



Tesi di Dottorato Internazionale in Matematica Applicata

XXV Ciclo

Analysis of Energy-Transport Models for semiconductors

Mariangela Ruscica

Advisors

Prof. Armando Majorana, Prof.ssa Rita Tracinà.

Università degli Studi di Catania

Dipartimento di Matematica e Informatica

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Mariangela Ruscica

A Dissertation Submitted in Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy

in

Applied Mathematics

University of Catania

Acknowledgements

I am profoundly grateful to my thesis advisors Prof. Armando Majorana and Prof. ssa Rita Tracinà for their assiduous support, patient help and many precious discussions and suggestions. I am very grateful to all the lecturers who taught, helped, and answered any questions to me during the study. I would also like to thank Prof V. Romano for his advices and constructive feedback. I would like to thank my parents for all their love and encouragement.

” What is essential is invisible to the eye”

The Little Prince

Dedicated to Marco

Abstract

In this thesis we study the energy transport models of the charge carriers in the semiconductors, in the unipolar and one-dimensional case. These are macroscopic models, that are useful to describe the thermal effects in the semiconductor devices. Usually the set of equations are given by the balance equations for density and energy of the charge carriers, coupled to the Poisson equation for the electric potential. Two energy transport models, with and without crystal heating, are presented with different approaches. The first energy transport model is the Chen model, in which the temperature lattice is assumed constant. We find some particular solutions and we discuss them behavior depending on physical parameters, as example for the silicon.

The second energy transport model includes as variable the lattice temperature. A symmetry analysis approach to this model is performed. We determine the group classification of the model equations, collecting them into equivalence classes and find the functional forms of the constitutive functions appearing in the equations. In some cases the reduced system solutions are found.

Contents

1	Introduction	5
2	Basic concepts about crystals with some mathematical details	10
2.1	Crystals	10
2.1.1	Lattice planes and Miller indices	14
2.1.2	Diamond and Zinblende structures	16
2.2	Crystal bonding	17
2.2.1	Ionic crystals	17
2.2.2	Covalent crystal	18
2.2.3	Other types of bonds	18
2.3	Reciprocal lattice	19
2.4	Energy levels in a periodic potential and Bloch's theorem	20
2.5	Doping	26
2.6	Effective mass	28
2.7	Physics of equilibrium of semiconductors and Fermi-Energy	30
2.8	Mobility, drift velocity, diffusion current	35
2.8.1	Diffusion current and Einstein Relation	37
2.9	Scattering mechanisms in a lattice	38

3	Classical Kinetic Transport Models	40
3.1	The Liouville equation	41
3.1.1	The conservation property	42
3.1.2	Zeroth and first order moments	42
3.1.3	The semiclassical Liouville equation	43
3.2	The semiclassical Vlasov Equation	44
3.2.1	The semiclassical Boltzmann equation	44
3.3	The collision operator	45
3.3.1	Scattering electron-phonon	47
3.3.2	Scattering mechanisms with ionized impurity	50
3.4	The Poisson equation	53
3.5	The recombination and generation processes in the bipolar semiconductor devices . .	53
4	From Kinetic to Fluid Dynamical models	56
4.1	Introduction to macroscopic models	56
4.2	Method of Moments	58
4.2.1	The Drift-Diffusion equations	62
4.2.2	Hydrodynamical models	64
4.2.3	The Energy Transport models	68
5	Energy-transport model equations with constant lattice temperature	70
5.1	Analysis of steady-state solution	72
5.2	A stable solution of energy-transport model	79
6	The symmetry analysis of differential equations	83
6.1	Basic theory of Lie Groups of transformation	84

6.1.1	Infinitesimal Transformations	85
6.1.2	Lie Groups of differential equations	88
7	Thermal lattice effects and Energy Transport model	92
7.1	An Energy Transport model with crystal heating	93
7.2	The symmetry classification in the one-dimensional case	94
7.3	Reduced system and exact solutions	100
	Bibliography	102

Chapter 1

Introduction

In the last years, the improvement of technology and design about semiconductor devices has been coupled to the development of mathematical models, to describe several phenomena in the performance of semiconductor devices. The miniaturization of the devices is more and more progressing and the transport equations, describing the charge carriers flow through a semiconductor device, depend on the device structure. The main transport phenomena may be very different, caused by diffusion, drift, scattering, or quantum-mechanical effects. Generally, we can classify kinetic and fluid-dynamical models.

At the kinetic level, in the semiconductors the charges transport is described by the semiclassical Boltzmann equation for the charge carriers, coupled to the Poisson equation for the electric potential. The semiconductor Boltzmann equation (BTE) gives quite accurate simulation results, but the numerical methods to solve this equation (for example Monte-Carlo method) are too expensive.

The main fluid-dynamical models are macroscopic semiconductor models, as the drift-diffusion, the hydrodynamic and the energy transport. In the literature, the drift-diffusion model is the simplest model and popular ones, since the efficient numerical algorithms are known and improved. Nevertheless it loses validity in the field of submicron-devices, owing to the rapidly changing electric fields and temperature effects.

The hydrodynamic and energy transport models are obtained from the semiclassical Boltzmann equation by the moments method [35]. In this way, we can simplify the BTE to a set of macroscopic transport equations. The zeroth to third-order moment equations can be generated from following moment variables: unity, the carrier velocity \mathbf{v} , the carrier energy \mathcal{E} and the carrier energy flow $\mathcal{E}\mathbf{v}$. The corresponding macroscopic moment quantities are defined, as charge density n (or p), electric current density (carrier flux) \mathbf{J} , energy W and energy flux \mathbf{S} . The different assumptions, formulations and the closure relations lead to different macroscopic models.

In this thesis, we focus our attention the energy-transport models. The energy-transport models, first presented by Stratton in 1962 [50], are derived from hydrodynamic models usually by neglecting certain convection terms. Generally, for these models the equations set is given by the continuity equation, balance equation for the electron energy and balance equation for the electron energy flux, including the phenomenological constitutive equations for the particle flux and energy flux. According to the moments method, the closure relations of these models can be based on the Maximum Entropy Principle (MEP) [3], [42].

Several and different kinds of energy transport models are proposed in [11], [44], [43], [13] et al., they are derived under various hypotheses on scattering terms, the semiconductor band structure and degeneracy. The energy-transport models describe the thermal effects related to the charge carriers flow through the crystal and to the lattice temperature. In some simpler models the temperature of lattice is constant. At characteristic micron/nano size features, thermal modeling of semiconductor devices are required. Due to the collision of the charge carriers with the crystal lattice, the increasing lattice temperature is described by heat equation, derived from thermodynamic principle. Therefore, we can obtain the energy transport models in which the thermal effects depend on the variance of the crystal lattice temperature. The scattering mechanisms, as scattering of electrons with acoustic and non-polar phonons and with impurities, are included, but we neglect electron-electron scatterings. This last assumption has validity, for example, for the low electron

density and in some semiconductors as the silicon. The scattering phenomena are included in the balance equation for the electron energy flux.

In this work we put our attention on two kinds of energy-transport model:

- the energy-transport model, proposed by Chen et al. in [13], where the lattice temperature is assumed constant;
- the energy-transport model with crystal heating.

In the first considered model, we have the continuity equation, the balance energy equation coupled with Poisson equation and two closure relations for the current density and flux energy. These closure relations depend on some physical parameters as mobility, thermal voltage, the characteristic length and relaxation time. Given a constant solution, we analyze the behavior of a stationary solution, which obtained as perturbation of constant solution. Using physical parameters of silicon semiconductor, we show how the amplitude of perturbation is related to the charge density and to the characteristic length of semiconductor device. Then, we study the asymptotic stability for a particular solution.

In the second part of the thesis, we present an energy-transport model, including the thermal effects depending on the lattice temperature. These results have been extracted by the preprint

- Ruscica M., Traciná R., Group classification of an energy transport model for semiconductors with crystal heating (submitted)

and have been presented in the

- 16th International Conference on Modern Group Analysis, Ufa, Russia: October 28- November 2, 2013.

We introduce a closure relation for the heat equation. This equation, introduced in [54], takes into account the physical parameters of semiconductor, as thermal conductivity and specific heat,

and the physical phenomena that depend on the scattering, on energy bands structure of lattice and on the environment temperature. The electron and lattice thermal conductivity as well as the electron energy and lattice thermal relaxation times are functions depending on the electron and lattice temperature, while other variables as charge density, electric field, electron temperature and lattice temperature are functions of space and time, finally the doping depends on only space.

For this last model we use an approach based on transformation method, a powerful tool in the field of nonlinear partial differential equations. We refer to the Lie point symmetries approach, which leaves the equations invariant [21], [37], [38]. Some applications in models for semiconductors can be found, as example, in [39], [45], [46], [47].

In several problems of mathematical physics, as in this case, the equations contain parameters or functions, that play the role of arbitrary elements. Due the presence of these arbitrary elements the search of Lie symmetries is more difficult. In these cases, we can classify all Lie symmetries depending on the forms of the arbitrary elements. By a Lie group classification, we can look for Lie symmetries for the specific pdes.

In many physical models some parameters can not be determined by a physical law, but only experimentally. The importance of the classification lies in the fact that we find the form of those quantities, as functions of the variables that appear in the equations of the model. By these results, we look for particular solutions for the equations model.

The plan of this work is as follows. In the next chapter we give a description of the main characteristics of semiconductors, we recall some fundamental concepts of the solid state physics, through mathematical means, as lattice, primitive cell, Bravais lattice, the first Brillouin zone, finally reciprocal lattice. Under assumption that the crystal lattice has a periodic structure, by the classical Hamiltonian function and Bloch's theorem, we introduce the energy bands model and describe those physical phenomena that influence the charge carriers transport through the crystal lattice, as doping and scattering.

In the chapter 3, we introduce classical Kinetic Transport Models and in particular the Boltzmann transport equation, describing characteristics and properties of collision operator.

In the chapter 4, by the moments method, we define those variables involved in the mathematical models, that are presented in this work. Then we give a general description of drift-diffusion model, hydrodynamic model and energy-transport model, explaining and underlying applicability range and weaknesses. The results about proposed energy-transport model are presented in the chapter 5, where we describe also some examples of solutions for this model.

After a short introduction on analysis of symmetries given in chapter 6, in the last chapter we compute the group classification for an energy-transport model with crystal heating. In some cases we solve the corresponding reduced system and obtain some exact solutions.

Chapter 2

Basic concepts about crystals with some mathematical details

In this chapter we present a summary about the physics and main properties of semiconductors. At the first, we give a description of the state of art of semiconductor solid physics, through mathematical means, introducing some fundamental concepts as lattice, primitive cell and reciprocal lattice. Then, we introduce an energy bands model for semiconductors and describe those physical phenomena, as doping and scattering, that play a fundamental role in the transport of the charges through the crystal lattice.

2.1 Crystals

The most important properties of semiconductors depend on the crystalline structure and on the transport of charge in crystal lattice, that is essentially influenced by regular periodic atomic order. The crystals structure is composed of a pattern, a set of large number of atoms, and a lattice exhibiting long-range order and symmetry, so that their properties are those of a ideal crystal and the surface effects influence these physical properties only near the edges. On the other hand,

today it is possible to fabricate and to study “nano-crystals” of very small dimensions, where the translational symmetry is completely lost, but we still call them crystals as long as the positions of their atoms are those predicted by the regular arrangement of the corresponding ideal crystal. There are, of course, intermediate cases, nowadays very frequent and important, where some of the bulk properties of the crystal can still be used, but the finite dimensions of the system play an important role [22]. An ideal crystal is constructed by the infinite repetition of identical groups of atoms, called the *basis*. The set of mathematical points to which the basis is attached is called the *lattice*, that in three dimensions is given by

$$L = \{l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3, (l, m, n) \in \mathbb{Z}^3\}. \quad (2.1)$$

The vector $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, called *primitive vectors*, are the basis vectors, so the lattice may be defined by three translation vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, such that the arrangement of atoms in the crystal looks the same when viewed from the point \mathbf{r} as when viewed from every point \mathbf{r}^* translated [27]

$$\mathbf{r}^* = \mathbf{r} + l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3.$$

There is no cell of smaller volume than $|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$, that represents a building block for the crystal structure. Introducing the primitive translation vectors, we define the crystal axes, which form three adjacent edges of the primitive parallelepiped. This primitive cell, defined by primitive axes $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, is called *primitive cell* and the basis associated with a primitive cell is called a *primitive basis*. No basis contains fewer atoms than a primitive basis contains.

Definition 1 *Primitive cell*

A primitive cell is a connected subset $D \subseteq \mathbb{R}^3$, that contains a unique elemental of L (usually the origin) and that its translated is a partition of \mathbb{R}^3 .

Besides translations, others symmetry operations bring the crystal over itself: rotations, reflections, rotary-reflections, and inversions. The total set of symmetry operations of a crystal is its

space group. The group of operations obtained by a space group setting to zero all translations is the point group of the crystal. Group theory indicates how to use the symmetry of the crystal, and in general of a physical system, to classify the eigenstates, evaluate degeneracies, selection rules, etc. For more details see [52].

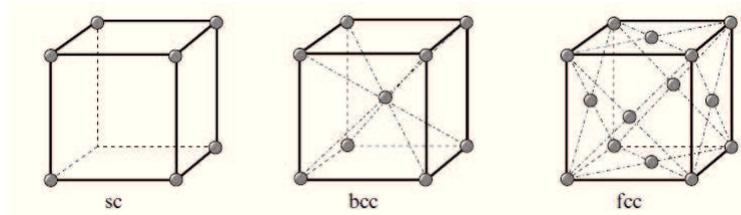


Figure 2.1: Cubic lattices. In the simple cubic (sc), lattice points are situated at the corners of the cube. In the body centered cubic (bcc), lattice points are situated at the corners and at the center of the cube. In the face centered cubic (fcc), lattice points are situated at the corners of the cube and at the centers of the faces of the cube.

In Fig.2.1, the three possible cubic lattices are shown. The simple cubic (sc), the body-centered cubic (bcc) and the face-centered cubic (fcc). A primitive cell of the (sc) lattice coincides with the cube. As any primitive cell, it contains, inside the cube, only one atom, more precisely $\frac{1}{8}$ of atom at each of the 8 corners. In the (bcc) lattice, the cube is not a primitive cell. It contains, besides the eight eighths of atom at the corners, a second atom at the center of the cube. A primitive cell of the (bcc) lattice is shown in Fig.2.2. The three primitive elementary translations link an atom at a center of the cube with three atoms at three nonadjacent corners. In the (fcc) lattice, the cube contains four atoms: eight eighths at the corners and six halves at the centers of the faces. A primitive unit cell, shown in Fig.2.2, is formed with elementary translations linking an atom at a corner of the cube with three atoms at the centers of three faces. Both the (bcc) and (fcc) primitive cells are formed by rhombohedrons where atoms are located at the eight corners and shared by eight primitive cells, as for the (sc) primitive cells [22].

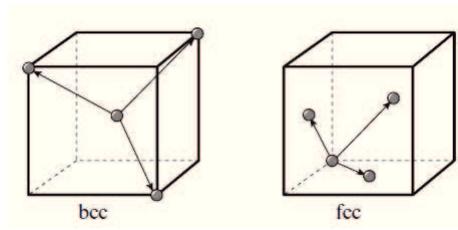


Figure 2.2: Primitive cells of body-centered and face-centered cubic lattices. For the simple cubic, the cubic cell shown in Fig.2.1 is also a primitive cell.

In the description of crystalline solid, a fundamental concept is the Bravais lattice, which specifies the periodic array, in which the repeated units of the crystal, are arranged. These units may be atoms, groups of atoms, molecules, ions. The Bravais lattice summarizes only geometry of the underlying periodic structure, without to specify the characteristic of units.

Definition 2 *Bravais Lattice*

A Bravais lattice is an infinity array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed.

The Bravais lattice is supposed with an infinite extension, but this is only a very useful idealization, because the crystal lattice is finite, of course. We must think of the crystal as filling up only a finite portion of the ideal Bravais lattice. For any given Bravais lattice the set of primitive vectors is not unique, consequently there are many non equivalent choices and it is not heavily need to rely on a definition that emphasizes a particular choice; usually we choose a basis with vectors of minimum length [5]. The conventional unit cell is generally chosen to be bigger than the primitive cell and to have satisfy the required symmetry.

Definition 3 *Primitive unit cell*

A primitive unit cell is a primitive cell with the basis vectors of minimal length, that is a region that just fills space without any overlapping when translated through some subset of the vectors of

a Bravais lattice.

A primitive cell may also be chosen following this procedure: draw lines to connect a lattice point to all nearby lattice points, draw the perpendicular bisectors of lines. The smallest volume enclosed in this way is the Wigner-Seitz primitive cell.

Definition 4 Wigner - Seitz primitive cell

The Wigner - Seitz primitive cell is the region of space, called D_{WS} , that is closer to that point than to any other point of lattice point, given by

$$D_{WS} = \{ \mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| \leq |\mathbf{x} + \mathbf{l}|, \forall \mathbf{l} \in L \} .$$

Wigner-Seitz cell is most compact, highest symmetry primitive cell possible.

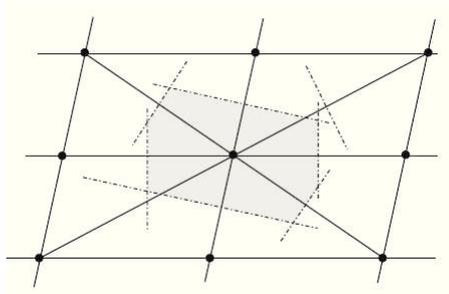


Figure 2.3: The Wigner-Seitz primitive cell of a lattice is formed by all points closer to one of the lattice points than to any other.

2.1.1 Lattice planes and Miller indices

In a crystal the points are identified by their coordinates in the crystallographic axes in units of the lattice vectors. For example, the point $(1/4, 1/4, 1/2)$ is the point given by

$$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 \tag{2.2}$$

where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are the conventional unit translations, not necessarily coincident with the primitive translations. The direction of an oriented straight line is indicated by the smallest integers proportional to the components, along the crystallographic axes, of a vector oriented in the considered direction. They are usually given inside square brackets: $[n_1, n_2, n_3]$. A negative component is indicated by a minus sign above the index: $[n_1, \bar{n}_2, n_3]$. If all directions equivalent by symmetry are to be indicated, they are usually put in angular brackets: $\langle n_1, n_2, n_3 \rangle$. In a crystal the orientation of a plane is specified by its *Miller indices*. To find the Miller indices of a plane we determine the intercepts of the plane on crystal axes, i.e. x_1, x_2 , and x_3 , in terms of fundamental vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, we take the reciprocal of these numbers in order and reduce them to three smallest integers having the same ratio. The Miller indices are usually given inside round brackets: (i, j, k) . The inverse are used to avoid infinities if a plane is parallel to a crystallographic direction. If all plane orientations equivalent by symmetry are to be indicated, they are often put in curly brackets $\{i, j, k\}$ [5],[22]. Miller indices of some important planes of cubic lattices are shown in the Fig. 2.4.

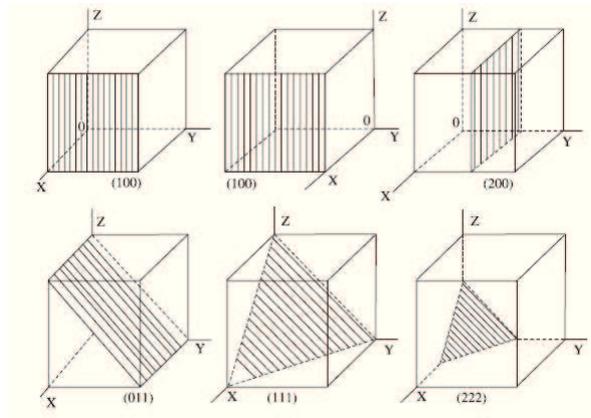


Figure 2.4: Miller indices of some important planes of cubic lattices

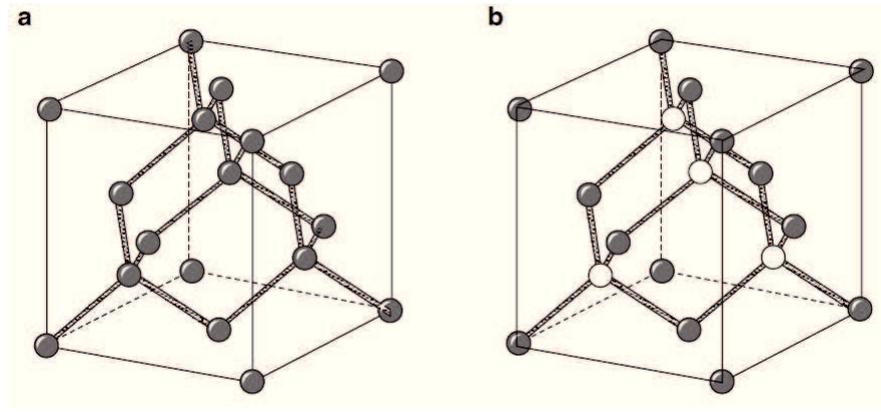


Figure 2.5: Diamond (a) and zincblende (b) structures. Not all atoms and bonds of the structures are shown in the figure to make more evident the tetrahedral structure of the bonds.

