CONDUCTION COEFFICIENTS FOR A TWO ENERGY BAND MODEL AND ITS APPLICATION

THESIS

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ABSTRACT

It is the purpose of the present thesis to try to establish a two-carrier conduction theory when the carriers are dragged by phonons. This work was aroused since the increasin[g] need (Issi, 1973; Dil[l]ner, 1983) for a two-carrier theory to account for the observations in narrow-gap semimetals where clear evidence proved that phonon-drag effect on carriers is playing an important role. The existing calculations in the field of the two carrier model are the results of the early work (see Issi, 1973 for references), using thermodynamic methods were able to establish the structural laws for the electrical resistivity, thermoelectric power and thermal conductivity in terms of contribution of both types of carriers to these coefficients.

In the present work, we apply the method of transport equations when the scattering effects on the carriers are due to phonons but taking into account the phonon-drag effect similar to the work of Hanna (1964).

For this purpose three cases were considered separately, [illegible]

A brief summary of the theory of conduction by electrons, when phonon-drag is taken into account, is given also.

In Chapter two the conduction theory by electrons and holes is established assuming both carriers to be scattered by impurities and lattice vibrations (phonons) and the transport coefficients were computed for holes alone as for the two-carrier model. The results obtained are simple and elegant though a lot of algebra was carried on to achieve these formulae. Some of the results were obtained before, but along different lines, but most of our results are quite new. These transport coefficients include many coefficients of different natures of the individual particles and it is quite difficult to put them to experimental comparison, unless these experiments are constructed to take into account the present results. On the other hand, the thermal conducvitiy k came out to contain a bipolar term which was established before experimentally (Issi 1973).

These results are much simplified when using complex variables (Chapter three). These complex formulae may be used for computation. The effect of the phonon drag on the transport coefficients is investigated in Chapter four where a solution in terms of operators is presented, and thus explicit formulae measuring this effect are provided both in the presence and absence of magnetic fields.

In Appendices A and B we provide the definitions of the transverse galvanomagnetic and thermomagnetic transport coefficients and suitable expressions for these coefficients in huge magnetic fields.

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CHAPTER ONE

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INTRODUCTION

1.1 Conduction in solids is fairly understood after the discovery of the electron and the solution of its quantum mechanical equation in a periodic lattice. The solution proved the existence of a series of energy bands each is made up of an equal number of energy levels equal to the number of electrons present, and are thus able to accommodate twice the number of electrons present (when we include the spin quantum number). The bands of greatest interest are the two neighbouring ones: the band of the "lowest energy levels" of the electrons (called the valence band) with a maximum energy E_v, and the band of the first excited levels", (called the conduction band), with a minimum energy E_c (see Fig. 1.1). The difference between E_c and E_v, defines the forbidden gap (or energy band gap) E_g,

$$E_g = E_c - E_v \tag{1.1}$$

Electronic energy bands provide the basis for electrical classification of solids, whether the solid is a good conductor (Metal, and certain types of semimetals) or bad conductors (other types of semimetals and semiconductors) or insulators. This depends gravely upon the width E_g of the energy gap and the concept of occupation or relative fullness of the allowed bands.

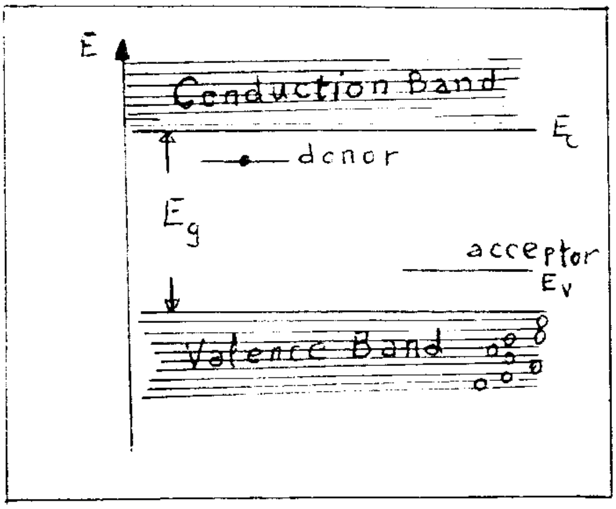

Fig.1.1 Schematic energy-band diagram, showing the valence band top E_v, the conduction band lowest energy level E_c and the energy gap E_g. Two types of impurity energy levels are shown.

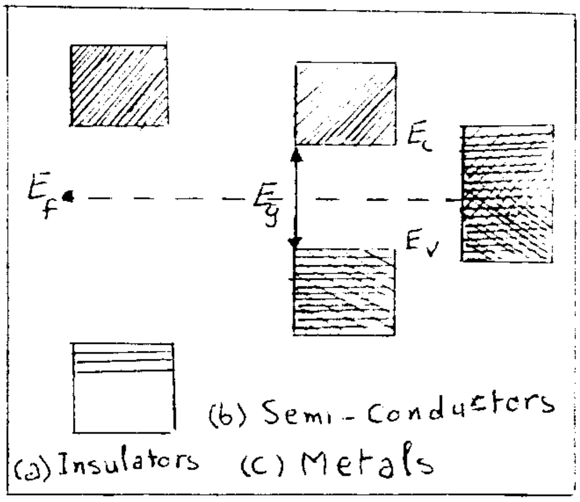

Fig.1.2 Schematic energy-band diagram showing the different structures for different solids. E_f is the Fermi energy level.

In a metal, either the valence and conduction bands overlap, so that both are partially filled, (see Fig. 1.2(e)), while in semiconductors and insulators, the valence band would be completely filled and the conduction band be completely empty (see Fig. 1.2(a) and (b)). The characteristic energy level that separates (in the case of metals) occupied from empty levels from the empty levels is called the Fermi level E_f.

