EFFECT OF LATTICE VIBRATION ON THE CONDUCTION OF SEMICONDUCTORS

THESIS

Submitted To Ain Shams University In Partial
Fulfilment Of The Requirements For The Degree Of
M. Sc.

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March, 1976.

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ACKNOWLEDGEMENT

I wish to express my deepest thanks to Professor I.I. Hanna, Head of Applied Mathematics Department for his helpful guidance, useful criticism under his supervision, and valuable discussions during my course of study.

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CHAPTER ONE

INTRODUCTION

Solids are, usually, divided according to its conductivity into two distinct categories; those of high conductivity and known as metals and those of no conductivity and classified under the term insulators. Midway between metals and insulators, we have a third type termed semi - conductors. These are essentially insulators and 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.

In a crystalline solid, we are dealing with two aggregates of interacting particles heavey ions and hight electrons, and the fundamental equation to solve is the many - particle schrödinger equation.

$$H_c \psi_c = E_c \psi_c \tag{1.1}$$

Where H_c is the crystal Hamiltonian made up of electronic and ionic keinetic operators T_e and T_n,

$$H_c = T_e + V + (T_n + V_n) \tag{1.2}$$

and V being the potential energy of the electrons and the interaction energies between the two aggregates, while V_n is the potential energy of the ions. The wave function ψ is a function of $\underline{r}$ and $\underline{R}$, the collective coordinates of electrons and ions respectively. The wave equation is solved approximately (Born - Oppenheimer) by treating the electrons and ions separately, assuming the electronic Hamiltonian $H_e = T_e + V$ and treating $H_n = T_n + V_n$ as a perturbation on H_e. This product separation is possible to the second order in k, the ratis of the electronic and ionic masses m and M, if ψ_c is expanded as a power series in k (see. Born and Huang, 1954). This type of approximation is still valid even when we consider the anharmonic terms in the equations of mation of the ions (terms heigher than the second order in lattice displacements).

The three-dimensional treatment of the lattice vibrations (ion motion) does not add much to the simple one - dimensional problem (see Patterson, 1970, P.66), thus we write X_i for the coordinate of the ion $\underline{R}_i$ and expand $V_n(\underline{R}) = V_n(X)$ as a power series in X_i , $i = 1, 2, 3, \ldots$. On using normal coordinates, H_n is over simplified to the form, assuming M_i to be mass of ion (i).

$$H_n = \sum_i \frac{M_i}{2} \left(-\hbar^2 \frac{\partial^2}{\partial q_i^2} + \omega_i^2 q_i^2 \right) \qquad (1.3)$$

keeping only quadratic terms in the expansion of V_n (x). Heigher (anharmonic) terms are of little importance and need to be considered when discussing phonon-phonon scattering. Its effect is calculated as a perturbation. The resulting Hamiltonian is the usual Hamiltonian of a certain number of uncoupled harmonic oscillators, the energy of each is

$$\epsilon_i = (n + \tfrac{1}{2}) \hbar w_i \qquad (1.4)$$

n being an integer. The results so far obtained using quantum mechanics may be obtained using classical mechanics except the eigenvalue relation.

It is now accepted to call each energy excitation of frequency w_i and energy $\hbar$ w_i a "phonon" which are treated as bosons that can be created (by emmision) or destroyed (by adsorbtion). The mean number of phonons of energy h w at temperature T is given by

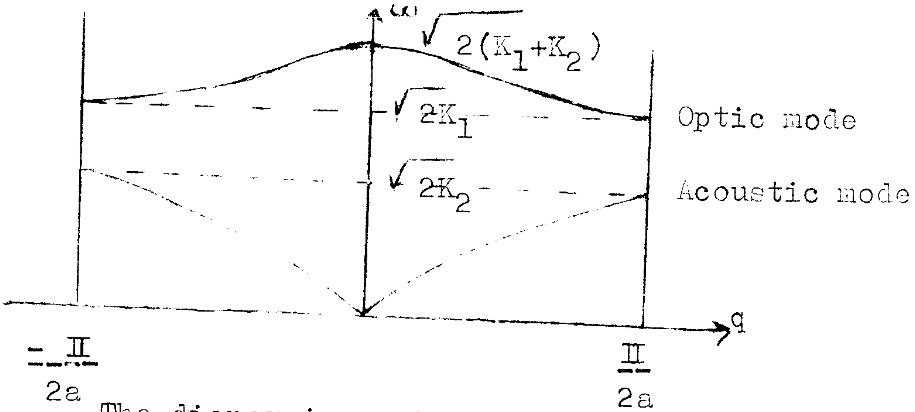
$$N (q) = 1/ (\exp (\hbar w/kT -1) \qquad (1.5)$$

Further consideration of linear lattices with two types of atoms in alternating positions has introduced two different types of modes of oscillations, the acoustic and optic modes. In an acoustic mode, the adjacent atoms vibrate almost in phase while in an optic mode, they are vibrating out of phase. The dispersion relations (w - q relation) are.

$$W_{op}^{2} = (k_1+k_2) + \left[(k_1+k_2)^2 - 4\ k_1\ K_2\ \sin^2\ q\ a\right]^{\frac{1}{2}} \qquad (1.6)$$

$$W_{ac}^{2} = (k_1+k_2) - \left[(k_1+k_2)^2 - 4\ k_1\ k_2\ \sin^2\ q\ a\right]^{\frac{1}{2}} \qquad (1.7)$$

where $k_i = b/Mi$, $i = 1,2$, b is the force constant and M_1, M_2 are the masses of the molecules ($M_2 < M_1$), while a is the lattice constant



The dispersion relation for optic and acoustic modes for a diatomic linear chain.