2.1.2 Diamond and Zincblende structures

Every crystal is characterized by its lattice and basis. The two-dimensional example in Fig.2.5 (in part (a)) shows the diamond structure, common to carbon (diamond), silicon, germanium, and gray tin. It is formed by a (fcc) lattice with a basis formed by two identical atoms, one at the corners of the cube and a second one along the diagonal of the cube at $1/4$ of its length. In the cubic crystallographic axes, the coordinates of the atoms of the basis are $(0, 0, 0)$ and $(1/4, 1/4, 1/4)$ then, the crystal is formed by two (fcc) interpenetrated structures at the distance of one fourth of the diagonal of the cube. The zincblende (ZnS) structure is common to many III-V semiconductors [22]. Its structure is similar to that of diamond, but in the zincblende structure the two atoms of the basis are different. This structure is shown in part (b) of Fig.2.5.

In Table 2.1, the crystal structures and lattice constants of some important semiconductors are given.

Material	Structure	Cube side at 300 K (\AA)
Silicon (Si)	Diamond	5.431
Germanium (Ge)	Diamond	5.646
Aluminum arsenide (AlAs)	Zincblende	5.661
Gallium arsenide (GaAs)	Zincblende	5.653
Gallium phosphide (GaP)	Zincblende	5.451
Indium arsenide (InAs)	Zincblende	6.058
Indium phosphide (InP)	Zincblende	5.869

Table 2.1: Crystallographic data of some semiconductors

2.2 Crystal bonding

There are different types of bonding of atoms and molecules in a crystals, due to the electron charge distribution around the nuclei, in particular due to the electrons that contribute to the binding are in the most external states, or valence states. The cohesive forces that hold together the atoms in a crystalline structure can have very different intensity. In many cases, these are real bonds, ionic or covalent, in other cases atoms or molecules interact through Van der Waals forces. Depending on the nature of cohesion forces, one identify some classes of solids, each characterized by a chemical and physical behavior and determined from the nature of the link: ionic, covalent bonding and other bonding.

2.2.1 Ionic crystals

The ionic bond is a chemical bond based on the electrostatic attraction forces between ions having opposite charge, for example between metal and non-metal ions. The metal gives one or more electrons, forming a positively charged ion. These electrons are transferred to non metal, that

becomes a negatively charged ion. Because the interaction between charges, given by Coulomb's law, is the same in all directions, ionic compounds do not form molecules. Instead, periodic lattices with many ions form, in which each ion is surrounded by many ions of opposite charge. If the ions get too close to each other electronic wavefunctions tend to overlap. According to Pauli exclusion principle, this overlap generates a repulsive force. The stable structure is determined by the minimum free energy due to competitive actions of these force [22]. Therefore, ionic compounds are almost always solids at room temperature. Typical ionic crystals are the salts formed by an element of the first group and one of the seventh group, such as NaCl.

2.2.2 Covalent crystal

When the atoms of a crystal are the same kind, the crystal binding can not be of ionic nature. For example, about the elements of group IV, the binding interaction results by sharing of electrons between two adjacent atoms. As for the hydrogen molecule, we have a covalent bond when two electrons of opposite spins have wavefunctions that overlap in the region between the atoms. This bonding state corresponds to a higher charge density in the region of low potential energy between the two atomic cores. Then, for III-V semiconductors, such as GaAs, the bond is partially ionic and partially covalent [22].

2.2.3 Other types of bonds

There are other types of crystal bonds, but these are less important for semiconductors. In the crystals, compound by elements noble-gas, the electronic shells are completely filled. In the solid atoms are alike isolated atoms and, in a static picture, no electrostatic force acting between them. However, there are Van der Waals forces, due to fluctuations of dipole that hold the crystal with small cohesive energy [5]. In metal crystals, the electrons in the outer shell of the atoms leave the parent atom and move freely inside the solid. This electron gas interacts electrostatically with

the positive ions of the lattice and this interaction determines the metallic bond of the crystal [17]. Another type of bond, especially important in organic crystals and ice, is the hydrogen bond. When a hydrogen atom is near a strongly electronegative atom, it transfers its electron to this atom, forming two bonded ions of opposite signs, as in ionic crystals [5], [27].

2.3 Reciprocal lattice

Let L be a set of a Bravais lattices and plane wave $e^{i\mathbf{k}\cdot\mathbf{l}}$, with $\mathbf{k}, \mathbf{l} \in L$. The plane wave will have the periodicity of the Bravais lattice only for the some special choices of wave vector \mathbf{k} . The set of all wave vectors \mathbf{k} that yields plane waves with periodicity of a given Bravais lattice is known as its *reciprocal lattice*. The vector \mathbf{k} belongs to the reciprocal lattice of a Bravais lattice of points of L , provided that the relationship $e^{i\mathbf{k}\cdot(\mathbf{l}+\mathbf{r})} = e^{i\mathbf{k}\cdot\mathbf{l}} \forall \mathbf{r}, \mathbf{l} \in L$ is true. The reciprocal lattice L^* is the set of wave vectors \mathbf{k} satisfying $e^{i\mathbf{k}\cdot\mathbf{l}} = 1 \forall \mathbf{l} \in L$ and it is itself a Bravais lattice

$$L^* = \{l\mathbf{b}_1 + m\mathbf{b}_2 + n\mathbf{b}_3, (l, m, n) \in \mathbb{Z}^3\},$$

where

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|}, \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|}, \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|}.$$

The reciprocal lattice of any Bravais lattice is still a Bravais lattice. Then, if $|D_L|$ is the volume of the primitive cell D_L of L and $|D_L^*|$ is the volume of the primitive cell D_L^* of reciprocal lattice L^* , we have

$$|D_L^*| = \frac{(2\pi)^3}{|D_L|}.$$

Definition 5 *The First Brillouin zone*

The Wigner - Seitz primitive cell of reciprocal lattice is known as the first Brillouin zone:

$$B = \{\mathbf{k} \in \mathbb{R}^3 : |\mathbf{k}| \leq |\mathbf{k} + \mathbf{l}^*|, \forall \mathbf{l}^* \in L^*\}.$$

It is the set of the points in \mathbb{R}^3 that are closest to the origin than to any other element of the inverse lattice L^* .

2.4 Energy levels in a periodic potential and Bloch's theorem

In the previous section we introduced the semiconductor solid by its crystalline structure and in this chapter we explain as this periodic structure influences the dynamic of a particle. By the classical Hamiltonian function and the Bloch's theorem, we explain and define the energy band model, that is useful and important to describe the features of semiconductors and the transport of charges in crystal lattice.

We define *momentum* the vector $\mathbf{p} = m\mathbf{v}$ of an elementary particle of mass m , charge q and velocity \mathbf{v} . The *phase space* is the space of all states $(\mathbf{x}, \mathbf{p}) \in \mathbb{R}^3 \times \mathbb{R}^3$, so that the path $\mathbf{x} = \mathbf{x}(t)$ identifies a curve $(\mathbf{x}, \mathbf{p}) = (\mathbf{x}(t), m\dot{\mathbf{x}})$. Then, to each path there is associated the total energy of the particle and, in particular, to each curve in this space is related a total energy. We can introduce the classical Hamiltonian function

$$\mathcal{H}(\mathbf{x}, \mathbf{p}) = \frac{|\mathbf{p}|^2}{2m} - q\phi(\mathbf{x}) \quad (2.3)$$

where ϕ is the electric potential. Using the Hamiltonian function, we can write the equation of motion for the charge q (with different expression from classical mechanics)

$$\dot{\mathbf{x}} = \nabla_{\mathbf{p}}\mathcal{H} \quad \dot{\mathbf{p}} = -\nabla_{\mathbf{x}}\mathcal{H}. \quad (2.4)$$

We can associate an energy $\mathcal{E}(t)$ to each path $\mathbf{x}(t)$ through the relationship $\mathcal{H}(\mathbf{x}, \mathbf{p}) = \mathcal{E}(t)$. In the quantum mechanical model an elementary charge is considered as a wave which is associated a vector \mathbf{k} and pulse wave ω , that is related by De Broglie relation

$$\mathbf{p} = \hbar\mathbf{k}, \quad (2.5)$$

where \hbar is reduced Planck constant, and by Planck - Einstein relation

$$\mathcal{E} = \hbar\omega. \quad (2.6)$$

Generally the dynamics of an elementary particle is described by a complex wave-function $\psi(\mathbf{x}, t)$, linked to the probability of finding the particle in the position \mathbf{x} at time t . If we consider a free elementary charge under the action of constant potential ϕ_0 , a most simple wave function is a plane wave

$$\psi(\mathbf{x}, t) = \exp i(\mathbf{k}\mathbf{x} - \omega t). \quad (2.7)$$

Then, from eq. (2.7),

$$\frac{\partial\psi}{\partial t} = -i\omega\psi \quad \Delta_{\mathbf{x}}\psi = -|\mathbf{k}|^2\psi. \quad (2.8)$$

Using (2.5) and (2.6), we have

$$i\hbar\frac{\partial\psi}{\partial t} = \mathcal{E}\psi \quad (2.9)$$

$$-\frac{\hbar^2}{2m}\Delta_{\mathbf{x}}\psi - q\phi_0\psi = \mathcal{H}(\mathbf{x}, \mathbf{p})\psi. \quad (2.10)$$

The last equation can be rewritten as following

$$H\psi = \mathcal{H}(\mathbf{x}, \mathbf{p})\psi \quad (2.11)$$

where the quantum operator $H = -\frac{\hbar^2}{2m}\Delta_{\mathbf{x}} - q\phi_0$ is obtained from Hamiltonian \mathcal{H} substituting $\mathbf{x} \rightarrow \mathbf{x}$ and $\mathbf{p} \rightarrow -i\hbar\nabla_{\mathbf{x}}$. Since $\mathcal{E}(t) = \mathcal{H}(\mathbf{x}(t), \mathbf{p}(t))$, from eq. (2.10), we have

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi. \quad (2.12)$$

This equation, known as Schrödinger equation, is postulated to be valid to describe the behavior of matter at the atoms scale or lower. Because the distance of two points in the crystal is of the same order of a typical electron de Broglie wavelengths ($\sim 10^{-8}cm$), a single electron dynamics

can be explained by

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi - q\phi(\mathbf{x}, t) \psi, \quad \mathbf{x} \in \mathbb{R}^3, \quad t > 0 \quad (2.13)$$

with initial condition $\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$.

If the atoms are located at the points of the lattice L , the potential ϕ_L will be a periodic with the same lattice periodicity, it will be invariant with respect to a translation for each element of L

$$\phi_L(\mathbf{x} + \mathbf{y}) = \phi_L(\mathbf{x}) \quad \forall \mathbf{x} \in \mathbb{R}^3, \mathbf{y} \in L. \quad (2.14)$$

In a physical system, as in a solid, electrons occupy stationary energy levels which are solutions of the stationary Schrödinger equation. Bloch waves are special solutions of Schrödinger's equation with a periodic real potential.

Theorem 1 *Bloch Theorem*

The bounded eigenstates of $H\psi = \mathcal{E}\psi$, with the periodic above Hamiltonian, have the form

$$\psi_{\mathbf{k}}(\mathbf{x}) = \exp(i\mathbf{k} \cdot \mathbf{x}) u_{\mathbf{k}}(\mathbf{x}), \quad \mathbf{k} \in \mathbb{R}^3 \quad (2.15)$$

and

$$u_{\mathbf{k}}(\mathbf{x} + \mathbf{y}) = u_{\mathbf{k}}(\mathbf{x}), \quad \forall \mathbf{y} \in L \quad (2.16)$$

This theorem claims that the eigenstates of H can be chosen, so that to each ψ there is associated a wavevector \mathbf{k} satisfying [5], [27]

$$\psi_{\mathbf{k}}(\mathbf{x} + \mathbf{y}) = \psi_{\mathbf{k}}(\mathbf{x}) \exp(i\mathbf{k} \cdot \mathbf{y}), \quad \mathbf{x} \in \mathbb{R}^3, \mathbf{y} \in L. \quad (2.17)$$

By replacing the eq. (2.15) in the eq.(2.12), one obtains a second order self-adjoint elliptic problem posed on a primitive cell of the crystal lattice L . It is possible to prove [5] the existence of an

infinite sequence of eigenpairs (energy-wave function) (ψ, \mathcal{E}) . The eigenfunctions ψ and $\mathcal{E}(\mathbf{k})$ are periodic with respect to reciprocal lattice L^* , in fact we have

$$\psi_{\mathbf{k}+\mathbf{l}^*} = \psi_{\mathbf{k}}, \quad \mathcal{E}_{\mathbf{k}+\mathbf{l}^*} = \mathcal{E}_{\mathbf{k}} \quad \forall \mathbf{l}^* \in L^*,$$

that is the set of eigenfunctions ψ and the $\mathcal{E}(\mathbf{k})$ are identical for any two wave-vectors which differ by a reciprocal lattice vector. Therefore one can constrain the wave vector \mathbf{k} to the Brillouin zone B . As a consequence, for any $\mathbf{k} \in B$ we have a sequence of eigenfunctions $\psi_{\mathbf{k}}^m$ with associated eigenvalues $\mathcal{E}_m(\mathbf{k})$, $m \in \mathbb{N}_0$.

The relation between $\psi_{\mathbf{k}}$ and ψ is given by

$$\psi_{\mathbf{k}}(\mathbf{x}) = \sum_{\mathbf{l} \in L} \exp(-i\mathbf{k} \cdot \mathbf{l}) \psi(\mathbf{x} + \mathbf{l}).$$

We can also write $\psi_{\mathbf{k}}^m$ as distorted waves

$$\psi_{\mathbf{k}}^m = u_{\mathbf{k}}^m(\mathbf{x}) \exp(i\mathbf{k} \cdot \mathbf{x}). \quad (2.18)$$

with $u_{\mathbf{k}}^m(\mathbf{x})$ periodic function in L , called *Bloch waves*

$$u_{\mathbf{k}}^m(\mathbf{x}) = \sum_{\mathbf{l} \in L} \exp(-i\mathbf{k} \cdot (\mathbf{x} + \mathbf{l})) \psi(\mathbf{x} + \mathbf{l}).$$

Then, we obtain an infinite sequence of eigenpairs $\mathcal{E}_m(\mathbf{k})$, $u_{\mathbf{k}}^m(\mathbf{x})$. Here $\hbar\mathbf{k}$ is called *crystal momentum*, it is not general momentum of the electron, but it reduces to this last in the case of the free space ($\phi_L = 0$). The function $\mathcal{E}_m = \mathcal{E}_m(\mathbf{k})$, called the *dispersion relation*, depends on the wave-vector \mathbf{k} and describes energy bands for each integer value of m . These energy bands represent the bands structure of the material. Whenever there is no overlapping between energy bands with different indices m there are energy ranges with no stationary values. In the classic crystalline semiconductors, electrons can have energies only within certain bands (i.e. ranges of levels of energy), so that the crystal is characterized by many different, spaced discrete energy levels, called quantum states of the electrons. In fact according to Pauli exclusion principle, in a given system,

two electrons can not occupy the same quantum state and each allowed electron energy level has a different energy. Each of the original quantized levels of the isolated atom is split many times and each resulting group of energy levels contains one level for each atom in the system. Some properties of semiconductors depend on the distribution of allowed energy levels and on the *energy gap*, that contains no available states. The total extension of the energy band is of the order of a few eV, the discrete different energy levels within each band is smaller than the thermal energy of an electron at room temperature, so that the electron can easily move between levels. The allowed energy levels are so close together that they are sometimes considered as being continuous. This is a useful and reasonable approximation in some calculations, but they are composed of a finite number of very closely spaced electron energy levels. The lower energy band is called the *valence band*, since it contains all the valence electrons, while the upper energy band is called *conduction band*, since excitation of electrons into this band is principal responsible for electrical conduction. The *energy gap* is the difference between the highest (in energy) filled band and the minimum of the lowest empty band

$$\mathcal{E}_g = \min_{\mathbf{k} \in B} \mathcal{E}_c(\mathbf{k}) - \max_{\mathbf{k} \in B} \mathcal{E}_v(\mathbf{k}) = \mathcal{E}_c - \mathcal{E}_v > 0. \quad (2.19)$$

The behaviour of electrons in the bands determines the electronic properties of a given material and it is a fundamental feature differentiating conductors, insulators and semiconductors. If the allowed energy bands are partially full, the crystal is a metal. In the presence of electric field the electrons near the top of the filled zone of the band can easily move into those empty states and become free electrons, carried through the lattice, and the conductivity is high, while in the insulators the allowed energy band is completely full or empty, all electrons do not move from band to another one. In semiconductor a certain set of bands is completely filled while the remaining ones are empty.

At absolute zero insulators and semiconductors have a similar band structure, the valence band of a semiconductor is completely full and conduction band is empty, so that at this temperature

the semiconductor behavior is the same of an insulator material. The only difference lies in the size of energy gap, which is smaller in semiconductors, generally of order of 1 eV, while in insulator it is generally of order of 5 eV. The energy gaps of some common semiconductors are shown in Table 2.2.

Material	Symbol	Energy gap (eV)
Silicon	(<i>Si</i>)	1.12
Germanium	(<i>Ge</i>)	0.67
Gallium arsenide	(<i>GaAs</i>) Zincblende	1.42
Aluminum gallium arsenide	(<i>Al_{0.3}Ga_{0.7}As</i>)	1.80
Gallium phosphide	(<i>GaP</i>)	2.20

Table 2.2: Energy gaps of some semiconductors [5],[32]

A small energy gap allows electrons to be excited across the forbidden gap, from filled valence band into the empty conduction band by thermal excitation at room temperature, leaving behind an empty bond. A positive charge is associated to vacant bond, called *hole*. Physically, a hole is a vacant orbital in an otherwise filled (valence) band. Then, the current flow in a semiconductor is given by the flow of electrons in the conduction band and the flow of holes in the valence band. At higher temperature the number of free electrons increases, the bottom of the conduction band is populated by electrons, while the top of the valence band by holes.

The existence of a band gap explains some characteristics of semiconductor [48],[51]:

- the conductivity increases with temperature, because with thermal excitation the number of free carriers is higher in the conduction band;
- the transparency of semiconductor to infrared radiation, in fact photons with energy $h\nu < \mathcal{E}_g$ can not be absorbed, as the electron can not reach a final state within the band gap. If $h\nu > \mathcal{E}_g$

electrons can be excited into the conduction band by absorbing photons. This phenomena explains the photo-conductivity in semiconductors.

2.5 Doping

We said that at absolute zero a pure semiconductor behaves like a perfect insulator, instead, at higher temperatures, thermal energy breaks some covalent bonds releasing a free electron, that leaves behind an empty bond. The semiconductor electrical resistivity lies in the range of $10^{-2} - 10^9 \Omega cm$, the conductivity is small compared with the conductivity of metals, because a small number of electrons and holes are involved, it is nonetheless sufficiently large for practical application in the semiconductor devices. Doping of semiconductors is the process of locally manipulating their charge carrier density and conductivity and it represents a key technology for semiconductor-based electronic devices [51].

Semiconductors occur in many different chemical compositions with a large variety of crystal structures. The best-know class is the group IV semiconductors (C, Si, Ge), that have been studied intensively for many applications in semiconductor devices. The fourth group semiconductors crystallizes in a structure known as the diamond structure, in which each atom is surrounded by four nearest neighbor atoms and has covalent bonds with them. Another important group of semiconductor is the groups III - V compounds, that contains two elements, one from third and other from the fifth column of the periodic table. In this structure, eight valence electrons are shared amongst neighbouring atoms; the bonding is not entirely covalent bond, but it is partially ionic too: three valence electrons are supplied by trivalent atom and five electrons by the pentavalent atom. Consequently, the valence electrons are bond with the atoms more strongly than the corresponding group IV semiconductor.

A semiconductor is defined as intrinsic, if the number of electrons n in the conduction band is

precisely equal to the number of holes p left behind in the valence band. Conventional doping is usually achieved through the bombardment of semiconductors with energetic ions followed by thermal annealing. This process, called ion implantation, allows external impurity atoms (dopants) with appropriate properties to be incorporated into the host lattice of the semiconductor. Depending on their number of valence electrons, the dopants (as donors) can either donate excess electrons as negative free charge carriers to the semiconductor conduction band at moderate temperature (n-type doping), or they (as acceptors) can accept additional electrons from surrounding atoms to complete the covalent chemical bonding, leaving positively charged and the holes as charge carriers in the semiconductor valence band (p-type doping). The density of donors (atoms cm^{-3}) is generally indicated with N_d , while the density of acceptors with N_a . For example, we consider the silicon (Si), which is a semiconductor with a band gap of about 1.1 eV. If a phosphorus (P) atom replaces one of the Si atoms in the lattice, a P atom can be thought as a Si atom plus an extra proton and an extra electron. Since the valence band is already filled this additional electron must go into the conduction band. The P atom is known as a donor (or electron donor) or an n -dopant. Analogously, if we can consider aluminum, the aluminum dopant provides one fewer electron than Si, so there will be one missing electron from the valence band. In this case Al is known as an electron acceptor, or equivalently as a p-dopant.

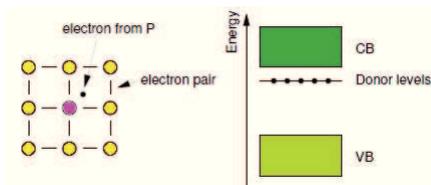


Figure 2.6: The donor levels created by substituting Si by P lie just below the bottom of the conduction band.