Conduction will occur when an electron is excited from the valence band to the conduction band, the number of excited electrons depends upon $e^{-E_g/T}$, where E_g/T is the ratio of the band gap E_g and the absolute temperature T, which is therefore very small for insulators, appreciable for semiconductors and high for metals. This may also occur if electrons are excited from impurity energy levels (donors) to the conduction band (see Fig. 1.1).

Conduction by holes is schematically understood when we have a completely filled valence band as in semiconductors and certain types of semimetals (having a narrow gap). This is simply illustrated as follows: when an electron is excited from the valence-band (completely filled), as well as from an impurity energy level (donor) to the conduction band, vacancies (holes) are created in the valence band. Similar "Holes" may be created in the valence-band when electrons are excited to the "acceptor" impurity levels which are very close to the top of the valence band (see Fig. 1.1).

So long as all energy levels of the valence band are occupied no current is to occur, and we may write:

$$\underline{J} = \sum_{n} n_i e \underline{v}_i = 0 \tag{1.2}$$

where n is the number of electrons in the filled valence band, if the band is partially filled, say with n_1 electrons, or $(n-n_1)$ holes a current will result

$$\begin{aligned} \underline{J} &= \sum_{n_1} n_i e \underline{v}_i \\ &= \sum_{n} n_i e \underline{v}_i - \sum_{n-n_1} n_i e \underline{v}_i = -\Sigma n_i e_i \underline{v}_i . \end{aligned} \tag{1.3}$$

Thus, the current due to electrons in a partially filled band is equal to the negative of what is due to the electrons which are absent from the band or from the so-created holes.

The number of the absent electrons being small, as they are from a narrow part of the band and may be assumed to have the same effective mass which must be negative, and, therefore, its acceleration ought to be in the opposite direction of the electrons occupying the lowest levels of the conduction band. The electrons which are absent would have, therefore, contributed a negative current, while that in the partially filled band, being the negative of this current is, however, positive. In order to avoid such a complication, the concept of holes was introduced, a hole being a particle having a positive charge and a positive effective mass both equal in magnitude to the corresponding parameters of the missing electron.

That was a schematic picture of the concept of holes in solid state physics. The theoretical approach is given in Ziman's (1969) book which is based upon Dirac's (1926) hypothesis concerning the positron and is equivalent to saying that every particle has its antiparticle. According to Dirac's relativistic theory an electron has two energy eigenvalues $\pm E_{\underline{k}}$, for each value of $\underline{k}$, those of negative energy are assumed to fill the valence-band and those of positive energy are quasi-particles created in the same band by excitations of those of negative energy to the conduction band.

To prove this statement, we calculate the total number of carriers (electrons and holes) in the conduction band and valence band which are treated as electrons of the distribution function

$$\bar{f}_o(\bar{E}) = 1/[e^{(\bar{E}-\bar{\xi})/kT} + 1]. \qquad (1.4)$$

This number is given by

$$n = \int_0^\infty \bar{f}_o(\bar{E})N(\bar{E})d\bar{E} \qquad (1.5)$$

where $N(\bar{E})d\bar{E}$ is equal to the number of states in the energy range dE. The range of integration in (1.5) is divided into two ranges (see Fig. 1.1):the ranges $0 \to E_v$ and $E_c \to$ the top of the conduction band and thus

$$n = \int_0^{E_v} \bar{f}_o(\bar{E})N_v(\bar{E})d\bar{E} + \int_{E_c}^\infty \bar{f}_o(\bar{E})N_c(\bar{E})d\bar{E} \qquad (1.6)$$

where $N_v(\bar{E})$ and $N_c(\bar{E})$ are the densities of states in the valence and the conduction bands respectively. The L.H.S. of (1.6) which is equal to the total number of electrons in the valence band at T = 0, where $\bar{f}_o(\bar{E})$ of (1.4) is just the unity, may be written as:

$$\int_0^{E_v} N_v(E)dE$$

and (1.6) will reduce to:

$$\int_{0}^{E_V} \{1 - \bar{f}_o(\bar{E})\} N_V(\bar{E}) d\bar{E}) = \int_{E_C}^{\infty} \bar{f}_o(\bar{E}) N_C(\bar{E}) d\bar{E} \ , \qquad (1.7)$$

which is just equivalent to saying, the total number of electrons excited into the conduction band is equal to the number of holes in the valence band. Moreover, the structure of (1.7) will lead to the statistical function of holes, as if we assume $f_o^+(E^+)$ to be the distribution function of holes, then

$$\begin{aligned} f_o^+ &= 1 - \bar{f}_o(\bar{E} - \bar{\xi}) \\ &= 1/[\exp\{-(\bar{E} - \bar{\xi})/kT\} + 1] \\ &= \bar{f}_o\{-(\bar{E} - \bar{\xi})\} \end{aligned} \qquad (1.8)$$

If we denote the energy of holes by E^+, which is to replace $-\bar{E}$ in (1.8), this equation may be written as:

$$f_o^+(E^+ + \xi^+) = \bar{f}_o\{-(\bar{E} - \bar{\xi})$$

and we deduce that Holes, like Electrons, obey the Fermi-Dirac statistics but, (see Ziman, 1972, p. 140), as if the axis of energy is drawn downwards.

In order to carry on calculations, using similar formulae for electrons and holes one may use the following frame of reference (see Ziman, 1972, p. 141). exhibited in Fig. 1.3, where the electron energy is measured from the bottom of the conduction band upward and the hole energy is measured from the top of the valence band downwards. This conversion may be altered as indicated by Wilson (1965) by assuming the origin of the electron energy axis to start at the top of the