline{q}$ there corresponds a number of normal modes in general having different frequencies w. Thus, the complete set of normal modes is specified by $w_j(\underline{q})$. The subscript j takes an integral values from 1 to 3s where "s" is the number of atoms per unit cell for the particular solid considered. This makes the total number of normal modes conform to the number of degrees of freedom of the whole system, which is three times the number of atoms in the system. The characteristic frequencies $w_j(\underline{q})$ can, in principle, be calculated from a knowledge of the mutual forces acting between the cores.

For a given value of j, as $\underline{q}$ varies, the frequency $w_j(\underline{q})$ varies continually with $\underline{q}$ throughout the Brillouin zone and defines a branch of the so-called vibrational spectrum. The three branches of lowest frequency