Semiconductors, in which the conduction depends primarily from carriers contributed by impurity atoms, are called extrinsic semiconductors. We observe that in metals the doping decreases the conductivity, because there are more scattering with lattice, but in the semiconductors the

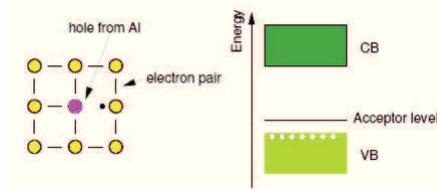


Figure 2.7: The acceptor levels created by substituting Si by Al lie just below the top of the valence band.

conductivity increases, because the donor atoms provide free electrons that did not exist in pure semiconductor. The intrinsic conductivity depends on the relationship $\mathcal{E}_g/k_B T$, where \mathcal{E}_g is gap band energy and T is the temperature. If this ratio is great, the density of intrinsic ionized carriers will be low. When doping is low, the atoms of impurity do not interact with each other and not alter the structure of the bands of the crystal. If the density of doping is about $5 \times 10^{15} \text{cm}^{-3}$, that is an atom for each 10^7 silicon atoms, increasing the density, the atomic structure can be modified, because the range of gap band decrease. Finally, with high doping, the atomic structure is modified, because the energy levels are not separate and the bands of impurity may overlap to near valence bands and conduction bands.

2.6 Effective mass

In the semiclassical theory, the motion of electron in an applied electric field is described by a packet of Bloch waves centered on $\mathbf{k} = \mathbf{k}_0$, that is built by introducing other neighboring states belonging to the same band m . Therefore, the electrons in a conduction band are essentially located in the neighborhoods of the lowest energy local minima, the so-called valleys. Fixed a wave number \mathbf{k} , the group velocity is given by definition

$$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}_{\mathbf{k}}. \quad (2.20)$$

Differentiating with respect to time, we have

$$\frac{\partial \mathbf{v}_n}{\partial t} = \frac{d^2 \mathcal{E}_n}{d\mathbf{k}^2} \frac{\partial \mathbf{k}}{\partial t} = \frac{1}{\hbar} \frac{d^2 \mathcal{E}_n}{d\mathbf{k}^2} \mathbf{F}, \quad (2.21)$$

where \mathbf{F} is the force of the electric field.

Using the Newton's law

$$\mathbf{F} = \frac{\partial \mathbf{p}}{\partial t} = m^* \frac{\partial \mathbf{v}_n}{\partial t} \quad (2.22)$$

where \mathbf{p} is the momentum and m^* is the *effective mass*, we obtain

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 \mathcal{E}_n}{d\mathbf{k}^2}. \quad (2.23)$$

The term $d^2 \mathcal{E}_n / d\mathbf{k}^2$ is a 3×3 matrix, then also the term m^* represents a matrix of the same order. If we evaluate the Hessian of \mathcal{E}_n near a local minimum, i.e. $\nabla_{\mathbf{k}} \mathcal{E}_n(\mathbf{k}_0) = 0$, we obtain a symmetric positive matrix, which can be diagonalized and that has the positive diagonal elements

$$\begin{pmatrix} \frac{1}{m_{xx}^*} & 0 & 0 \\ 0 & \frac{1}{m_{yy}^*} & 0 \\ 0 & 0 & \frac{1}{m_{zz}^*} \end{pmatrix} = \frac{1}{\hbar^2} \frac{d^2 \mathcal{E}_n}{d\mathbf{k}^2}(\mathbf{k}_0)$$

Under assumption that the energy value are shifted, so the energy vanishes at the local minimum (\mathbf{k}_0). For wave vector \mathbf{k} "close" to \mathbf{k}_0 , we have from Taylor's formula and we have

$$\begin{aligned} \mathcal{E}_n(\mathbf{k}) &= \mathcal{E}_n(\mathbf{k}_0) + \nabla_{\mathbf{k}} \mathcal{E}_n(\mathbf{k}_0) \cdot \mathbf{k} + \frac{1}{2} \mathbf{k}^\top \frac{d^2 \mathcal{E}_n}{d\mathbf{k}^2}(\mathbf{k}_0) \mathbf{k} + O(|\mathbf{k} - \mathbf{k}_0|^3) \\ &= \frac{\hbar^2}{2} \left(\frac{k_x^2}{m_x^*} + \frac{k_y^2}{m_y^*} + \frac{k_z^2}{m_z^*} \right) + O(|\mathbf{k} - \mathbf{k}_0|^3) \end{aligned}$$

where $\mathbf{k} = (k_x, k_y, k_z)^\top$. If the effective mass is isotropic, we can neglect higher - order terms and the dispersion relation can be rewritten as

$$\mathcal{E}_n(\mathbf{k}) = \frac{\hbar^2}{2m^*} |\mathbf{k}|^2. \quad (2.24)$$

We remark that the energy of an electron, near a band minimum, is equal to energy of a free electron in vacuum, where the mass of the particle is replaced by the effective mass. Moreover, the effects of the crystal potential are represented by the effective mass. The (2.24) is referred to the parabolic band approximation, but taking into account the non - parabolic effect, we have to introduce a factor of non parabolicity $\alpha > 0$. In this case we use an *approximation of Kane* for dispersion relation

$$\mathcal{E}_n (1 + \alpha \mathcal{E}_n) = \frac{\hbar^2}{2m^*} |\mathbf{k}|^2. \quad (2.25)$$

Assuming value of the effective mass near a band maximum, we find that the Hessian of \mathcal{E}_n is a negative definite, which would lead to a negative effective mass. For a positive charge, the hole, the effective mass is positive.

2.7 Physics of equilibrium of semiconductors and Fermi-Energy

In this section we determine the equation of state for the density of electrons and holes number in the conduction band and in the valence band, respectively.

In a semiconductor, the statistical distribution of particles (electrons and holes) can be described by the concept of *Fermi Energy*. The three thermodynamics quantities, taken into account, are the density of number of particles, the temperature and the chemical potential. The chemical potential represents the energy required to increase by one the number of particles, when the temperature and volume are both constant. When the energy \mathcal{E} is equal to the chemical potential, obviously the distribution function is equal to 1/2, this value for the energy is called Energy Fermi. According Pauli exclusion principle, electrons in solids follow *Fermi - Dirac* statistics, which describes that probability $f_D(\mathcal{E})$ that a state at energy \mathcal{E} is filled by an electron, at the thermal equilibrium. This

statistical function is given by

$$f_D(\mathcal{E}) = \frac{1}{1 + \exp[(\mathcal{E} - \mathcal{E}_F)/k_B T]} \quad (2.26)$$

where \mathcal{E}_F is a reference energy *Fermi energy* or *Fermi level*. Some properties of Fermi Dirac function are as follows

- at $T \rightarrow 0$ K the distribution function has a simple rectangular as shown in Fig. 2.8. All states above \mathcal{E}_F are empty and all state below \mathcal{E}_F are filled with electrons, that is for $\mathcal{E} > \mathcal{E}_F \implies f_D(\mathcal{E}) \rightarrow 0$, while for $\mathcal{E} < \mathcal{E}_F \implies f_D(\mathcal{E}) \rightarrow 1$.
- at temperature $T > 0$ K, we observe that the $f_D(\mathcal{E})$ is a decreasing function of temperature, that is at higher energies ($\mathcal{E} > \mathcal{E}_F$) the state has a lesser probability of being occupied by an electron. On the other hand, for $\mathcal{E} < \mathcal{E}_F$, at lower energies, it has a small probability of being empty.
- it can be shown that the probability of a state at an energy $\Delta\mathcal{E}$ above \mathcal{E}_F being occupied is exactly the same of a state at an energy $\Delta\mathcal{E}$ below \mathcal{E}_F being vacant. In other words the function $f_D(\mathcal{E})$ is symmetrical about \mathcal{E}_F at all temperatures. A filled state in the conduction band indicates the presence of an electron in the conduction band and an empty state in the valence band, occupied by an hole.

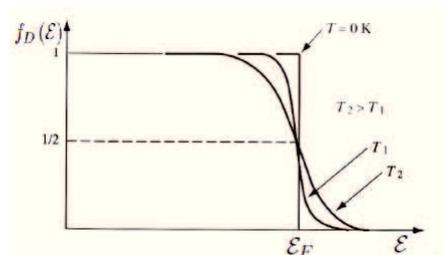


Figure 2.8: Fermi-Dirac Distribution for some temperatures.

The Fermi function represents only a probability of occupancy, it does not give information about

the states and charge at a given energy; but applying quantum physics we can obtain information about the density of available states as a function, that depends on energy. The number of possible states within all energy bands per unit of volume $(2\pi)^3$ is given by

$$g(\mathcal{E}) = \frac{2}{(2\pi)^3} \sum_{\nu} \int_B \delta(\mathcal{E} - \mathcal{E}_{\nu}(\mathbf{k})) d\mathbf{k}. \quad (2.27)$$

The function $g(\mathcal{E})$ is called *density of states*.

The factor 2 comes from the two possible states of the spin of an electron, B is the Brillouin zone and the function δ distribution is defined by

$$\int_{-\infty}^{+\infty} \delta(\mathcal{E}_0 - \mathcal{E}) \varphi(\mathcal{E}) d\mathcal{E} = \varphi(\mathcal{E}_0) \quad (2.28)$$

of all continuous function φ .

Using the (2.28), we can express the electron concentration in the conduction band

$$n_c = \frac{1}{4\pi^3} \sum_{\nu} \int_B \int_{-\infty}^{+\infty} \delta(\mathcal{E} - \mathcal{E}_{\nu}(\mathbf{k})) f_D(\mathcal{E}) d\mathcal{E} d\mathbf{k}$$

$$n_c = \int_{\mathcal{E}_c}^{\infty} g(\mathcal{E}) f_D(\mathcal{E}) d\mathcal{E}$$

with \mathcal{E}_c is the minimum of the conduction band $\mathcal{E}_c(\mathbf{k})$. Similarly we can express the holes concentration in the valence band

$$p_v = \int_{-\infty}^{\mathcal{E}_v} g(\mathcal{E}) (1 - f_D(\mathcal{E})) d\mathcal{E} \quad (2.29)$$

The distribution function $f_D(\mathcal{E})$ can be approximated by *Maxwell - Boltzmann distribution* if $\mathcal{E}_c - \mathcal{E}_F \gg k_B T$ for any energy level \mathcal{E} in the conduction band and if $\mathcal{E}_F - \mathcal{E}_v \gg k_B T$ in the valence band

$$f_M(\mathcal{E}) = \exp\left(-\frac{\mathcal{E} - \mathcal{E}_F}{k_B T}\right) \quad \forall \mathcal{E} < \mathcal{E}_c \quad (\text{for electrons})$$

$$f_M(\mathcal{E}) = \exp\left(-\frac{\mathcal{E}_F - \mathcal{E}}{k_B T}\right) \quad \forall \mathcal{E} < \mathcal{E}_v \quad (\text{for holes}).$$

These hypothesis might be not valid if semiconductor is very heavily doped (degenerate case).

Using these approximations the carrier concentration, respectively, in the conduction band and valence one is

$$n_c = N_c(T) \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_F}{k_B T}\right) \quad p_v = N_v(T) \exp\left(-\frac{\mathcal{E}_F - \mathcal{E}_v}{k_B T}\right) \quad (2.30)$$

with

$$N_c(T) = \int_{\mathcal{E}_c}^{\infty} g_c(\mathcal{E}) \exp\left(-\frac{\mathcal{E} - \mathcal{E}_c}{k_B T}\right) d\mathcal{E} \quad (2.31)$$

$$N_v(T) = \int_{\mathcal{E}_{-\infty}}^{\mathcal{E}_v} g_v(\mathcal{E}) \exp\left(-\frac{\mathcal{E}_v - \mathcal{E}}{k_B T}\right) d\mathcal{E}. \quad (2.32)$$

If in the conduction and valence bands the densities of states are equal (*intrinsic semiconductor*), the Fermi level is exactly at the middle of the band gap and we have the *law of mass action*

$$n_c p_v = n_i^2 \quad (2.33)$$

where n_i is the intrinsic concentration that, in this case, depends only on the temperature and that is given by

$$n_i^2 = N_c N_v \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_v}{k_B T}\right) = N_c N_v \exp\left(-\frac{\mathcal{E}_g}{k_B T}\right) \quad (2.34)$$

$$n_i(T) = \sqrt{N_c N_v} \exp\left(-\frac{\mathcal{E}_g}{2k_B T}\right). \quad (2.35)$$

Using (2.30) it is possible to determine the chemical potential (Fermi-level) depending of temperature

$$N_c(T) \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_F}{k_B T}\right) = N_v(T) \exp\left(-\frac{\mathcal{E}_F - \mathcal{E}_v}{k_B T}\right). \quad (2.36)$$

Hence, we have

$$\mathcal{E}_F = \mathcal{E}_{F,i}(T) = \frac{1}{2}(\mathcal{E}_c - \mathcal{E}_v) + \frac{1}{2}k_B T \ln\left(\frac{N_v(T)}{N_c(T)}\right). \quad (2.37)$$

To analyze non-equilibrium case, we must define quasi-Fermi levels so that the relationship between the intrinsic carrier n_i and the electron and hole densities is expressed at thermal equilibrium in the equations (2.30). If we replace the Fermi-level \mathcal{E}_F with $\mathcal{E}_{F,c}$ for the electron in conduction band and with $\mathcal{E}_{F,v}$ for holes in valence band, we obtain

$$n_c = N_c(T) \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_{F,c}}{k_B T}\right), \quad p_v = N_v(T) \exp\left(-\frac{\mathcal{E}_{F,v} - \mathcal{E}_v}{k_B T}\right) \quad (2.38)$$

with

$$N_c(T) = n_i \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_{F,i}}{k_B T}\right), \quad N_v(T) = n_i \exp\left(-\frac{\mathcal{E}_{F,i} - \mathcal{E}_v}{k_B T}\right). \quad (2.39)$$

Using (2.39) equations, we can rewrite (2.38) as

$$n_c = n_i \exp\left(-\frac{\mathcal{E}_{F,c} - \mathcal{E}_{F,i}}{k_B T}\right), \quad p_v = n_i \exp\left(-\frac{\mathcal{E}_{F,i} - \mathcal{E}_{F,v}}{k_B T}\right). \quad (2.40)$$

From the above expressions, we obtain

$$\mathcal{E}_{F,c} = \mathcal{E}_{F,i} + k_B T \ln \frac{n_c}{n_i}, \quad \mathcal{E}_{F,v} = \mathcal{E}_{F,i} + k_B T \ln \frac{p_v}{n_i}. \quad (2.41)$$

Under non-equilibrium condition $np \neq n_i^2$, but np can be expressed as function of the two quasi-Fermi levels. From (2.39) and (2.40) we can derive

$$np = n_i^2 \exp\left(\frac{\mathcal{E}_{F,c} - \mathcal{E}_{F,v}}{k_B T}\right). \quad (2.42)$$

The difference between the two quasi-Fermi levels is a measure of deviation from thermal equilibrium of the semiconductor free-carrier density and it is zero at thermal equilibrium.

It is interesting to know the carrier concentration or the position the Fermi energy level when the semiconductor is highly doped. We can use a simple approximation $n_c = N_D$ and $p_v = N_A$, where N_D is the donor concentration in *n-type* semiconductor and N_A is the acceptor concentration in *p-type* semiconductor. Let us \mathcal{E}_d and \mathcal{E}_a the energy level of a donor electron and an acceptor

hole, respectively. The energies $\mathcal{E}_c - \mathcal{E}_d$ and $\mathcal{E}_a - \mathcal{E}_v$ are small with respect to $k_B T$, this means that additional particles contribute at room temperature to the electrons and holes density.

The Fig. (2.9) shows the electron concentration depending on temperature for a *n-type* semiconductor. At low temperatures the electron concentration is low, because complete ionization has not taken place. Increasing the temperature, the degree of ionization of the donors increases and consequently also the electron concentration. Then, it remains nearly constant over a range of temperature, because the ionization is complete. In this range of temperature the semiconductor is strongly extrinsic. Finally at higher temperatures, n_i increases and when the thermally generated electron and hole concentration becomes comparable to the dopant concentration, the material have a nearly intrinsic behavior.

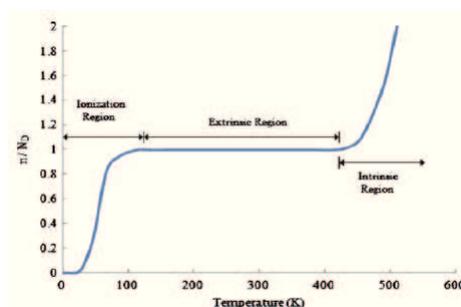


Figure 2.9: Temperature dependence of n in a doped semiconductor.

2.8 Mobility, drift velocity, diffusion current

We described the concentrations of carriers in a semiconductor, now we turn our attention to the dynamics of the carriers in presence of electric fields and of density gradients. We said that electrons (and holes) in semiconductors are free-particles, then they are not associated with any particular lattice site. On the other hand, the effective mass, that differs somewhat from the free-electron mass, points out the influence of crystal force. According to the laws of statistical mechanics, we can claim that the electrons and the holes have a thermal energy associated with classical free-particles.

In not stationary conditions, the charge carriers are in random motion through the lattice, colliding among themselves and with lattice, with average kinetic energy proportional to $k_B T$. If v_{th} is the mean-square thermal velocity [51], we have

$$\frac{1}{2}m_n^*v_{th}^2 = \frac{3}{2}k_B T.$$

At thermal equilibrium the motion of the electrons ensemble is completely random so that the semiconductor is in electrostatic equilibrium and the net current is zero. Collisions with the lattice produce an energy transfer between the electrons and the atomic cores of the lattice.

If we apply a small electric field, the electrons are accelerated along the same direction of field during collisions. When they collide with the lattice and drop toward their thermal-equilibrium position, the energy exchanged is small and the crystal lattice is not enough heated by passage of current, because the electric field is small and the lost energy in each collision is much less the mean thermal energy of an electron. The net carrier velocity in presence of an electric field is called *drift velocity* v_d , it can be found by equating the impulse applied to an electron, between two collision, with the momentum gained by electron in the same period of time. We have this equality when all momentum gained between collisions is lost to the crystal lattice in the collisions. Thus from the condition $-qE\tau_c = m_n^*v_d$, we obtain

$$v_d = -\frac{qE\tau_c}{m_n^*}. \quad (2.43)$$

This equation points out that the drift velocity v_d is proportional to the electric field and it depends on the mean scattering time and the effective mass. The proportionally factor is called *mobility* and it is designed by the symbol μ_n :

$$\mu_n = \frac{q\tau_n}{m_n^*}. \quad (2.44)$$

From (2.43), we can assume the current density flowing in the direction of the applied electric field

in this way

$$J_n = - \sum_{i=1}^n qv_i = -nqv_d = nq\mu_n E. \quad (2.45)$$

Similarly for holes, if μ_p is the holes mobility, we can write

$$J_p = pq\mu_p E. \quad (2.46)$$

As a consequence the total current density is

$$J = J_n + J_p = (nq\mu_n + pq\mu_p) E.$$

Let us $\sigma = nq\mu_n + pq\mu_p$, we obtain $J = \sigma E$, where σ is the conductivity.

2.8.1 Diffusion current and Einstein Relation

The term diffusion current is used for the electric current due to a density gradient of charge. The lower conductivity and nonuniform density of carriers produce often diffusion and important process involving current flow in semiconductors. For example, we consider a n-type semiconductor, with a gradient of charge concentration $n(x)$. Let us l the mean free path between two subsequent collisions, so that $l = v_{th}\tau_c$, the diffusion current can be written as following

$$J_n = qlv_{th} \frac{dn}{dx}, \quad (2.47)$$

that is proportional to the spatial derivative of the electron density; if the electron density increases then the gradient is positive, like diffusion current. Using the theorem of the equipartition of energy to this one dimensional case, we can rewrite the (2.47) in the following form known as Einstein relation

$$J_n = qD_n \frac{dn}{dx} \quad (2.48)$$

where $D_n = \frac{k_B T}{q} \mu_n$ is called diffusion coefficient .

Finally, we can assert that in presence of electric field, we must take into account the drift and diffusion current

$$J_n = q\mu_n nE + qD_n \frac{dn}{dx}. \quad (2.49)$$

We can obtain a similar expression for the holes, so that the total hole current is:

$$J_p = q\mu_p pE - qD_p \frac{dp}{dx}. \quad (2.50)$$

2.9 Scattering mechanisms in a lattice

Taking into account an ideal and perfect lattice, the carriers scattering with crystal is neglected and the electrons do not interchange energy with (stationary), perfect lattice. Nevertheless, at any temperature above $T = 0$ K the atoms of lattice vibrate. These vibrations alter the periodicity and the energy is exchanged between the carriers and the lattice. This interaction is known as collisions with energetic particles, called phonons. The scattering phenomena lead to heating of semiconductor, the dissipation of this heat is often a limiting factor in the size of semiconductor devices. From the electron scattering, we can have an absorption or emission of a phonon, that may be an acoustic or an optical phonon. The interaction mechanism may also be electrostatic, as we have for polar optical or piezoelectric acoustic phonons in compound semiconductors, or it can be due to the variation of the band edge produced by the deformation of the lattice. In these cases we talk of polar interaction, piezoelectric interaction, and deformation-potential interaction, respectively. In many mathematical models, it is useful the assumption that the optical phonon scattering is anelastic, while acoustic phonons carry a very small amount of energy, and the scattering can be considered elastic at room temperature.

In the doped semiconductors, if the impurities are ionized, they interact with electrons through a long-range Coulomb field, but if they are neutral impurities, the interaction occurs with a short-range interaction and with much weaker effect in bulk transport properties. Owing to the large

mass of the impurities, this kind of scattering can be always considered elastic. The effect of the impurities becomes more important at lower temperatures, when phonons become less effective.