For small qa, the acoustic dispersion relation reduces to

$$\left.\begin{aligned} w_{ac} &= \left[(2\ k_1\ k_2) \ / \ (k_1 + k_2) \right]^{1/2} qa \\ \text{Thus} \\ \frac{d\ w_{ac}}{dq} &= w_{ac}/q \end{aligned}\right) \qquad (1.8)$$

and hence the phase and group velocities are the same, and consequently we expect to have no acoustic dispersion for long wavelength. On the other hand, for long wavelengths (qa ---→ 0), the optic branch show that

$$w_{ap} \doteq 2\ (k_1 + k_2) + \frac{2\ k_1\ k_2}{(k_1 + k_2)} q^2 a^2 \qquad (1.9)$$

The only addition in 3- dimensional space, is that there are 3k dispersion relations (if there are k atoms per unit cell), three of which are acoustic and the rest will determine the optic modes.

Turning to the wave equation

$$\left[(H_e + V) \right] \psi_e = E_e\ \psi_e \qquad (1.10)$$

of the electrons, where the potential energy V contains the potential energy of the electrons in the field of the atoms and the interaction energies between the electrons itself. It is usual to reduce the above equation to a one-electon wave equation (Hartree approximation) by neglecting the effect of antisymmetry of the may electron wave function ψ_e as well as the carrelations of the electrons. As a matter of fact this is the only type of problem that we know how to solve exactly.

The method of describing the eigen states of the valence electrons by the one - electron model is considered as the starting point in the modern theory of solids. Electron - electron as well as electron - core interaction are usually treated as part of the potential V ($\underline{r}$) of such valence electron as it moves through the crystal lattice. The potential V ($\underline{r}$) is supposed to be calculated as a Hartree or Hartree-Fock potential of the ion (see Ziman, 1972 P.77).

To proceed with the calculations, an over simplification about V ($\underline{r}$) is always assumed; thus, V ($\underline{r}$) is taken as a constant leading to the usual free electron model (or the summerfeld model, See Wilson, 1933 P.25) The valence electrons then fall into the eigen-states

$$\psi_k = N_{\exp} \; (i \; \underline{k} \; . \; \underline{r}) \qquad (1.11)$$

with eigenvalues

$$E_k = h^2 \underline{k}^2 / 8 \Pi^2 m \qquad (1.12)$$

The surfaces of constant energy are thus spheres in the k-space. The volume of such energy sphere (containing all the energy states of the solid) is governed by the number of electrons per unit volume. Near the top of this distribution (at the Fermi level) the electrons have wavelengths comparable with lattice spacing and we have a bragg diffraction, and the electron energy spectrum may show gaps, or forbidden energy states.

As a consequence, the electronic energy levels fall into bands. The nature of these bands depends completely on the type of solid considered at the beginning of this chapter and is also responsible for its properties.

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. 113) has proved that the perisdic nature of the solid, particularly when we are concerned with law concentrations of electrons (as in the case of semi-conductors), may be taken into account by using an effective electronic mass m^* in (1,1) 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 semiconductors.

In the presence of a temperature gradiant. The heavy ions cited at lattice points are no longer at rest but will excute a small ascillations about its positions of equilibrium. The lattice vibrations distort the lattice periodicity and hence the electrons cannot propagate through the lattice without being scattered. Such deformation in the potential energy V ($\underline{r}$) is considered as a perturbation and the matrix element is calculated by the time dependent perturbation theory. This results into the following restrictions (Ziman, 1960 P.).

i- Energy is conserved.

ii- The total wave vector of the system before the scattering process can differ only be a reciprocal lattice vector from the total wave vector of the system after the scattering process.

The first of these equations is interpreted as

$$E_{\underline{k}'} = E_{\underline{k}} \pm \hbar w_{\underline{q}} \qquad (1.13)$$

resulting from the absorption or emission of a lattice quanta (phonon). The latter may be looked upon as a selection rule on the wave vector and is usually written as

$$\underline{k}' = \underline{k} + \underline{q} + \underline{G} \qquad (1.14)$$

where $\underline{G}$ is a reciprocal lattice vector. If $G = 0$ we have normal processes, which is equivalent to the conservation of the linear momentum of the electron-phonon pair, otherwise ($G \neq 0$) we have Umklapp processes. The transport phenomenae in solids involve a flow of either charge or energy or both, arising from certain external effects acting on the solid which are the electric field , the temperature gradient $\underline{\nabla}\, T$ and the magnetic field $\underline{H}$. The relations between the current densities (electric or thermal) and these effects (see chapters 3 and 4) define the transport coefficients, such as the electrical, thermal conductivity, the various thermoelectric coefficients, thermo - and galvano - magnetic coefficients. These coefficients are obtained essentially, interms of the distribution function $f_{\underline{k}}\,(\underline{r}, \underline{v})$ of electrons (see chapter 2) which is determined by the solution of a transport equation (Boltzmann equation, equation 2.3). This function f is affected by the external effects as well as the scattering mechanisms present in the crystal