The scattering between electrons is type of Coulomb interaction, that depends on the probability of an electron to scatter with another electron with a given momentum. Therefore, it depends on the electron distribution function (see chapter 4). In a collision between two electrons, the total momentum and the total energy of the electrons do not change. This type of interaction is not dissipative, but the shape of the distribution function changes and, as a consequence, this collision influences the effect of the other scattering mechanisms. Its effect is relevant at high electron concentrations ($\geq 10^{17} - 10^{18} \text{ cm}^{-3}$).

An other important factor is the relationship between the mobility and the doping, because also impurities cause local distortions in the lattice and scatter with the free carriers. About phonon scattering, this scattering is less significant at higher temperatures, in fact the carriers move faster and remain near the impurity atom for a shorter time; consequently, when impurity scattering is dominant, the mobility increases if the temperature increases. At high electric fields, the energy of hot electrons reaches a critical value, in this case there is an other important scattering phenomena (collisions with high energy optical phonons) and the mobility decreases from its low-field value. In this case the carriers can not gain significant additional energy and reach a limiting value of velocity, called velocity of *saturation* v_{sat} at high field.

Chapter 3

Classical Kinetic Transport Models

This chapter deals with the classical kinetic transport equations, modeling the flow of charge carriers in the semiconductors, as the Liouville, Vlasov, and Boltzmann equation [35]. According to a probabilistic approach, the charge carriers are specified by a distribution function depending on the phase space variable and on the time.

At the first we introduce the classical Liouville equation, which describes the evolution distribution function of a single particles, neglecting interference from the environment. Then, this equation is rewritten for a particle ensemble. Including the quantum effects of the semiconductor lattice via the band-diagram of the material, the semiclassical Liouville equation is needed.

The Vlasov equation is presented in the semiclassical formulation. This equation has the form of Liouville equation, but supplemented by an effective field equation, which depends on the position space number density of the particles. The effective field equation represents the average effect of the many-body physics.

Finally, we focus on the description of the semiclassical Boltzmann equation and in particular on the collisional operator and its features. This equation describes the short interactions of the particles with each other and with lattice. The specific form of the kernel of the collisional operator are shown.

3.1 The Liouville equation

In the classical models the description of the motion of particle ensembles is based on Newton's second law. A probabilistic reformulation of these canonical equations of motion is given by the classical Liouville equation. Let us $f_I = f_I(\mathbf{x}, \mathbf{v})$ the joint probability density of the initial position and velocity associated to an elementary particle (an electron, for example)[35]. Assume that

$$f_I = f_I(\mathbf{x}, \mathbf{v}) \geq 0, \quad \iint f_I(\mathbf{x}, \mathbf{v}) d\mathbf{x}d\mathbf{v} = 1 \quad (3.1)$$

then

$$\iint_B f_I(\mathbf{x}, \mathbf{v}) d\mathbf{x}d\mathbf{v} \quad (3.2)$$

is the probability to find the particle ensemble in the subset B of the (\mathbf{x}, \mathbf{v}) -space at time $t = 0$.

Given $f = f(\mathbf{x}, \mathbf{v}, t)$ the probability density of the electron at time t , we postulate that this function does not change along the trajectories $w = w(t; \mathbf{x}, \mathbf{v})$

$$f(w(t; \mathbf{x}, \mathbf{v}), t) = f_I(\mathbf{x}, \mathbf{v}) \quad \forall \mathbf{x}, \mathbf{v} \quad t \geq 0. \quad (3.3)$$

Differentiating (3.3) with respect to time, we have

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f + \frac{d\mathbf{v}}{dt} \cdot \nabla_{\mathbf{v}} f = 0. \quad (3.4)$$

In the presence of electric field, we obtain

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \frac{q}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}} f = 0, \quad t > 0. \quad (3.5)$$

This equation is the *Liouville equation* governing the evolution of the position-velocity probability density $f = f(\mathbf{x}, \mathbf{v}, t)$ of the electron in the electric field \mathbf{E} under the hypothesis that the electron moves according to the laws of classical mechanics, without to interact with crystal lattice. If we consider a particle ensemble (electrons), the classical Liouville becomes

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f = 0 \quad (3.6)$$

where $\mathbf{x} \in \mathbb{R}^{3M}$, $\mathbf{v} \in \mathbb{R}^{3M}$ and $f = f(\mathbf{x}, \mathbf{v}, t)$ represents the joint position–velocity probability density of the M –particle ensemble at time t . In the following, we assume that the electric field force \mathbf{F} is divergence–free with respect to the velocity, so that

$$\operatorname{div}_{\mathbf{v}} \mathbf{F} = 0 \quad \mathbf{x} \in \mathbb{R}^{3M} \quad \mathbf{v} \in \mathbb{R}^{3M} \quad t \geq 0.$$

3.1.1 The conservation property

We integrate (3.6) over $\mathbb{R}^{3M} \times \mathbb{R}^{3M}$, assume that solution decays to zero sufficiently fast as $|\mathbf{x}| \rightarrow \infty$, $|\mathbf{v}| \rightarrow \infty$ and obtain

$$\frac{1}{m} \int_{\mathbb{R}^{3M}} \mathbf{F} \cdot \nabla_{\mathbf{v}} f \, d\mathbf{v} = -\frac{1}{m} \int_{\mathbb{R}^{3M}} f \operatorname{div}_{\mathbf{v}} \mathbf{F} \, d\mathbf{v} = 0$$

and

$$\frac{d}{dt} \int_{\mathbb{R}^{3M}} \int_{\mathbb{R}^{3M}} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{v} d\mathbf{x} = 0$$

that is, the integral of f over the whole position–velocity space is conserved in time

$$\int_{\mathbb{R}^{3M}} \int_{\mathbb{R}^{3M}} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{v} d\mathbf{x} = \int_{\mathbb{R}^{3M}} \int_{\mathbb{R}^{3M}} f_I(\mathbf{x}, \mathbf{v}) \, d\mathbf{v} d\mathbf{x} = 1, \quad t \geq 0. \quad (3.7)$$

3.1.2 Zeroth and first order moments

In this subsection we introduce the concepts of moment to define the density and current density and to obtain the *continuity equation*.

We define moment of order zero

$$n(\mathbf{x}, t) = \int_{\mathbb{R}^{3M}} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{v} \quad (3.8)$$

and the first order moment

$$\mathbf{J}(\mathbf{x}, t) = -q \int_{\mathbb{R}^{3M}} \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{v}. \quad (3.9)$$

The function $n = n(\mathbf{x}, t)$ is the position probability density of the particle ensemble, known as *classical microscopic particle position density*, while $J(\mathbf{x}, t)$ represents a flux density, called *microscopic particle current density*. The conservation property (3.7) can be rewritten as

$$\int_{\mathbb{R}^{3M}} n(\mathbf{x}, t) d\mathbf{x} = \int_{\mathbb{R}^{3M}} n_I(\mathbf{x}) d\mathbf{x}, \quad t \geq 0 \quad (3.10)$$

with $n_I(\mathbf{x}) = \int_{\mathbb{R}^{3M}} f_I(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$. By formally integrating the Liouville equation (3.6) over \mathbb{R}^{3M} we obtain the conservation law

$$q\partial_t n - \operatorname{div}_{\mathbf{x}} J = 0 \quad (3.11)$$

which is referred to as macroscopic particle continuity equation.

3.1.3 The semiclassical Liouville equation

We described the energy band model taking into account a semiclassical theory, in which the electrons are subjected to periodic potential of lattice. For this reason we introduce the semiclassical Liouville equation, that takes in account the quantum effects of the crystal lattice. Consider the phase space with seven coordinates: $\mathbf{x} = (x_1, x_2, x_3)^\top$ (spatial coordinates), $\mathbf{k} = (k_1, k_2, k_3)^\top$ (wave vector associated to momentum of lattice), and time $t > 0$, the semi-classical Liouville equation is

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f + \frac{1}{\hbar} F \cdot \nabla_{\mathbf{k}} f = 0 \quad t \geq 0 \quad (3.12)$$

where $\mathbf{x} \in \mathbb{R}^{3M}$, $\mathbf{k} = (k_1, k_2, \dots, k_M) \in B$ for $i = 1, 2, \dots, M$. As the Brillouin zone is a bounded subset, we have to impose boundary conditions for \mathbf{k} . We choose the periodic boundary conditions

$$f(\mathbf{x}, k_1, k_2 \dots k_i \dots k_M, t) = f(\mathbf{x}, k_1, k_2 \dots -k_i \dots k_M, t), \quad k_i \in \partial B.$$

The definition of the electron ensemble position density (3.8) and of the electron ensemble current density (3.9) have to be modified

$$n_B = \int_{B^M} f(\mathbf{x}, \mathbf{k}, t) d\mathbf{k}, \quad (3.13)$$

$$J_B = -q \int_{B^M} \mathbf{v}(\mathbf{k}) f(\mathbf{x}, \mathbf{k}, t) d\mathbf{k}. \quad (3.14)$$

The periodicity of f in k_i and the point-symmetry of the Brillouin zone B involve that the conservation property (3.10) and the conservation law (3.11) are hold for the semi-classical Liouville equation.

3.2 The semiclassical Vlasov Equation

Assuming that the electrons move in a vacuum, the scattering is neglected, the force field \mathbf{F} acting on the ensemble is independent of the velocity vector (in particular magnetic field effects are neglected) and the motion is governed by an external electric field and by two particles interaction force. The semiclassical Vlasov equation is given by

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f = 0 \quad t \geq 0. \quad (3.15)$$

The Vlasov equation is a kinetic equation describing the motion of a weakly interacting large particle ensemble. However, when the time scale is enough large, the motion of particles is more influenced by strong short range force, that is we must consider the scattering phenomena between the particles and the lattice, for example. The Vlasov equation describes the electrons motion in an ideal perfectly periodic lattice, but this is only approximation, because the periodicity of the lattice is impaired some features as crystal dislocation, defects of lines or plane missing atoms (called vacancy), interstitials defects, mechanical stresses, doping, thermal vibration of the ions of their equilibrium position in the lattice.

3.2.1 The semiclassical Boltzmann equation

Since the crystal is not perfectly periodic (ideal crystal), it can be think as a perturbative way and the weak deviations from periodicity are treated as small perturbations of the background

periodic potential and they are described quantum mechanically as scattering with quasi-particles (phonons) representing the thermal lattice vibrations. Formally these effects are taken into account by introducing a non zero right hand side in the semiclassical Vlasov equation. In this way we obtain the Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f - \frac{e\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_{Coll} \quad (3.16)$$

where \mathbf{E} is external electric field [35], [12], the term $\left(\frac{\partial f}{\partial t} \right)_{Coll}$ represents the scattering due to the lattice vibrations (phonons), internal force, and to internal localized crystal features like impurity atoms or ions, vacancies. In semiconductor crystals, there are three main classes of scattering mechanisms: electron-phonon scattering, ionized impurity scattering, electron-electron scattering. At finite temperature, the crystal ions vibrate around the equilibrium position represented by the point of the ideal Bravais lattice. These lattice vibrations are quantized and the quantum of lattice vibrations are the phonons. The interaction with the phonons produces a change in the energy and momentum of the electrons. The exchange of energy can leave the electron in the same band (intraband transition) or pull it into another band (interband transition), e.g for holes. In the conduction bands, the electrons are essentially located in the valleys. After a collision the electron can remain in the same valley (intravalley scattering) or be drawn in another valley (intervalley scattering).

3.3 The collision operator

Let us that the scattering interactions are confined in a limited space with respect to total space and they are instantaneous. We define the *Transition Rate* $S(\mathbf{k}, \mathbf{k}')$ as the density probability per unit time of an electron transition from state with wave number \mathbf{k} into an empty state with wave number \mathbf{k}' . Let us suppose that the particle variation rate $P(t, \mathbf{x}, \mathbf{k}' \rightarrow \mathbf{k},)$ is proportional to occupation probability $f(t, \mathbf{x}, \mathbf{k}')$ of state $(\mathbf{x}, \mathbf{k}')$ at time t and to probability that the state (\mathbf{x}, \mathbf{k})

is not occupied, that can be expressed by $1 - f(t, \mathbf{x}, \mathbf{k})$ in agreement with of the Pauli exclusion principle. As a consequence we have

$$P(t, \mathbf{x}, \mathbf{k}' \rightarrow \mathbf{k},) = S(\mathbf{k}, \mathbf{k}') f(t, \mathbf{x}, \mathbf{k}') (1 - f(t, \mathbf{x}, \mathbf{k})) \quad (3.17)$$

and

$$\left(\frac{\partial f}{\partial t}\right)_{Coll} = \int_B [P(t, \mathbf{x}, \mathbf{k}' \rightarrow \mathbf{k},) - P(t, \mathbf{x}, \mathbf{k} \rightarrow \mathbf{k}')] d^3\mathbf{k}'. \quad (3.18)$$

The first term of the right side of (3.18) represents the gain and the second one the loss. Let us

$Q(f) = \left(\frac{\partial f}{\partial t}\right)_{Coll}$, we can rewrite the collision operator

$$Q(f)(t, \mathbf{x}, \mathbf{k}) = \int_B [S(\mathbf{k}', \mathbf{k}) f'(1 - f) - S(\mathbf{k}, \mathbf{k}') f(1 - f')] d^3\mathbf{k}' \quad (3.19)$$

with $f = f(t, \mathbf{x}, \mathbf{k})$, $f' = f(t, \mathbf{x}, \mathbf{k}')$.

By these assumptions, the semiclassical Boltzmann equation assumes a form of an integral-differential equation

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f - \frac{e\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = Q(f). \quad (3.20)$$

If we integrate the (3.19) we obtain

$$\int_B Q(f) d^3\mathbf{k}' = 0 \quad (3.21)$$

as required to satisfy the law of conservation of mass. It is shown that the balance distribution functions, where $Q(f) = 0$, have the following expression

$$f = \frac{1}{\exp\left(-\frac{\mathcal{E} - \mu}{k_B T_L}\right) + 1} \quad (3.22)$$

where $\mathcal{E} = \mathcal{E}(\mathbf{k})$, $\mu = \mathcal{E}_F$ and T_L is temperature of lattice. As a consequence, at equilibrium the electron distribution must obey the Fermi-Dirac statistics. However this hypothesis is not satisfied by some scattering mechanism (as with phonons, etc.). The problem of determining the null space

for the physical electron-phonon operator was tackled and solved in [33] where it is proved that the equilibrium solutions form an infinite sequence of functions of the kind

$$f = \frac{1}{h(\mathcal{E}) \exp\left(\frac{\mathcal{E}}{k_B T_L}\right) + 1}$$

where $h(\mathcal{E}) = h(\mathcal{E} + \hbar\omega_q)$ is a periodic function of period $\hbar\omega_q/n$ with $n \in \mathcal{N}$. This property implies a numerable set of collisional invariants and hence of conservation laws. The physical meaning is that the density of electrons whose energy \mathcal{E} differs from a given value u by a multiple of $\hbar\omega_q/n$ is constant.

In many applications we suppose $0 \leq f(t, \mathbf{x}, \mathbf{k}) \ll 1$, then the quadratic terms of the collision operator can be neglected (the non-degenerate case) and the collision operator can be replaced by

$$Q_L(f) = \int_B [S(\mathbf{k}', \mathbf{k}) f' - S(\mathbf{k}, \mathbf{k}') f] d^3\mathbf{k}'$$

where the balance distribution functions, with $Q_L(f) = 0$, are the Maxwellian approximation

$$f \simeq \text{const} \ e^{-\frac{\mathcal{E}}{k_B T_L}}. \quad (3.23)$$

The collisional operator (3.20) is given by the sum of each operator collisional related to different scattering mechanisms. We describe in the following subsection the expression about “transition rate” $S(\mathbf{k}, \mathbf{k}')$ for the scattering mechanisms, for more details see [23], [53].

3.3.1 Scattering electron-phonon

We said that at nonzero temperature, the atoms in the crystal lattice vibrate around their fixed equilibrium and we defined these as quantized vibrations and the quantum of lattice vibrations as phonon. We can distinguish so-called acoustic phonons and optical phonons. Acoustic phonons arise from displacements of lattice atoms in the same direction such as sound waves, while optical phonons describe displacements in the wave vector and they are able to interact strongly with

light. The phonon occupation number depends on thermic energy and it is given by Bose - Einstein distribution

$$N_B = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T_L}\right) - 1} \quad (3.24)$$

where $\hbar\omega$ is the energy phonon. The Bose - Einstein statistics has to be used for the particles, that do not obey the Pauli exclusion principle and therefore also for phonons, so two phonons can occupied the same quantum state. In the electron-phonon scattering, we can have two effects: an absorption or emission of a phonon. In the first case, a phonon with energy $\hbar\omega$ and wave-vector ξ is absorbed by an electron with energy $\mathcal{E}_c(\mathbf{k})$ and we have:

$$\mathbf{k}' = \mathbf{k} + \xi + \mathbf{l} \quad \mathcal{E}_c(\mathbf{k}') = \mathcal{E}_c(\mathbf{k}) + \hbar\omega$$

where \mathbf{l} is a vector of the reciprocal lattice, so that also $\mathbf{k}' \in B$. This means that these interactions conserve energy or momentum. While, if there is an emission of a phonon, we have:

$$\mathbf{k}' = \mathbf{k} - \xi + \mathbf{l} \quad \mathcal{E}_c(\mathbf{k}') = \mathcal{E}_c(\mathbf{k}) - \hbar\omega.$$

The transition rate [32] can be written usually as

$$S_{ph}(\mathbf{k}, \mathbf{k}') = \phi_{ph}(\mathbf{k}, \mathbf{k}') [(N_B + 1)\delta(\mathcal{E}' - \mathcal{E} + \hbar\omega) + N_B\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega)]$$

where the terms $\mathcal{E} = \mathcal{E}(\mathbf{k})$, $\mathcal{E}' = \mathcal{E}(\mathbf{k}')$ are the energy before and after collision, respectively, while δ is the delta distribution. The first delta distribution contributes when an energy of $\hbar\omega$ has been absorbed, whereas the second term contributes when an energy of $\hbar\omega$ has been emitted. The factors $1 + N_B$ and N_B come from the eigenvalues of the so-called creation and annihilation operators. The function $\phi_{ph}(\mathbf{k}, \mathbf{k}')$ depends on the kind of phonon interaction, with acoustic phonons or optical ones. For this reason, we consider this function as follow

$$\phi_{ph}(\mathbf{k}, \mathbf{k}') = \phi_{ph}^0(\mathbf{k}, \mathbf{k}') G(\mathbf{k}, \mathbf{k}') \quad (3.25)$$

where $\phi_{ph}^0(\mathbf{k}, \mathbf{k}')$ depends on kind of electron-phonon scattering and $G(\mathbf{k}, \mathbf{k}')$ is the overlap factor. Let us $u_{\mathbf{k}}(\mathbf{x})$ the periodic factor of Bloch function and $u_{\mathbf{k}'}^*(\mathbf{x})$ the complex conjugate, we define the overlap factor

$$G(\mathbf{k}, \mathbf{k}') = \left| \int_B u_{\mathbf{k}'}^*(\mathbf{x}) u_{\mathbf{k}}(\mathbf{x}) d^3\mathbf{x} \right|^2 \quad (3.26)$$

that depends on energy band structure and on the kind of interaction. This function satisfies the symmetry condition

$$G(\mathbf{k}, \mathbf{k}') = G(\mathbf{k}', \mathbf{k}), \quad G(\mathbf{k}, \mathbf{k}') \geq 0.$$

In the conduction band, the overlap factor can be approximate to a constant value, in particular we can assume $G(\mathbf{k}, \mathbf{k}') = 1$, while in the valence band a useful and good approximation it is given by

$$G(\mathbf{k}, \mathbf{k}') = \frac{1}{4} (1 + 3\cos^2\theta) \quad (3.27)$$

where θ is the angle between \mathbf{k} and \mathbf{k}' [23].

The allowed electron-phonon scattering in the conduction bands can be summarized as follows:

- intravalley acoustic phonon scattering (approximately elastic);
- intervalley acoustic phonons scattering (inelastic);
- non polar optical phonons scattering (inelastic).

Generally, the phonon energy $\hbar\omega$ can be considered as a function that depends on the wave vectors \mathbf{k} and \mathbf{k}' before and after a scattering event only [8]. For optical (nonpolar) phonon scattering, this dependency is weak such that ω_{op} can be considered to be constant. On the other hand, the energy of acoustic phonons is rather small compared to the kinetic energy of a carrier and it can be neglected near room temperature, $\hbar\omega_{ac} \approx 0$. At high temperature the scattering could be

considered an elastic collision

$$S_{ph}(\mathbf{k}, \mathbf{k}') \simeq \phi_{ph}^0(\mathbf{k}, \mathbf{k}') (1 + 2N_B) \delta(\mathcal{E}' - \mathcal{E}). \quad (3.28)$$

Under these assumption, the transition rate, regarding to the electron-acoustic phonon collision, is expressed by

$$S(\mathbf{k}, \mathbf{k}') = K_{ac} \delta(\mathcal{E} - \mathcal{E}') \quad (3.29)$$

with $\phi_{ph}^0(\mathbf{k}, \mathbf{k}') = K_{ac}$, where the physical parameter K_{ac} is defined by

$$k_{ac} = \frac{k_B T_L \Xi_d^2}{4\pi^2 \hbar \rho_0 v_s^2}$$

with Ξ_d the acoustic - phonon deformation potential, ρ_0 the mass density and v_s the sound velocity of the longitudinal acoustic mode. For inelastic scatterings between electron and non polar optical phonons, we have

$$S(\mathbf{k}, \mathbf{k}') = K_{np} \left[(N_B^{(np)} + 1) \delta(\mathcal{E}' - \mathcal{E} + \hbar\omega) + N_B^{(np)} \delta(\mathcal{E}' - \mathcal{E} - \hbar\omega) \right] \quad (3.30)$$

with $\phi_{ph}^0(\mathbf{k}, \mathbf{k}') = K_{np}$ and

$$K_{np} = Z_f \frac{(D_t K)}{8\pi^2 \rho \omega}$$

where Z_f is the number of final equivalent valleys in the intervalley scattering, $D_t K$ is the deformation potential for optical phonons. The factors (3.30) and (3.31) contain physical parameters that depend on kind of semiconductor. In the following Table 3.1 we report some value of these physical parameters about the silicon.

3.3.2 Scattering mechanisms with ionized impurity

These interactions are elastic collisions, as a consequence the electron energy $\mathcal{E}(\mathbf{k}')$ after the collision is equal to the energy $\mathcal{E}(\mathbf{k})$ before of interaction and the transition rate for the scattering

m_e	mass of electron	9.1095×10^{-28} g
m^*	effective mass of electron	$0.32 m_e$
T_L	lattice temperature	300 K
ρ_0	density	2330 g/cm^3
v_s	sound velocity	$9.18 \times 10^5 \text{ cm/sec}$
α	non parabolicity factor	0.5 1/eV
ϵ_s	Silicon relative dielectric constant	11.7
ϵ	vacuum dielectric constant	$8.85 \times 10^{-18} \text{ C/V } \mu\text{m}$

Table 3.1: Physical parameters and constants about Si

with impurities is

$$S^{imp}(\mathbf{k}, \mathbf{k}') = \frac{K_{imp}}{[|\mathbf{k} - \mathbf{k}'|^2 + \beta^2]^2} \delta(\mathcal{E}' - \mathcal{E})$$

with $\phi_{ph}^0(\mathbf{k}, \mathbf{k}') = K_{imp}$. The term β is the inverse Debye length

$$\beta = \left[\frac{q^2 N_I}{\epsilon} k_B T_L \right]^{\frac{1}{2}} \quad (3.31)$$

and the term k_{imp} depends on some physical parameters

$$K_{imp} = \frac{N_I Z^2 q^4}{4\pi \hbar \epsilon^2}$$

with N_I doping concentration.

If the carrier concentration is high, then it would take into account the electron-electron collision, in fact when an electron is near another electron, it will feel the Coulomb potential generated from the other as a perturbation of the periodic potential of the lattice. In this case, unlike the scattering with impurities, both electrons are subjected to the scattering and this is not in agreement with the use of the linearized operator. The collisional operator for the scattering electron-electron has

this expression [23], [35]:

$$Q_{ee}(f)(\mathbf{k}) = \int_B \int_B \int_B [f' f'_1 (1-f)(1-f_1) - f f_1 (1-f')(1-f'_1)] \phi_{ee}(\mathbf{k}, \mathbf{k}') \\ \delta(\mathcal{E}' + \mathcal{E}'_1 - \mathcal{E} - \mathcal{E}_1) \delta_p(\mathbf{k}' + \mathbf{k}'_1 - \mathbf{k} - \mathbf{k}_1) d^3\mathbf{k}_1 d^3\mathbf{k}' d^3\mathbf{k}'_1$$

where \mathbf{k} and \mathbf{k}_1 are the wave vectors of electrons before of scattering, while \mathbf{k}' and \mathbf{k}'_1 after scattering and the function $\phi_{ee}(\mathbf{k}, \mathbf{k}')$ is

$$\phi_{ee}(\mathbf{k}, \mathbf{k}') = \frac{e^4}{4\pi^4 \epsilon^2 \hbar^2} \frac{1}{[|\mathbf{k} - \mathbf{k}'|^2 + \beta^2]^2}.$$

The distribution $\delta(\mathcal{E}' + \mathcal{E}'_1 - \mathcal{E} - \mathcal{E}_1)$ ensures the energy conservation, while by $\delta_p(\mathbf{k}' + \mathbf{k}'_1 - \mathbf{k} - \mathbf{k}_1)$ it follow that the moment is conserved to less than a factor of reciprocal lattice

$$\mathbf{k} + \mathbf{k}_1 = \mathbf{k}' + \mathbf{k}'_1 + \mathbf{g} \quad \mathbf{g} \in L^*$$

If the vector \mathbf{g} is not zero, the collision is called *umklapp* [27],[5]. (Umklapp processes, discovered by Peierls, occur when the pseudo-wave vector of an electron or phonon interacting with other particles leaves the Brillouin zone and it is brought back to this zone by adding a reciprocal lattice vector). Generally the collision electron-electron can be neglected because it is small compared to collision electron-photon. For low electron density, the intensity of the electron-electron interaction is proportional to the density, but at higher densities the combined effects of shielding and the principle of Pauli make the frequency of collisions decreasing with increasing density. Regarding to the collision electron-electron, the maximum of the collision frequency is obtained for an intermediate value of the electron density, which depends on the material.

3.4 The Poisson equation

The Maxwell equations for the electrostatic field are

$$\nabla \times \mathbf{E} = 0 \quad (3.32)$$

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}. \quad (3.33)$$

Since the electric field depends on electrostatic potential $\phi(x)$ through the relation $\mathbf{E} = -\nabla_x \phi(x)$, the (3.33) can be written as

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0 \epsilon_r} \quad (3.34)$$

which is known as Poisson equation. For a semiconductor, in Poisson equation, we have to consider the density due to electrons and that one to holes, finally the ionized impurities

$$\nabla^2 \phi(x) = -\frac{q}{\epsilon_0 \epsilon_s} [p - n - N_a + N_d]. \quad (3.35)$$

The Boltzmann equation coupled Poisson equation is known as *Boltzmann-Poisson system*. In the unipolar case only one carrier is involved in current transport, so the Poisson equation is:

$$\nabla^2 \phi(x) = -\frac{q}{\epsilon_0 \epsilon_s} [N_d - N_a - n] \quad (3.36)$$

3.5 The recombination and generation processes in the bipolar semiconductor devices

As it has been shown in subsection 2.5, through the doping it is possible to change the concentration of charge in a semiconductor device or in some of its parts. A semiconductor device is *unipolar device* if the semiconductor is doped with a prevalence of one type of charge carriers, electrons or holes, called majority carriers, and the current due to the remaining minority carriers is negligible. While, if the both charge carriers contribute to electrical conduction, a device is a *bipolar device* and

in this case it is necessary to take into consideration the effects of the electron-hole interaction. We define the *generation* of an electron-hole the process in which an electron moves from the valence band to the conduction band, leaving a hole behind it in the valence band. For example, in silicon, the electron has to overcome the energy gap, which is of the order of $1eV$. On the other hand, the thermal energy of an electron is only of the order of $k_B T \approx 0.026eV$ at room temperature. Therefore, a lot of absorption energy is necessary for such processes. In the inverse process, called the *recombination* of an electron-hole pair, an electron moves from the conduction to the valence band, occupying an empty state, with emission of energy.

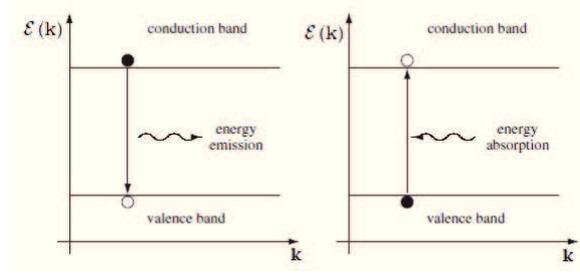


Figure 3.1: Recombination (left) and generation (right) of an electron-hole pair.

From a microscopic point of view, the equations (3.16), (3.36) represent a *Boltzmann-Poisson system* for a unipolar device, while about the bipolar device, we have

$$\frac{\partial f_e}{\partial t} + \mathbf{v}_e(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_e - \frac{eE}{\hbar} \cdot \nabla_{\mathbf{k}} f_e = Q_e(f_e) + I_e(f_n f_p) \quad (3.37)$$

$$\frac{\partial f_h}{\partial t} + \mathbf{v}_h(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_h + \frac{eE}{\hbar} \cdot \nabla_{\mathbf{k}} f_h = Q_h(f_e) + I_h(f_n f_p), \quad (3.38)$$

coupled with (3.35) Poisson equation. The collisional operators $Q_e(f_e)$ and $Q_h(f_e)$ have been described in the above subsection, while $I_e(f_n f_p)$ and $I_h(f_n f_p)$ represents the generation-recombination mechanism

$$I_e(f_n f_p) = \int_B [g(\mathbf{x}, \mathbf{k}', \mathbf{k}) (1 - f_n) (1 - f'_p) - r(\mathbf{x}, \mathbf{k}', \mathbf{k}) f_n f'_p] d^3 \mathbf{k}' \quad (3.39)$$

$$I_h(f_n f_p) = \int_B [g(\mathbf{x}, \mathbf{k}, \mathbf{k}') (1 - f'_n) (1 - f_p) - r(\mathbf{x}, \mathbf{k}, \mathbf{k}') f'_n f_p] d^3 \mathbf{k}'. \quad (3.40)$$

We consider these terms as a balance coefficient, which is given by a contribute of generation term, increasing the concentration of the charge, and an other of recombination one, decreasing the concentration of the charge. The term $g(\mathbf{x}, \mathbf{k}, \mathbf{k}')$ is the generation rate of an electron in the state (\mathbf{x}, \mathbf{k}) and a hole in the state $(\mathbf{x}, \mathbf{k}')$ and $r(\mathbf{x}, \mathbf{k}, \mathbf{k}')$ is the recombination rate. The recombination and generation rates are related by the equation

$$r(\mathbf{x}, \mathbf{k}, \mathbf{k}') = \exp\left(\frac{\mathcal{E}_n(\mathbf{k}) - \mathcal{E}_p(\mathbf{k}')}{k_B T}\right) g(\mathbf{x}, \mathbf{k}', \mathbf{k}), \quad (3.41)$$

which can be derived assuming Maxwell-Boltzmann statistics.

In the generation-recombination processes the basic mechanisms are:

- Auger/impact ionization generation-recombination,
- radiative generation-recombination,
- thermal generation-recombination.

An Auger process is defined as an electron-hole recombination followed by a transfer of energy to a free carrier which is then excited to a higher energy state. The inverse Auger process, in which an electron-hole pair is generated, is called impact ionization. The energy for the pair generation comes from the collision of a high-energy free carrier with the lattice or from electron-electron or hole-hole collision. In a radiative recombination, an electron from the conduction band recombines with a hole from the valence band emitting a photon. The energy, that is lost by the electron, is equal to the energy gap of the material, and a photon is produced with same band energy gap. Radiative generation occurs when a photon with energy larger than or equal to the gap energy is absorbed. These processes are important in narrow-gap semiconductors. Finally, thermal recombination or generation come from lattice vibrations or phonons and arise from phonon emission or absorption, respectively.

Chapter 4

From Kinetic to Fluid Dynamical models

4.1 Introduction to macroscopic models

In modern semiconductor devices, characterized by small size, thermal effects play an important role together to strongly inhomogeneous distributions of electric field, drift velocity, carrier concentration, carrier energy, etc. Under these conditions, the carriers transport is significantly different from transport in bulk materials and in sub-micrometer devices. Since the simulation of sub-micron devices by directly integrating the semi-classical electron transport equation (semi-classical BTE) presents many computational difficulties and the numerical methods to solve this equation (for instance with Monte-Carlo methods [23]) are still computationally expensive, other macroscopic models have been proposed for the description of charge transport in semiconductors. The main classes of macroscopic semiconductor models are the drift-diffusion, energy-transport and hydrodynamic equations [35],[49]. The simplest model and the most popular one is the set of the drift-diffusion equations, first proposed in 1950 by Van Roosbroeck [40] and for which very efficient numerical algorithms are available [24].

The drift-diffusion equations give satisfactory results for semiconductor devices with a typical size of a few microns and moderately applied voltage, whereas energy-transport models can also be used for certain submicron devices [15]. The hydrodynamic equations have been introduced by Bløtekjaer [9] and subsequently thoroughly investigated by Bacarani and Wordeman [6]. They can be derived from the Boltzmann equation by using the moments method. This yields usually a set of equations for the carrier density, momentum and energy, and it is not in closed form. To obtain a closed set of equations, often, as example, the Fourier law for the heat flux is taken into account[9]. For many details on different approaches of the derivation of the hydrodynamic equations and a discussion of the closing problem, we refer to [4], [19] and [25]. In the moments method, the BTE is multiplied by a number of linearly independent functions of velocity and integrated over velocity space. In some cases not all integrations can be carried out explicitly and these terms are usually replaced by phenomenological models. The ET models, first presented by Stratton in 1962 [50], are derived from hydrodynamic models usually by neglecting certain convection terms, but include the carrier energy (or temperature). These models improve the standard drift-diffusion model, based only on the balance equation of density and upon the condition (violated in the sub-micron devices) of thermal equilibrium. As a consequence the ET models include two balance equations, for density and energy flux. A systematic approach can be obtained using the Principle of Maximum Entropy in the context of extended thermodynamics and the theory of moments of Levermore [29] in the case of parabolic approximation for the energy bands of electrons. Nevertheless, the parabolic band is too poor for realistic simulations and models with a more complex energy bands are guaranteed. The energy-transport equations can be also obtained from the Boltzmann equation by means of the Hilbert expansion method [8], so-called spherical harmonic expansion model (SHE). This model is derived from the Boltzmann equation in the diffusion limit, under the strong and rather unphysical assumption that the dominant scattering mechanism is the electron-electron interaction [26], [35]. The advantage of this approach lies in the fact that it is can be performed under quite weak

assumptions on the semiconductor band structure and that we can obtain explicit expressions for the diffusion coefficients and for the energy relaxation term [15].

4.2 Method of Moments

Macroscopic models for charge transport can be obtained from the Boltzmann equation by the moments method. This method transforms the BTE into an equivalent, infinite set of equations. An approximation of this set is the truncation to a finite number of equations (normally three or four). The equation of highest order contains the moment of the next order, which has to be suitably approximated using available information, typically the lower order moments. Furthermore, the set of equations has more unknowns than equations, for this reason the closure relations are required.

As in gas - dynamics, multiplying the Boltzmann equation by a number of linearly independent functions we obtain the macroscopic physical quantities as moments of the distribution function, respect to the weight functions. At the first we introduce the *Drift-Diffusion model* and subsequently the hydrodynamic models and its derivation and extension models.

Multiplying the Boltzmann equation by a sufficiently regular function $\psi(\mathbf{k})$ and integrating over B , we obtain the generic moment equation

$$\frac{\partial M_\psi}{\partial t} + \int_B \psi(\mathbf{k}) v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} d^3\mathbf{k} - \frac{e}{\hbar} E^j \int_B \psi(\mathbf{k}) \frac{\partial f}{\partial k_j} d^3\mathbf{k} = \int_B \psi(\mathbf{k}) C[f] d^3\mathbf{k} \quad (4.1)$$

where

$$M_\psi = \int \psi(\mathbf{k}) f d^3\mathbf{k}$$

is the moment related to the weight function ψ .

Since

$$\int_B \psi(\mathbf{k}) \frac{\partial f}{\partial k_j} d^3\mathbf{k} = \int_{\partial B} \psi(\mathbf{k}) f n_j d\sigma - \int_B f \frac{\partial \psi(\mathbf{k})}{\partial k_j} d^3\mathbf{k} \quad (4.2)$$

with n_j is j -th component of $\hat{\mathbf{n}}$ outward unit on the boundary ∂B of the domain B and $d\sigma$ surface element of ∂B , the equation (4.1) becomes

$$\frac{\partial M_\psi}{\partial t} + \frac{\partial}{\partial x^i} \int_B f \psi(\mathbf{k}) v^i(\mathbf{k}) d^3\mathbf{k} - \frac{e}{\hbar} E^j \left[\int_{\partial B} \psi(\mathbf{k}) f n_j d\sigma - \int_B f \frac{\partial \psi(\mathbf{k})}{\partial k_j} d^3\mathbf{k} \right] = \int_B \psi(\mathbf{k}) C[f] d^3\mathbf{k}. \quad (4.3)$$

The term $\int_{\partial B} \psi(\mathbf{k}) f \hat{\mathbf{n}} \sigma$ is zero when B is expanded to \mathbb{R}^3 , as in the parabolic and Kane approximation, because in order to guarantee the integrability condition the function f must tend to zero sufficiently fast as $k \rightarrow \infty$ and when B is compact and $\psi(\mathbf{k})$ is periodic and continuous on ∂B . This latter condition is a consequence of the periodicity of f on B and the symmetry of B with respect to the origin. Under these assumptions, with the term $\int_{\partial B} \psi(\mathbf{k}) f \hat{\mathbf{n}} \sigma$ is zero, the (4.3) becomes

$$\frac{\partial M_\psi}{\partial t} + \frac{\partial}{\partial x^i} \int_B f \psi(\mathbf{k}) v^i(\mathbf{k}) d^3\mathbf{k} + \frac{e}{\hbar} E^j \int_B f \frac{\partial \psi(\mathbf{k})}{\partial k_j} d^3\mathbf{k} = \int_B \psi(\mathbf{k}) C[f] d^3\mathbf{k}. \quad (4.4)$$

The different models employ different expression of the weight functions set $\psi(\mathbf{k})$ and number of moments. We write the moment equations with weight functions $(1, \hbar\mathbf{k}, \mathcal{E}(\mathbf{k}))$ to obtain the law of mass conservation and laws of impulse and energy balance

$$\frac{\partial n}{\partial t} + \frac{\partial (nV^i)}{\partial x^i} = 0 \quad (4.5)$$

$$\frac{\partial (nP^i)}{\partial t} + \frac{\partial (nU^{ij})}{\partial x^j} + neE^i = nC_P^i \quad (4.6)$$

$$\frac{\partial (nW)}{\partial t} + \frac{\partial (nS^i)}{\partial x^j} + neV_k E^k = nC_W \quad (4.7)$$

with

$$n = \int_B f d^3\mathbf{k} \quad (4.8)$$

$$V^i = \frac{1}{n} \int_B f v^i d^3\mathbf{k} \quad (4.9)$$

$$W = \frac{1}{n} \int_B f \mathcal{E}(\mathbf{k}) d^3\mathbf{k} \quad (4.10)$$

$$S^i = \frac{1}{n} \int_B f v^i \mathcal{E}(\mathbf{k}) d^3\mathbf{k} \quad (4.11)$$

$$P^i = \frac{1}{n} \int_B f \hbar k^i d^3\mathbf{k} \quad (4.12)$$

$$U^{ij} = \frac{1}{n} \int_B f v^i \hbar k^j d^3\mathbf{k} \quad (4.13)$$

where n is the electron density, W is the average electron velocity, S^i is the flux of energy, P^i is the average crystal momentum and U^{ij} is the flux of crystal momentum. The collisional terms have the following expression

$$C_P^i = \frac{1}{n} \int_B C[f] \hbar k^i d^3\mathbf{k} \quad (4.14)$$

$$C_W = \frac{1}{n} \int_B C[f] \mathcal{E}(k) d^3\mathbf{k} \quad (4.15)$$

and they represent the production of the crystal momentum balance equation and the production of the energy balance equation, respectively.

We can choose a new set of weight functions $(1, \mathbf{v}(\mathbf{k}), \mathcal{E}(\mathbf{k}))$, but under parabolic band approximation both of sets are equivalent.

For time-dependent simulation, a convenient choice of the set $(1, \hbar\mathbf{k}, \mathcal{E}(\mathbf{k}), \mathcal{E}(\mathbf{k})\mathbf{v}(\mathbf{k}))$ [41], from which one obtains the balance equation for the crystal momentum, the balance equation for the electron energy and the balance equation for the electron energy flux and the continuity equation. In this last equation on the right-hand side it should appear a term due to the generation-recombination mechanism, but this effect is relevant for times of order 10^{-9} that in most applications can be neglected because the characteristic times are the order of a fraction of

picoseconds. The set of balance equations reads as:

$$\frac{\partial n}{\partial t} + \frac{\partial (nV^i)}{\partial x^i} = 0 \quad (4.16)$$

$$\frac{\partial (nP^i)}{\partial t} + \frac{\partial (nU^{ij})}{\partial x^j} + neE^i = nC_P^i \quad (4.17)$$

$$\frac{\partial (nW)}{\partial t} + \frac{\partial (nS^i)}{\partial x^j} + neV_k E^k = nC_W \quad (4.18)$$

$$\frac{\partial (nS^i)}{\partial t} + \frac{\partial (nF^{ij})}{\partial x^j} + neE_j G^{ij} = nC_W^i \quad (4.19)$$

with

$$F^{ij} = \frac{1}{n} \int_B f v^i v^j \mathcal{E}(k) d^3 \mathbf{k} \quad (4.20)$$

$$G^{ij} = \frac{1}{n} = \int_B \frac{1}{\hbar} f \frac{\partial}{\partial k_j} (\mathcal{E} v_i) d^3 \mathbf{k} \quad (4.21)$$

$$C_W^i = \frac{1}{n} \int_B C[f] \mathcal{E}(\mathbf{k}) d^3 \mathbf{k} \quad (4.22)$$

where F^{ij} is the flux of energy, C_W^i is the energy production.

For example, the continuity equation (4.16) can be obtained from (4.3), assuming $\psi(\mathbf{k}) = 1$. In fact, it follows that:

$$\int_B \frac{\partial f}{\partial t} d^3 \mathbf{k} + \int_B \frac{\partial}{\partial x^i} f(\mathbf{k}) v^i(\mathbf{k}) d^3 \mathbf{k} = 0$$

$$\frac{\partial}{\partial t} \int_B f d^3 \mathbf{k} + \frac{\partial}{\partial x^i} \int_B f(\mathbf{k}) v^i(\mathbf{k}) d^3 \mathbf{k} = 0$$

because

$$\int_B f \frac{\partial(1)}{\partial \mathbf{k}} d\mathbf{k} = 0 \quad \int_B C[f] d\mathbf{k} = 0. \quad (4.23)$$

Then,

$$\frac{\partial n(\mathbf{x}, t)}{\partial t} + \frac{\partial}{\partial x^i} (n(\mathbf{x}, t) V(\mathbf{x}, t)) = 0 \quad (4.24)$$

where $V(\mathbf{x}, t)$ is the macroscopic velocity.

4.2.1 The Drift-Diffusion equations

In this subsection we introduce a derivation of DD model from Boltzmann transport equation by the method of moments [49]. This model is introduced from merely macroscopic considerations regarding to the gradient of the electric potential and the gradient of the density, as a consequence we take into account the first order and the second order moments (4.5) and (4.6). Assuming that if the external electric field is zero, we have the relaxation of the system to equilibrium and, in the (4.6) equation, the production of the crystal momentum balance can be approximated to

$$nC_p^i \simeq -\frac{nP^i}{\tau_p} \quad (4.25)$$

where $\tau_p > 0$ is the impulse relaxation time. Then the (4.6) equation can be rewrite

$$\frac{\partial (nP^i)}{\partial t} + \frac{\partial}{\partial x^j} + neE^i = -\frac{nP^i}{\tau_p}. \quad (4.26)$$

Under assumption of the parabolic band, we have

$$nP^i = \int_B f \hbar k^i d^3 \mathbf{k} = m^* \int_B f v^i d^3 \mathbf{k} = m^* V^i, \quad nU^{ij} = \int_B f v^i \hbar k^j d^3 \mathbf{k} = \int_B \hbar^2 \frac{k^i k^j}{m^*} f d^3 \mathbf{k}. \quad (4.27)$$

From (4.27), we have

$$tr(nU) = \int_B \frac{\hbar^2 k^2}{m^*} f d^3 \mathbf{k} = 2nW. \quad (4.28)$$

Let us the closure relation

$$enU^{ij} = nP\delta^{ij} \quad \text{with} \quad nP = nk_B T_L. \quad (4.29)$$

The ideal gas law can be used under condition of the parabolic band approximation and the low electron densities. From (4.28) and (4.29) equations, we obtain

$$W = \frac{3}{2} k_B T_L. \quad (4.30)$$

This means that in these approximations only the internal energy contributes to the total energy of the electrons. Since the DD model is valid for the macroscopic time scale, we can assume

$$\left| \frac{\partial n P^i}{\partial t} \right| \ll \frac{n P^i}{\tau_p}, \quad (4.31)$$

so that the term $\frac{\partial n P^i}{\partial t}$ can be neglected. Under previous conditions, the (4.6) becomes

$$k_B T_L \frac{\partial n}{\partial x^i} + n e E^i = -\frac{n P^i}{\tau_p}. \quad (4.32)$$

Moreover $n P^i = m^* n V^i = -m^* J_n^i$, the current density is given by

$$J_n^i = \frac{k_B T_L \tau_p}{m^*} \frac{\partial n}{\partial x^i} + \frac{e \tau_p}{m^*} n E^i. \quad (4.33)$$

Let us $\mu_n = \frac{e \tau_p}{m^*}$ e $D_n = \frac{k_B T_L \tau_p}{m^*}$, we obtain

$$J_n^i = \mu_n n E^i + D_n \frac{\partial n}{\partial x^i}. \quad (4.34)$$

For a unipolar n-type semiconductor device, the DD equations are given by

$$\frac{\partial n}{\partial t} - \nabla_{\mathbf{x}} \mathbf{J}_n = 0 \quad (4.35)$$

$$\mathbf{J}_n = \mu_n n \mathbf{E} + D_n \nabla_{\mathbf{x}} n \quad (4.36)$$

$$\nabla^2 \phi(x) = -\frac{e}{\epsilon_0 \epsilon_s} [N_d(\mathbf{x}) - N_a(\mathbf{x}) - n(\mathbf{x}, t)]. \quad (4.37)$$

While for the bipolar semiconductor device, the DD equations are given by

$$\frac{\partial n}{\partial t} - \nabla_{\mathbf{x}} \mathbf{J}_n = G_n - R_n \quad (4.38)$$

$$\frac{\partial p}{\partial t} - \nabla_{\mathbf{x}} \mathbf{J}_p = G_p - R_p \quad (4.39)$$

$$\mathbf{J}_n = \mu_n n \mathbf{E} + D_n \nabla_{\mathbf{x}} n \quad (4.40)$$

$$\mathbf{J}_p = -\mu_p p \mathbf{E} + D_p \nabla_{\mathbf{x}} p \quad (4.41)$$

$$\nabla^2 \phi(x) = -\frac{e}{\epsilon_0 \epsilon_s} [p(\mathbf{x}, t) - n(\mathbf{x}, t) - N_a(\mathbf{x}) + N_d(\mathbf{x})] \quad (4.42)$$

where G_n , R_n , G_p and R_p are the terms of generation and recombination, respectively for the electrons and holes.

We remark that at the sub-micrometer regime, some assumptions of the DD model lost their validity. At small length scales, the increasing and rapidly change of the electric field inside the devices give non-local and hot-carrier effects, which dominate device performance. For these reasons, the modern industrial applications must take into account these phenomena in the miniaturize of semiconductor devices. To overcome some of the limitations of the DD model, an extensions have been proposed which basically add an additional balance equation for the average carrier energy [50], [9]. Since in the DD model the electron gas has been assumed to be in equilibrium with the lattice temperature, in its extensions an additional driving term is added to the current relation, which will be proportional to the gradient of the carrier temperature. In fact, if the electric field rapidly increases, the average energy lags behind the electric field, and the assumption of local equilibrium becomes invalid. Due to this lag, that the maximum energy could be considerably smaller than the one predicted by the local energy balance equation. In some cases, the lag of the average energy gives rise to an overshoot in the carrier velocity. The velocity overshoot is risen because the mobility depends, to first order, on the average energy and it does not on the electric field. Since the mobility has not yet been reduced by the increased energy, but the electric field is already large, in the velocity an overshoot is observed until the carrier energy comes into equilibrium with the electric field again [19].

4.2.2 Hydrodynamical models

Bløtekjaer [9] derived conservation equations by taking into account the moments of the BTE using the weight functions one, \hbar , \mathcal{E} . As shown in previous section, these weight functions define

the moments of zeroth, first, and second order. Under following assumptions

$$C_n = 0 \quad (4.43)$$

$$C_p = -\frac{P}{\tau_p} \quad (4.44)$$

$$C_W = -\frac{W - W_0}{\tau_W} \quad (4.45)$$

with τ_p and τ_W the momentum and energy relaxation times, respectively, the moment equations (4.16), (4.18) and (4.19) can be written as follows

$$\frac{\partial n}{\partial t} + \frac{\partial (nV^i)}{\partial x^i} = 0 \quad (4.46)$$

$$\frac{\partial (nP^i)}{\partial t} + \frac{\partial (nU^{ij})}{\partial x^j} + neE^i = -\frac{nC_P^i}{\tau_p} \quad (4.47)$$

$$\frac{\partial (nW)}{\partial t} + \frac{\partial (nS^i)}{\partial x^i} + neV_k E^k = -\frac{W - W_0}{\tau_W}. \quad (4.48)$$

This equations set is not closed, but it contains more unknowns than equations. Closure relations have to be found to express the equations in terms of the unknowns n , \mathbf{V} and W . Assuming the approximation of the parabolic band and that the term $\hbar\mathbf{k}$ can be separated into a random part $m^*\mathbf{c}$ and the mean value $m^*\mathbf{V}$ [9], [6]

$$\hbar\mathbf{k} = m^* (\mathbf{V} + \mathbf{c}) \quad (4.49)$$

where \mathbf{V} is given by (4.10) and

$$\int_B f \mathbf{c}^i d^3\mathbf{k} = 0. \quad (4.50)$$

From the equation (4.13), the tensor U^{ij} can be expressed by

$$\begin{aligned} nU^{ij} &= \frac{1}{m^*} \int_B f \hbar k^i \hbar k^j d^3\mathbf{k} \\ &= m^* n V^i V^j + m^* \int_B f \mathbf{c}^i \mathbf{c}^j d^3\mathbf{k}. \end{aligned}$$

Let us $\theta^{ij} = \frac{1}{n} \int_B f \mathbf{c}^i \mathbf{c}^j d^3\mathbf{k}$, expressed by

$$\theta^{ij} = \frac{1}{3} \theta_k^k \delta^{ij} + \theta^{<ij>} \quad (4.51)$$

where $\theta_k^k = \frac{1}{n} \int_B f c^2 d^3\mathbf{k}$, with $c = |\mathbf{c}|$. Then we have

$$nU^{ij} = m^* n V^i V^j + \frac{1}{3} m^* \theta_k^k \delta^{ij} + m^* n \theta^{<ij>}. \quad (4.52)$$

Neglecting anisotropic tensor $\theta^{<ij>}$, we obtain

$$nW = \frac{1}{2} \text{tr}(nU) = \frac{1}{2} \left(m^* n V^2 + m^* n \theta_k^k \right). \quad (4.53)$$

Supposed that the energy band is parabolic, it is reasonable to assume that the electrons temperature T and lattice one are different, so that the energy is given by

$$nW = \frac{1}{2} m^* n V^2 + \frac{3}{2} n k_B T. \quad (4.54)$$

By comparing (4.53) and (4.54)

$$n\theta_k^k = \frac{3n k_B T}{m^*} \quad \text{and} \quad n\theta^{ij} = \frac{n k_B T}{m^*} \delta^{ij}. \quad (4.55)$$

the balance impulse equation becomes

$$\frac{\partial n V^i}{\partial t} + \frac{\partial}{\partial x^j} \left[n V^i V^j + \frac{n k_B T}{m^*} \delta^{ij} \right] + \frac{n e E^i}{m^*} = -\frac{n V^i}{\tau_p}. \quad (4.56)$$

Furthermore, using the condition (4.50) a suitable approximation for the energy flux density is given by

$$\begin{aligned} nS^i &= \int_B f v^i \mathcal{E} \mathbf{k} d^3\mathbf{k} = \int_B f \frac{\hbar k^i}{m^*} \frac{\hbar^2 k^2}{2m^*} d^3\mathbf{k} \\ &= \frac{m^*}{2} \int_B f [V^i V^2 + 2V^i V^j c^j + V^i c^2 + c^i V^2 + 2c^i V^j c^j + c^i c^2] d^3\mathbf{k} \\ &= \frac{m^*}{2} \left[n V^i V^2 + n V^i \theta_k^k + 2V^j \left(\frac{1}{3} n \theta_k^k \delta^{ij} \right) + \int_B f c^i c^2 d^3\mathbf{k} \right] \\ &= \left(\frac{1}{2} n m^* V^2 + \frac{5}{2} n k_B T \right) V^i + \frac{m^*}{2} \int_B f c^i c^2 d^3\mathbf{k}. \end{aligned}$$

We define the heat flux

$$nq^i = \frac{m^*}{2} \int_B f c^i c^2 d^3\mathbf{k} \quad (4.57)$$

and using (4.54), the energy flux density can be approximated to

$$nS^i = \left(\frac{1}{2}nm^*V^2 + \frac{5}{2}nk_B T \right) V^i + nq^i = (nW + nk_B T) V^i + nq^i. \quad (4.58)$$

Bløtekjaer used as closure relation the heat flux by Fourier's law

$$nq^i = -\kappa \frac{\partial T}{\partial x^i}, \quad (4.59)$$

where κ is thermal conductivity, that is given by the Wiedemann-Franz law as

$$\kappa = \left(\frac{5}{2} - p \right) \left(\frac{k_B}{e} \right)^2 ne\mu_n T$$

with p is a correction factor. With previous approximations, the HD model equations can be rewritten as follow

$$\frac{\partial n}{\partial t} + \frac{\partial (nV^i)}{\partial x^i} = 0 \quad (4.60)$$

$$\frac{\partial (nV^i)}{\partial t} + \frac{\partial}{\partial x^j} \left(nV^i V^j + \frac{nk_B T}{m^*} \delta^{ij} \right) + \frac{neE^i}{m^*} = -\frac{nV^i}{\tau_p} \quad (4.61)$$

$$\frac{\partial (nW)}{\partial t} + \frac{\partial}{\partial x^j} \left[(nW + nk_B T) V^j - \kappa \frac{\partial T}{\partial x^i} \right] + neV_k E^k = -\frac{nW - nW_0}{\tau_W} \quad (4.62)$$

$$nW = \frac{1}{2}m^*nV^2 + \frac{3}{2}nk_B T \quad (4.63)$$

$$\nabla^2 \phi(\mathbf{x}) = -\frac{e}{\epsilon_0 \epsilon_s} [N_d(\mathbf{x}) - N_a(\mathbf{x}) - n(\mathbf{x}, t)]. \quad (4.64)$$

The energy balance equation is frequently simplified by the assumption that the time derivative of the mean electron energy $\frac{\partial W}{\partial t}$ is small compared to the other terms and that the kinetic part in W can also be neglected

$$W \approx \frac{3}{2}k_B T. \quad (4.65)$$

This non-degenerate approximation is justified for the low electron densities in the every region of the simulation, where velocity overshoot can be observed. The velocity overshoot in hydrodynamic models depends on the choice of the energy relaxation time. The energy relaxation times are parameters which depend on material, device geometry and doping, so their determination ahead

of time is not possible. To avoid the best choice of the energy relaxation times, an useful and important method is a direct solution of the BTE, using the Monte Carlo.

4.2.3 The Energy Transport models

The Energy-Transport models are now widely used in practical and industrial applications. These models are based on a general assumption about the distribution function is isotropic and, in particular, normally a Maxwellian distribution. The model equations are given by the phenomenological constitutive equations for the particle flux and energy flux and the closure relation of this model is based on the Maximum Entropy Principle (MEP). This model takes into account all the relevant scattering mechanisms, i.e. scattering of electrons with acoustic and non-polar phonons and with impurities, and has been formulated also for non-parabolic bands [3]. For example, for the silicon semiconductors, the scattering mechanisms regard to those of electrons with non-polar optical phonons, acoustic phonons and impurities of the crystal. Instead the electron-electron scatterings as well as the degeneration effects may be neglected, but the thermal effects related to the electron flow through the crystal are not neglected. The MEP-ET model is represented, except the Poisson equation for the electric potential, by a hyperbolic quasilinear system of balance law.

To obtain the ET model, we assume that the following scaling holds

$$t = O\left(\frac{1}{\delta^2}\right), \quad x^i = O\left(\frac{1}{\delta}\right), \quad \mathbf{V} = O(\delta), \quad \mathbf{S} = O(\delta), \quad \tau_W = O\left(\frac{1}{\delta^2}\right). \quad (4.66)$$

Relation (4.66)₁ means a long time scaling, while the (4.66)₂ indicates a diffusion approximation. The assumptions (4.66)₃ and (4.66)₄ are consistent with the small anisotropy condition in the derivation of the f_M , while the relation (4.66)₅ means that the energy must relax to equilibrium slower than the velocity and energy flux.

The set of equation is given by

$$\frac{\partial n}{\partial t} + \operatorname{div}(n\mathbf{V}) = 0 \quad (4.67)$$

$$\frac{\partial(nW)}{\partial t} + \text{div}(n\mathbf{S}) - qn\mathbf{V}\nabla\phi = nC_W \quad (4.68)$$

$$h^2\Delta\phi = q(n - c) \quad (4.69)$$

with $\mathbf{E} = -\nabla\phi$ and c the doping profile that is a given function of the position.

Some special cases considered in the literature are

- the Chen model *et al* [13]:

$$\begin{aligned} C_W &= -\frac{3}{2}k_B\frac{(T - T_L)}{\tau_W} \\ n\mathbf{V} &= -\frac{\mu_0k_B T_L}{q}\left(\nabla n - \frac{qn}{k_B T}\nabla\phi\right) \\ n\mathbf{S} &= -\frac{3}{2}\frac{\mu_0k_B T_L}{q}\left[\nabla(k_B n T) - qn\nabla\phi\right] \end{aligned}$$

- the Lyumkis model *et al* [31]:

$$\begin{aligned} C_W &= -\frac{2}{\sqrt{\pi}}\frac{(T - T_L)}{\tau_W T^{\frac{1}{2}}} \\ n\mathbf{V} &= -\frac{2\mu_0}{\sqrt{\pi}}\left[\nabla\left(nT^{\frac{1}{2}}\right) - \frac{n}{T^{\frac{1}{2}}}\nabla\phi\right] \\ n\mathbf{S} &= -\frac{4\mu_0}{\sqrt{\pi}}\left[\nabla\left(nT^{\frac{3}{2}}\right) - nT^{\frac{1}{2}}\nabla\phi\right] \end{aligned}$$

where μ_0 is the low-field mobility and τ_0 is the energy relaxation time, usually taken as a constant.

We observed that in the standard DD model

$$\frac{\partial n}{\partial t} + \text{div}(n\mathbf{V}) = 0 \quad (4.70)$$

$$\mathbf{J} = -D_n\nabla n + \mu_0 n\mathbf{E}, \quad (4.71)$$

consequently, we have the following relationship $\mathbf{J} = n\mathbf{V}$.

Chapter 5

Energy-transport model equations with constant lattice temperature

In this chapter we consider an energy-transport model, in the case of homogeneous silicon semiconductor, and find some particular constant solutions. If let us a constant solution as a solution of an initial value problem, we can study the perturbation which will be amplified by a factor depending on device length, with physical parameters fixed [34].

We consider the ET equations (4.67),(4.68),(4.69), (according to Chen model) in the one-dimensional case, under condition of a low electric field

$$\frac{\partial n}{\partial t} + \frac{\partial J}{\partial x} = 0 \quad (5.1)$$

$$\frac{\partial(nW)}{\partial t} + \frac{\partial(nS)}{\partial x} - qJ\frac{\partial\phi}{\partial x} = nC_W \quad (5.2)$$

$$h^2\frac{\partial^2\phi}{\partial x^2} = q(n - c(x)) \quad (5.3)$$

with

$$J = -\frac{\mu_0 k_B T_L}{q} \left(\frac{\partial n}{\partial x} - \frac{qn}{k_B T} \frac{\partial \phi}{\partial x} \right) \quad (5.4)$$

$$nS = -\frac{3}{2} \frac{\mu_0 k_B T_L}{q} \left[\frac{\partial(k_B n T)}{\partial x} - qn \frac{\partial \phi}{\partial x} \right] \quad (5.5)$$

$$C_W = -\frac{3}{2} k_B \frac{(T - T_L)}{\tau_W}. \quad (5.6)$$

The scaled variables have been obtained from the original ones by the transformations

$$n = \tilde{n}c^* \quad t = \tilde{t}t^* \quad x = \tilde{x}l^* \quad \phi = U_T \tilde{\phi} \quad W = \tilde{W}W^* \quad J = \tilde{J}J^* \quad (5.7)$$

with $W^* = k_B T_L$, l^* , c^* , t^* are typical values of the energy, characteristic length, doping density and time respectively, $U_T = \frac{k_B T}{q}$ is the thermal voltage and $J^* = -\frac{\mu_0 U_T}{l^{*5}}$ is the characteristic electron momentum density.

We can rewritten the set of equations. The (5.1) equation becomes

$$\frac{\partial(\tilde{n}c^*)}{\partial(\tilde{t}t^*)} - \mu_0 U_T \frac{\partial}{\partial x} \left(\frac{\partial c^* \tilde{n}}{\partial l^* \tilde{x}} - \frac{q c^*}{k_B T_L} \frac{\tilde{n}}{\tilde{T}} \frac{U_T}{l^*} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} \right) = 0$$

from which we get

$$\frac{l^{*3}}{t^*} \frac{\partial \tilde{n}}{\partial \tilde{t}} - \frac{\mu_0 U_T}{l^{*5}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial \tilde{n}}{\partial \tilde{x}} + \frac{\tilde{n}}{\tilde{T}} \tilde{E} \right] = 0. \quad (5.8)$$

In order to write the (5.2) equation, taking in account the (5.7) and using (5.4), (5.5) e (5.6), we have

$$\frac{c^* W^*}{t^*} \frac{\partial(\tilde{n} \tilde{W})}{\partial \tilde{t}} - \frac{3}{2} \mu_0 U_T \frac{W^* c^*}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial(\tilde{n} \tilde{T})}{\partial \tilde{x}} + \tilde{n} \tilde{E} \right] - q \tilde{J} J^* \frac{U_T}{l^*} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} = n C_W = -\frac{3}{2} \frac{c^*}{t^*} \tilde{n} \frac{(k_B T_L \tilde{T} - k_B T_L)}{\tilde{\tau}_W}.$$

Then the second equation reads

$$\frac{l^{*3} k_B T_L}{t^*} \frac{\partial(\tilde{n} \tilde{W})}{\partial \tilde{t}} - \frac{3}{2} \frac{\mu_0 U_T k_B T_L l^{*3}}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial(\tilde{n} \tilde{T})}{\partial \tilde{x}} + \tilde{n} \tilde{E} \right] - \frac{k_B T_L l^{*3} \mu_0 U_T}{l^{*2}} \tilde{J} \tilde{E} = -\frac{3}{2} \frac{l^{*3} k_B T_L}{t^*} \tilde{n} \frac{(\tilde{T} - 1)}{\tilde{\tau}_W}$$

that, simplified, becomes

$$\frac{1}{t^*} \frac{\partial(\tilde{n} \tilde{W})}{\partial \tilde{t}} - \frac{3}{2} \frac{\mu_0 U_T}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial(\tilde{n} \tilde{T})}{\partial \tilde{x}} + \tilde{n} \tilde{E} \right] - \frac{\mu_0 U_T}{l^{*2}} \tilde{J} \tilde{E} = -\frac{3}{2} \frac{1}{t^*} \tilde{n} \frac{(\tilde{T} - 1)}{\tilde{\tau}_W} \quad (5.9)$$

Now, the Poisson equation is given by

$$-\frac{h^2 U_T l^*}{q} \frac{\partial \tilde{E}}{\partial \tilde{x}} = \tilde{n} - \tilde{c}$$

from which, we have

$$\frac{\partial \tilde{E}}{\partial \tilde{x}} = -\tilde{h}(\tilde{n} - \tilde{c}). \quad (5.10)$$

$$\text{with } \tilde{h} = -\frac{q}{U_T h^2 l^*}.$$

5.1 Analysis of steady-state solution

Using the new variables, we want to find a stationary solution. Then, we consider the following set of equations

$$-\frac{\mu_0 U_T}{l^{*5}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial \tilde{n}}{\partial \tilde{x}} + \frac{\tilde{n} \tilde{E}}{\tilde{T}} \right] = 0 \quad (5.11)$$

$$-\frac{3 \mu_0 U_T}{2 l^{*2}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial(\tilde{n} \tilde{T})}{\partial \tilde{x}} + \tilde{n} \tilde{E} \right] + \frac{\mu_0 U_T}{l^{*2}} \tilde{J} \tilde{E} = -\frac{3 \tilde{n}}{2 t^*} \frac{(\tilde{T} - 1)}{\tau_W} \quad (5.12)$$

$$-\frac{h^2 U_T l^*}{q} \frac{\partial \tilde{E}}{\partial \tilde{x}} = \tilde{n} - \tilde{c}, \quad (5.13)$$

which becomes

$$\frac{\partial}{\partial \tilde{x}} \left[\frac{\partial \tilde{n}}{\partial \tilde{x}} + \frac{\tilde{n} \tilde{E}}{\tilde{T}} \right] = 0 \quad (5.14)$$

$$\frac{\partial}{\partial \tilde{x}} \left[\frac{\partial(\tilde{n} \tilde{T})}{\partial \tilde{x}} + \tilde{n} \tilde{E} \right] + \frac{2}{3} \tilde{J} \tilde{E} = \frac{l^{*2}}{\mu_0 U_T t^*} \tilde{n} \frac{(\tilde{T} - 1)}{\tau_W} \quad (5.15)$$

$$\frac{\partial \tilde{E}}{\partial \tilde{x}} = -\tilde{h}(\tilde{n} - \tilde{c}). \quad (5.16)$$

Now, we determine a constant solution and choose as variables the charge concentration n , the current density J and temperature T . Under condition of constant concentration we have that $n_0 = c$, while from (5.14) we obtain J_0 , that is expressed by

$$\frac{n_0 E_0}{T_0} = J_0. \quad (5.17)$$

Finally from (5.15), we find the expression for temperature T as

$$\frac{2}{3}J_0E_0 = An_0(T_0 - 1)$$

with $A = \frac{l^{*2}}{t^*\mu_0U_T\tau_W}$. Hence, replacing (5.17) in the last expression, we have

$$T_0 = \frac{3A \pm \sqrt{9A^2 + 24AE_0^2}}{6A}.$$

Summarizing, the constant solution is given by

$$\begin{aligned} n_0 &= c \\ \frac{n_0E_0}{T_0} &= J_0 \\ T_0 &= \frac{3A + \sqrt{9A^2 + 24AE_0^2}}{6A} \end{aligned}$$

Let us linearize the equations to analyse the behavior near the constant solution. We consider

$$\tilde{n} = n_0 + \delta\tilde{n}$$

$$\tilde{T} = T_0 + \delta\tilde{T}$$

$$\tilde{E} = E_0 + \delta\tilde{E}$$

Then, the set of equations (5.14), (5.15) and (5.16) becomes

$$\frac{\partial\delta\tilde{n}}{\partial\tilde{x}} + \frac{n_0E_0}{T_0} + \frac{E_0}{T_0}\delta\tilde{n} + \frac{n_0}{T_0}\delta\tilde{E} - \frac{n_0E_0}{T_0^*}\delta\tilde{T} = J_0 \quad (5.18)$$

$$n_0\frac{\partial^2(\delta\tilde{T})}{\partial\tilde{x}^2} + J_0\frac{\partial(\delta\tilde{T})}{\partial\tilde{x}} + \frac{2}{3}J_0E_0 + \frac{2}{3}J_0\delta\tilde{E} = A\left(n_0(T_0 - 1) + \delta\tilde{n}(T_0 - 1) + n_0\delta\tilde{T}\right) \quad (5.19)$$

$$\frac{\partial(\delta\tilde{E})}{\partial\tilde{x}} = -\tilde{h}(n_0 + \delta\tilde{n} - c). \quad (5.20)$$

We write the characteristic equation, so we assume

$$\delta\tilde{n} = k_1e^{\lambda x} \quad (5.21)$$

$$\delta\tilde{T} = k_2e^{\lambda x} \quad (5.22)$$

$$\delta\tilde{E} = k_3e^{\lambda x}. \quad (5.23)$$

Replacing the (5.21), (5.22) and (5.23) in the set of equations, we have:

$$\left[k_1 \lambda e^{\lambda x} + \frac{n_0 E_0}{T_0} + \frac{n_0}{T_0} k_3 e^{\lambda x} + \frac{E_0}{T_0} k_1 e^{\lambda x} - \frac{n_0 E_0}{T_0^2} k_2 e^{\lambda x} \right] = J_0 \quad (5.24)$$

$$n_0 \lambda^2 k_2 e^{\lambda x} + J_0 \lambda k_2 e^{\lambda x} + \frac{2}{3} J_0 E_0 + \frac{2}{3} J_0 k_3 e^{\lambda x} = A \left[n_0 (T_0 - 1) + k_1 e^{\lambda x} (T_0 - 1) + n_0 k_2 e^{\lambda x} \right] \quad (5.25)$$

$$\lambda k_3 e^{\lambda x} = -\tilde{h} \left(n_0 + k_1 e^{\lambda x} - c \right). \quad (5.26)$$

Hence, we can obtain the characteristic equation

$$\begin{pmatrix} \lambda + \frac{E_0}{T_0} & -\frac{n_0 E_0}{T_0^2} & \frac{n_0}{T_0} \\ -A(T_0 - 1) & n_0 \lambda^2 + J_0 \lambda - A n_0 & \frac{2}{3} J_0 \\ \tilde{h} & 0 & \lambda \end{pmatrix} = 0.$$

Let us study the dependence on charge density of the real part of the term λl^* , where λ are eigenvalues [34]. These results are obtained numerically from the characteristic equations for typical values of silicon parameters, that are shown in table.

Parameter	Physical meaning	Numerical value
q	elementary charge	1.6×10^{-19} C
U_T	thermal voltage at $T_0 = 300$ K	0.026 V
μ_0	mobility constant (low field)	$0.145 \mu\text{m}^2/\text{V}$ ps
l^*	length of device	$0.1 - 1 \mu\text{m}$
c^*	doping concentration	$1 \mu\text{m}^{-3}$
k_B	the Boltzmann constant	1.38×10^{-23} J/K
τ_W	energy relaxation time	0.4 ps
n	concentration of charge	$10^2\text{-}10^4 \mu\text{m}^{-3}$
ε_s	Silicon relative dielectric constant	11.7
ε	vacuum dielectric constant	8.85×10^{-18} C/V μm

Table 5.1: Physical parameters (Si)

The $\mathcal{Re}(\lambda l^*)$ are plotted against the longitudinal mean electric field for several values of charge density n and characteristic length l^* . Let be the applied electric field between $0.1\text{V}/\mu\text{m}$ and $0.5\text{V}/\mu\text{m}$, the charge density n between $10\mu\text{m}^{-3}$ and $10^3\mu\text{m}^{-3}$ and characteristic length l^* between $0.1\mu\text{m}$ and $0.8\mu\text{m}$. In some cases we note how two branches collapse into one when the terms λl^* become complex.

These plots point out the dependence critically of the characteristic length. For small fixed value of n and l^* , in particular $n = 10\mu\text{m}^{-3}$, $l^* = 0.1\mu\text{m}$ or $l^* = 0.2\mu\text{m}$, the $\mathcal{Re}(\lambda l^*)$ is rather small in absolute value. Then the stationary solution of the system has value near constant solution. At

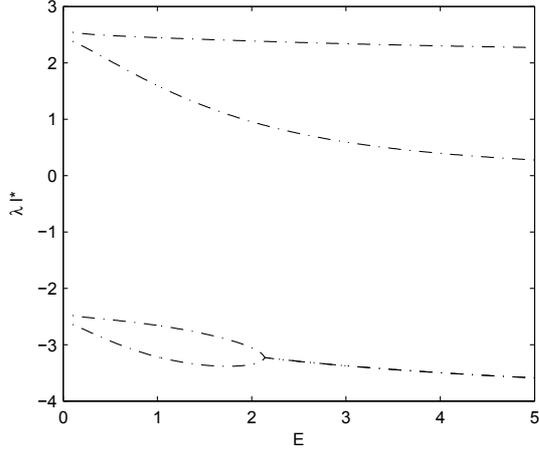


Figure 5.1: $n = 10\mu\text{m}^{-3}$ $l^* = 0.1\mu\text{m}$

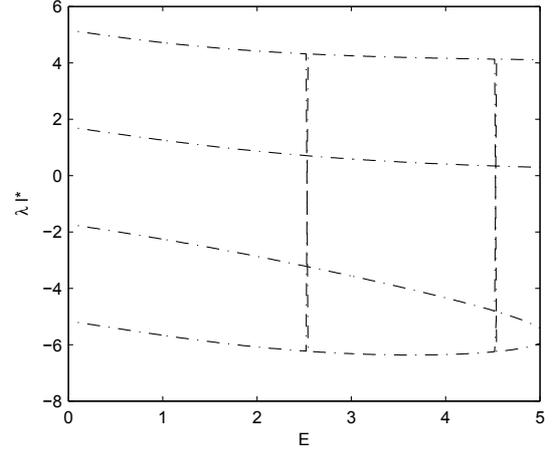


Figure 5.2: $n = 10\mu\text{m}^{-3}$ $l^* = 0.2\mu\text{m}$

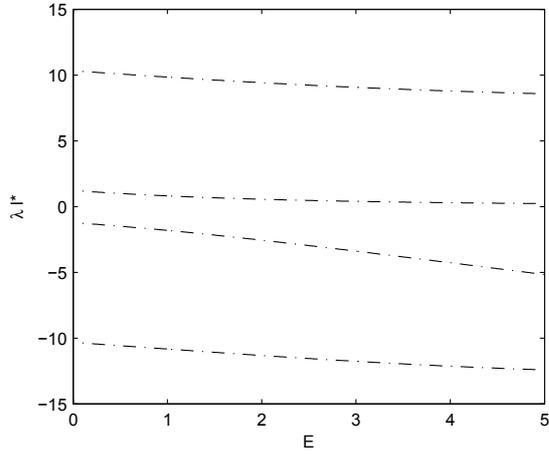


Figure 5.3: $n = 10\mu\text{m}^{-3}$ $l^* = 0.4\mu\text{m}$

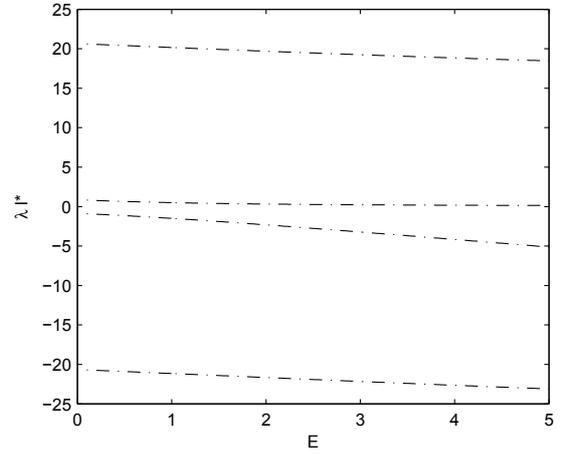


Figure 5.4: $n = 10\mu\text{m}^{-3}$ $l^* = 0.8\mu\text{m}$

the same charge density, with increasing of l^* , for example $l^* = 0.8\mu\text{m}$, some $\mathcal{R}e(\lambda^*)$ become large in absolute value and the gap between steady-state and constant solutions increases.

If let us the charge density is $n = 10^2\mu\text{m}^{-3}$ and $l^* = 0.1\mu\text{m}$ or $l^* = 0.2\mu\text{m}$, some $\mathcal{R}e(\lambda^*)$ are small, while others assume value rather large in absolute value. Same results are obtained for $n = 10^3\mu\text{m}^{-3}$.

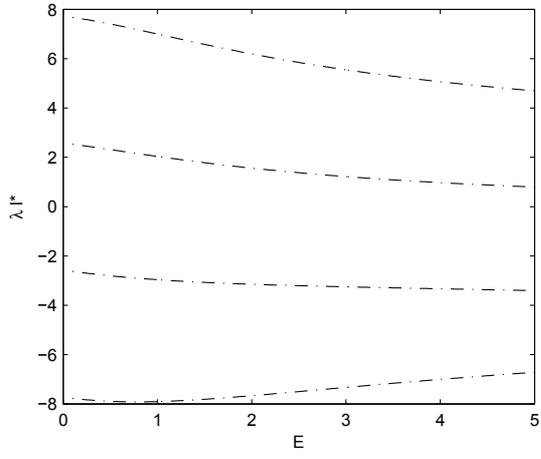


Figure 5.5: $n = 10^2 \mu\text{m}^{-3}$ $l^* = 0.1 \mu\text{m}$

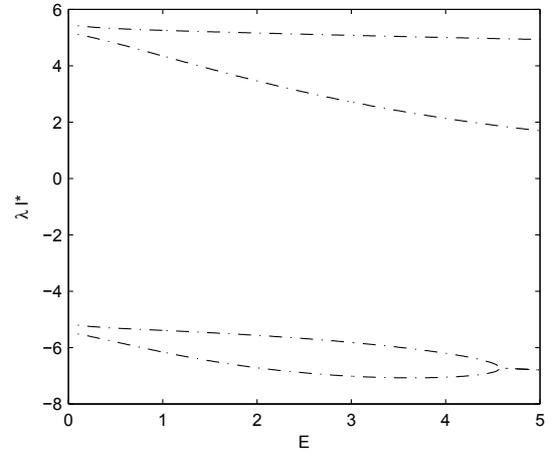


Figure 5.6: $n = 10^2 \mu\text{m}^{-3}$ $l^* = 0.2 \mu\text{m}$

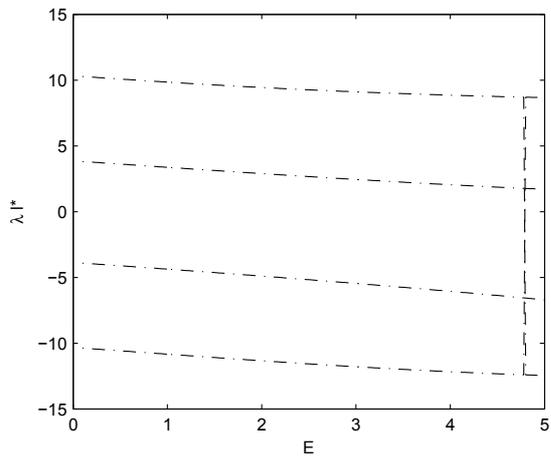


Figure 5.7: $n = 10^2 \mu\text{m}^{-3}$ $l^* = 0.4 \mu\text{m}$

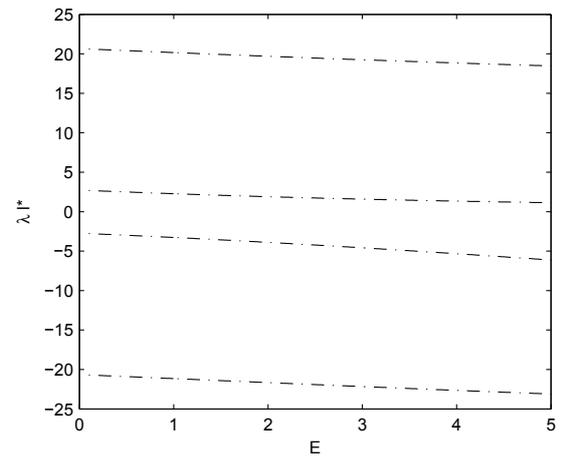


Figure 5.8: $n = 10^2 \mu\text{m}^{-3}$ $l^* = 0.8 \mu\text{m}$

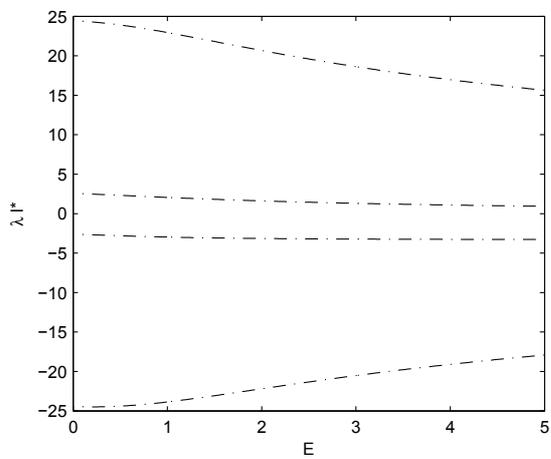


Figure 5.9: $n = 10^3 \mu\text{m}^{-3}$ $l^* = 0.1 \mu\text{m}$

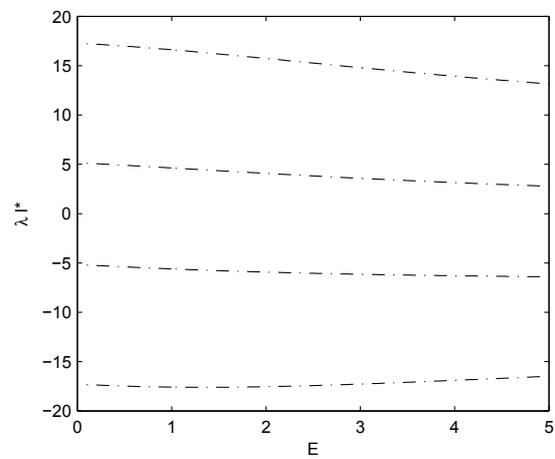


Figure 5.10: $n = 10^3 \mu\text{m}^{-3}$ $l^* = 0.2 \mu\text{m}$

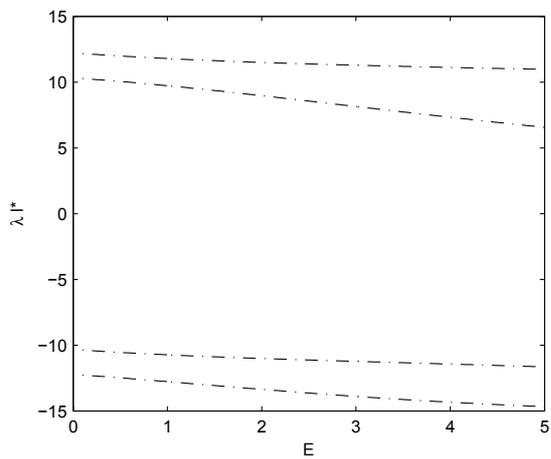


Figure 5.11: $n = 10^3 \mu\text{m}^{-3}$ $l^* = 0.4 \mu\text{m}$

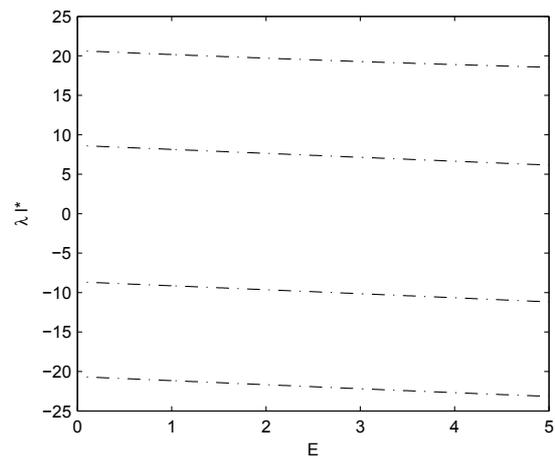


Figure 5.12: $n = 10^3 \mu\text{m}^{-3}$ $l^* = 0.8 \mu\text{m}$

5.2 A stable solution of energy-transport model

In this section we study the stability of a particular solution. We consider a perturbation, around constant solution, depending on the space and on the time. In this case we choose as variables n, nW, ϕ and rewrite the scaling equations of the mathematical model. As a consequence, we obtain a new set of ET equations (with the Chen model), in one-dimensional case. The equation (5.1) becomes

$$\frac{\partial(\tilde{n}c^*)}{\partial(\tilde{t}t^*)} - \frac{\mu_0 U_T}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left(c^* \frac{\partial \tilde{n}}{\partial \tilde{x}} - \frac{3}{2} \frac{qc^{*2} \tilde{n}^2}{c^* \tilde{W} W^*} U_T \frac{\partial \tilde{\phi}}{\partial \tilde{x}} \right) = 0$$

from which we have

$$\frac{\partial \tilde{n}}{\partial \tilde{t}} - \frac{\mu_0 U_T t^*}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left(\frac{\partial \tilde{n}}{\partial \tilde{x}} - \frac{\tilde{n}^2}{\tilde{W}} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} \right) = 0.$$

The equation (5.2) is given by

$$\frac{c^* W^*}{t^*} \frac{\partial \tilde{W}}{\partial \tilde{t}} + \frac{\partial}{\partial \tilde{x}} \left[-\mu_0 U_T \left(\frac{c^* W^*}{l^*} \frac{\partial \tilde{W}}{\partial \tilde{x}} - \frac{3}{2} q U_T \frac{c^* \tilde{n}}{l^*} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} \right) \right] - q J^* \tilde{J} \frac{U_T}{l^*} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} = -\frac{c^* W^*}{t^*} \frac{(\tilde{W} - 1)}{\tilde{\tau}_W}$$

that can be simplified

$$\frac{\partial \tilde{W}}{\partial \tilde{t}} - \frac{\mu_0 U_T t^*}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial \tilde{W}}{\partial \tilde{x}} - \tilde{n} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} \right] + \frac{2}{3} \frac{\mu_0 U_T t^*}{l^{*2}} \tilde{J} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} = -\frac{c^* W^*}{t^*} \frac{(\tilde{W} - 1)}{\tilde{\tau}_W}.$$

At the least, we rewritten the Poisson equation

$$h^2 \frac{U_T}{l^{*2}} \frac{\partial^2 \tilde{\phi}}{\partial \tilde{x}^2} = q (c^* \tilde{n} - c^* \tilde{c})$$

$$\frac{\partial^2 \tilde{\phi}}{\partial \tilde{x}^2} = h (\tilde{n} - \tilde{c}(x)) \quad \text{with} \quad h = \frac{qc^* l^{*2}}{h^2 U_T}.$$

The set of equations is

$$\frac{\partial \tilde{n}}{\partial \tilde{t}} - \frac{\mu_0 U_T t^*}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left(\frac{\partial \tilde{n}}{\partial \tilde{x}} - \frac{\tilde{n}^2}{\tilde{W}} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} \right) = 0 \tag{5.27}$$

$$\frac{\partial \tilde{W}}{\partial \tilde{t}} - \frac{\mu_0 U_T t^*}{l^{*2}} \frac{\partial}{\partial \tilde{x}} \left[\frac{\partial \tilde{W}}{\partial \tilde{x}} - \tilde{n} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} \right] + \frac{2}{3} \frac{\mu_0 U_T t^*}{l^{*2}} \tilde{J} \frac{\partial \tilde{\phi}}{\partial \tilde{x}} = -\frac{c^* W^*}{t^*} \frac{(\tilde{W} - 1)}{\tilde{\tau}_W} \tag{5.28}$$

$$\frac{\partial^2 \tilde{\phi}}{\partial \tilde{x}^2} = h (\tilde{n} - \tilde{c}(x)). \tag{5.29}$$

Let us linearize the equations and study the behavior near the constant solution, then we consider

$$\tilde{n}(x, t) = n_0 + \delta\tilde{n}(x, t) \quad (5.30)$$

$$\tilde{W}(x, t) = W_0 + \delta\tilde{W}(x, t) \quad (5.31)$$

$$\tilde{\phi}(x, t) = \phi_0 + \delta\tilde{\phi}(x, t) \quad (5.32)$$

Then the set of equations can be rewritten as follow

$$\frac{\partial(\delta\tilde{n})}{\partial\tilde{t}} - \frac{\mu_0 U_T t^*}{l^{*2}} \frac{\partial}{\partial\tilde{x}} \left[\frac{\partial(\delta\tilde{n})}{\partial\tilde{x}} - \frac{n_0^2}{W_0} \frac{\partial(\delta\tilde{\phi})}{\partial\tilde{x}} \right] = 0 \quad (5.33)$$

$$\frac{\partial(\delta\tilde{W})}{\partial\tilde{t}} - \frac{\mu_0 U_T t^*}{l^{*2}} \left[\frac{\partial^2(\delta\tilde{W})}{\partial\tilde{x}^2} - n_0 \frac{\partial^2(\delta\tilde{\phi})}{\partial\tilde{x}^2} \right] + \frac{2}{3} \frac{\mu_0 U_T t^*}{l^{*2}} \tilde{J} \frac{\partial(\delta\tilde{\phi})}{\partial\tilde{x}} = -\frac{W_0 + \delta\tilde{W} - 1}{\tau_{\tilde{W}}} \quad (5.34)$$

$$\frac{\partial^2(\delta\tilde{\phi})}{\partial\tilde{x}^2} = h(n_0 + \delta\tilde{n} - c_0 - \delta\tilde{c}(x)) \quad (5.35)$$

The characteristic equation

We search solutions $\tilde{n}(x, t)$, $\tilde{W}(x, t)$ and $\tilde{\phi}(x, t)$ in which

$$\delta\tilde{n}(x, t) = c_1 e^{i(kx - \omega t)}$$

$$\delta\tilde{W}(x, t) = c_2 e^{i(kx - \omega t)}$$

$$\delta\tilde{\phi}(x, t) = c_3 e^{i(kx - \omega t)}$$

To study the stability, we must take into account the characteristic equation. For this reason we assume that the family of functions (5.30), (5.31) and (5.32) are solutions of the set of given equations (5.33), (5.34), (5.35) and we write the characteristic equation. If we consider the first equation (5.33), we have

$$-c_1 i\omega e^{i(kx - \omega t)} - A \left[-c_1 k^2 e^{i(kx - \omega t)} + \frac{n_0^2}{W_0} k^2 c_3 e^{i(kx - \omega t)} \right] = 0. \quad (5.36)$$

From the (5.34) equation, we obtain

$$-i c_2 \omega e^{i(kx - \omega t)} - A \left[-c_2 k^2 e^{i(kx - \omega t)} + n_0 k^2 c_3 e^{i(kx - \omega t)} \right] + i \frac{2}{3} A J k c_3 e^{i(kx - \omega t)} = -\frac{W_0 + c_2 e^{i(kx - \omega t)} - 1}{\tau_{\tilde{W}}}, \quad (5.37)$$

and from the (5.35) Poisson equation, we have

$$-k^2 c_3 e^{i(kx - \omega t)} = h \left(n_0 + c_1 e^{i(kx - \omega t)} - c_0 \right). \quad (5.38)$$

So, we can obtain the characteristic equation by the determinant of the following matrix

$$\begin{pmatrix} -i\omega + Ak^2 & 0 & \frac{-An_0^2 k^2}{W_0} \\ 0 & -i\omega + Ak^2 + \frac{1}{\tau_{\tilde{W}}} & -An_0 k^2 + i\frac{2}{3}AJk \\ -h & 0 & -k^2 \end{pmatrix} = 0.$$

We obtain:

$$i\omega = Ak^2 + \frac{1}{\tau_{\tilde{W}}}; \quad i\omega = Ak^2 + \frac{hAn_0^2}{W_0}. \quad (5.39)$$

We find the eigenvectors \mathbf{b}_1 and \mathbf{b}_2 solving the follow systems

- if $i\omega = AK^2 + \frac{1}{\tau_{\tilde{W}}}$

$$\begin{cases} -c_1 \left(AK^2 + \frac{1}{\tau_{\tilde{W}}} \right) - A \left(-c_1 k^2 + \frac{n_0^2}{W_0} k^2 c_3 \right) = 0 \\ -c_2 AK^2 + \frac{1}{\tau_{\tilde{W}}} - A \left(-c_2 k^2 + n_0 k^2 c_3 \right) + i\frac{2}{3}AJk c_3 + \frac{c_2}{\tau_{\tilde{W}}} = 0 \\ -k^2 c_3 = hc_1 \end{cases}$$

$$\mathbf{b}_1 = (0, c_2, 0)$$

- If $i\omega = Ak^2 + \frac{hAn_0^2}{W_0}$

$$\begin{cases} -c_1 \left(\frac{hAn_0^2}{W_0} + Ak^2 \right) - A \left(-c_1 k^2 + \frac{n_0^2 k^2}{W_0} c_3 \right) = 0 \\ -c_2 \left(\frac{hAn_0^2}{W_0} + Ak^2 \right) - A \left(-c_2 k^2 + n_0 k^2 c_3 \right) + i \frac{2}{3} A J k c_3 + \frac{c_2}{\tilde{\tau}_W} = 0 \\ -k^2 c_3 = hc_1 \end{cases}$$

$$\mathbf{b}_2 = \left(c_3 \frac{k^2}{h}, -\frac{\left(An_0 k^2 - i \frac{2}{3} A J k \right)}{\left(\frac{1}{\tilde{\tau}_0} - \frac{hAn_0^2}{W_0} \right)} c_3, c_3 \right).$$

We have the solution

$$(n, W, \phi) = (n_0, W_0, \phi_0) + \mathbf{b}_1 e^{i(kx - \omega t)} + \mathbf{b}_2 e^{i(kx - \omega t)} \quad (5.40)$$

Since $k \in \mathbb{C}$, we find

- $k^2 = \frac{1}{A} \left(i\omega - \frac{1}{\tilde{\tau}_W} \right)$, from which we find

$$k_n = \sqrt[4]{\frac{\omega^2 \tilde{\tau}_W^2 + 1}{A^2 \tilde{\tau}_W^2}} e^{i\theta_n}, \quad n = 0, 1 \quad (5.41)$$

$$\text{with } \theta_0 = \frac{\arctan(-\omega \tau_0) + \pi}{2} \quad \text{and} \quad \theta_1 = \theta_0 + \pi,$$

- $k^2 = \frac{i\omega}{A} - \frac{hn_0^2}{W_0}$, from which we find

$$k_n = \sqrt[4]{\left(\frac{\omega}{A} \right)^2 + \left(\frac{hn_0^2}{W_0} \right)^2} e^{i\theta_n}, \quad n = 0, 1 \quad (5.42)$$

$$\text{with } \theta_0 = \frac{1}{2} \arctan \left(-\frac{\omega W_0}{A h n_0^2} \right) \quad \text{and} \quad \theta_1 = \theta_0 + \pi.$$

We can conclude that (5.40) is an asymptotic stable solution for a unlimited domain.

Chapter 6

The symmetry analysis of differential equations

The symmetry analysis of differential equations was introduced by Sophus Lie in latter part of 19th century, and it played an important role in the theory of continuous groups. These groups, known as Lie's Groups, have had a fundamental impact on all areas of mathematics, pure and applied, as algebraic topology, differential geometry, invariant theory, bifurcation theory, numerical analysis, classic and quantum mechanics and so on.

Lie's theory represents an efficient and powerful tool to solve complicated problems, that involve ordinary and partial differential equations. It is useful as example to determine invariant solutions of initial and boundary value problems, to study conservation laws, to construct relations between different differential equations that turn out be equivalent. The symmetry analysis is a completely algorithmic procedure and, in the last years, a several symbolic manipulation computer programs have been developed for this task, because it involves a lot of cumbersome and many calculations.

A symmetry group of a system of differential equations is a group that transforms solutions of the system to the other solutions of the same system. The non-linear conditions of invariance of

the system under group transformations could, in the case of a continuous group, be replaced by equivalent, but simpler, linear conditions, reflecting a form of infinitesimal invariance of system under generators of the group.

We can use the symmetry groups to make a classification of families of differential equations, depending on arbitrary functions or parameters. Another, we can start from a known solution and find a means of classifying different families of symmetry solutions, in fact two solutions are equivalent if one can be transformed into the other by some group element. Lie's fundamental theorems show that symmetry groups are characterized by their infinitesimal generators. Lie groups and hence their infinitesimal generators, can be naturally extended or "prolonged" to act on the space of independent variables, dependent variables and derivatives of the dependent variables up to any finite order. As a consequence, the seemingly intractable non-linear conditions of group invariance of a given system of differential equations reduce to linear equations determining the infinitesimal generators of the group. Since these determining equations form an overdetermined system of linear partial differential equations, one can usually determine the infinitesimal generators in closed form. Given a system of differential equations, Lie groups transformations are useful to lower the order or eventually reduce order of the equations, to determine particular solutions, called *invariant solution* or generate new solutions, once a special solution is known. If a system of partial differential equations is invariant under a Lie group of point transformations, the invariant solutions are invariant under some subgroup of the full group admitted by the system. These solutions result from solving a reduced system of differential equations with fewer independent variables.

6.1 Basic theory of Lie Groups of transformation

In this subsection, we introduce the basic ideas of Lie Groups of transformations necessary to study invariance properties of differential equations.

Definition 6 *One-parameter group of transformations.*

Let us consider a domain $D \subseteq \mathbb{R}^n$ and a subset $S \subseteq \mathbb{R}$. The set of transformations

$$\mathbf{x}^* = \mathbf{Z}(\mathbf{x}, a) \quad \mathbf{Z}: D \times S \rightarrow D \quad (6.1)$$

defined for each $\mathbf{x} \in D$ and depending on the parameter $a \in S$, with $\mu(\varepsilon, \delta)$ defining a law of composition of parameters a and δ in S , forms a one-parameter group of transformations on D if:

- (i) for each value of $a \in S$ the transformations are one-to-one onto D ;
- (ii) S , with the law of composition μ , forms a group G with identity a_0 ;
- (iii) $\mathbf{Z}(\mathbf{x}, a_0) = \mathbf{x}, \quad \forall \mathbf{x} \in D$;
- (iv) $\mathbf{Z}(\mathbf{Z}(\mathbf{x}, a), \delta) = \mathbf{Z}(\mathbf{x}, \mu(a, \delta)), \quad \forall \mathbf{x} \in D, \quad \forall a, \delta \in D$

Definition 7 *Lie Group transformation*

A set of transformations (6.1) defines a one-parameter Lie group of transformations if, in addition to satisfying axiom (i) – (iv) of the previous definition, satisfies these properties:

- (v) a is a continuous parameter, i.e. S is an interval in \mathbb{R} ;
- (vi) $\mathbf{Z} \in C^\infty$ with respect to $\mathbf{x} \in D$ and it is an analytic function of $a \in S$;
- (vii) $\mu(a, \delta)$ is an analytic function of a and $\delta, \forall a, \delta \in S$.

We can always re-parametrize a given group in terms of a parameter a such that for parameter a_1 e a_2 the law of composition becomes $\phi(a_1, a_2) = a_1 + a_2$.

6.1.1 Infinitesimal Transformations

We consider a one-parameter (a) Lie group of transformations

$$\mathbf{x}^* = \mathbf{Z}(\mathbf{x}, a) \quad (6.2)$$

with identity $a = 0$ and law of composition μ . Let us the function $\mathbf{Z}(\mathbf{x}, a)$ into the Mc Laurin series respect to the parameter a in the neighbourhood of $a = 0$

$$\mathbf{x}^* = \mathbf{x} + a \left(\frac{\partial \mathbf{Z}(\mathbf{x}; a)}{\partial a} \Big|_{a=0} \right) + \frac{a^2}{2} \left(\frac{\partial^2 \mathbf{Z}(\mathbf{x}; a)}{\partial a^2} \Big|_{a=0} \right) + \dots = \mathbf{x} + a \left(\frac{\partial \mathbf{Z}(\mathbf{x}; a)}{\partial a} \Big|_{a=0} \right) + O(a^2). \quad (6.3)$$

Let us

$$\zeta(\mathbf{x}) = \frac{\partial \mathbf{Z}(\mathbf{x}; a)}{\partial a} \Big|_{a=0}, \quad (6.4)$$

the transformation $\mathbf{x} + a\zeta(\mathbf{x})$ is called the *infinitesimal transformation* of the Lie group of transformations (6.2) and the components of $\zeta(\mathbf{x})$ are called the *infinitesimal* of (6.2).

The following theorem ensures that the infinitesimal transformations contain the essential information to characterize a one-parameter Lie group of transformations.

Theorem 2 *First fundamental Theorem of Lie*

There exists a parametrization $\tau(a)$ such that the Lie group of transformations (6.2) is equivalent to the solution of the initial value problem for the system of first order differential equations

$$\frac{d\mathbf{x}^*}{da} = \zeta(\mathbf{x}^*) \quad \text{with} \quad \mathbf{x}^* = \mathbf{x}, \tau = 0. \quad (6.5)$$

For a given differential equation we must know the admitted infinitesimal generators.

Definition 8 *Infinitesimal generators*

The infinitesimal generator of the one-parameter Lie group of transformations (6.2) is

$$X = \zeta(\mathbf{x}) \cdot \nabla = \sum_{i=1}^n \zeta_i(\mathbf{x}) \frac{\partial}{\partial x_i} \quad (6.6)$$

where ∇ is the gradient operator

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \dots, \frac{\partial}{\partial x_n} \right).$$

and for any differential function $F(\mathbf{x}) = F(x_1, x_2, \dots, x_n)$, we have

$$XF(\mathbf{x}) = \zeta(\mathbf{x}) \cdot \nabla F(\mathbf{x}) = \sum_{i=1}^n \zeta_i(\mathbf{x}) \frac{\partial F(\mathbf{x})}{\partial x_i}. \quad (6.7)$$

As a consequence a one-parameter Lie group of transformations, which is “equivalent” to its infinitesimal transformation, is also equivalent to its infinitesimal generator.

Now, we can introduce the concept of invariance of a function with respect to a Lie group of transformations and give the relative corresponding invariance criterion.

Definition 9 Invariants.

An infinitely differentiable function $F(\mathbf{x})$ is an invariant function (or, simply, an invariant) of the Lie group of transformations (6.2) if, for any group transformation (6.2),

$$F(\mathbf{x}^*) \equiv F(\mathbf{x}).$$

The invariance of a function is characterized in a simple way by means of the infinitesimal generator of the group, as the following theorem shows.

Theorem 3 $F(\mathbf{x})$ is invariant under a Lie group of transformations (6.2) if and only if

$$XF(\mathbf{x}) = 0.$$

Given an invariant $F(\mathbf{x})$, any function $\Phi(F(\mathbf{x}))$ is also invariant.

We can also define the invariance of a surface with respect to a Lie group.

Definition 10 Invariant surfaces.

A surface $F(\mathbf{x}) = 0$ is an invariant surface with respect to the Lie group of transformations (6.2) if $F(\mathbf{x}^*) = 0$ when $F(\mathbf{x}) = 0$.

This theorem immediately follows.

Theorem 4 *A surface $F(\mathbf{x}) = 0$ is invariant under a Lie group of transformations (6.2) if and only if*

$$XF(\mathbf{x}) = 0 \quad \text{when} \quad F(\mathbf{x}) = 0.$$

6.1.2 Lie Groups of differential equations

In this section we describe the analytical method for calculation of infinitesimal generators of differential equations. We consider a system Σ of q differential equations of order s , with independent variables $\mathbf{x} \in \mathbb{R}^n$ and m dependent variables $\mathbf{u} \in \mathbb{R}^m$. The space (\mathbf{x}, \mathbf{u}) of independent and dependent variables will be called the base space of the differential equations. It is useful to introduce an adapted notation

$$\mathbf{u}_{(1)} \equiv \left(\frac{\partial u^1}{\partial x_1}, \dots, \frac{\partial u^1}{\partial x_n}, \dots, \frac{\partial u^m}{\partial x_1}, \dots, \frac{\partial u^m}{\partial x_n} \right) \quad (6.8)$$

and, in general, $\mathbf{u}_{(s)}$ indicates the set of all s th- order partial derivatives of \mathbf{u} with respect to \mathbf{x} .

Let us a system Σ

$$\mathbf{F}(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \dots, \mathbf{u}_{(s)}) = 0 \quad (6.9)$$

with $\mathbf{F} = (F_1, F_2, \dots, F_q)$ and

$$\mathbf{u} = \boldsymbol{\theta}(\mathbf{x}) \equiv (\theta^1(\mathbf{x}), \theta^2(\mathbf{x}), \dots, \theta^m(\mathbf{x})) \quad (6.10)$$

an its solution.

Definition 11 *A one parameter Lie group of point transformations admitted by a system Σ is a group of transformations of the form*

$$\hat{\mathbf{x}} = \mathbf{X}(\mathbf{x}, \mathbf{u}, a), \quad \hat{\mathbf{u}} = \mathbf{U}(\mathbf{x}, \mathbf{u}, a) \quad (6.11)$$

acting on the base space \mathbb{R}^{n+m} of the independent and dependent variables that satisfies the following two equivalent properties

1. a transformation of the group maps any solution $\mathbf{u} = \boldsymbol{\theta}(\mathbf{x})$ of Σ into another solution of Σ ;
2. a transformation of the group leaves Σ invariant, in the sense that the form of Σ is unchanged in terms of the transformed variables for any solution $\mathbf{u} = \boldsymbol{\theta}(\mathbf{x})$ of Σ .

A Lie group of transformations admitted by a differential equation corresponds to a mapping of each of its solutions to another solution of the same differential equation.

The transformations (6.11) of the base space determine suitable transformations for the derivatives of the dependent variables \mathbf{u} with respect to the independent variables \mathbf{x} .

The transformations of the derivatives of the dependent variables lead to natural extensions (prolongations) of the one-parameter Lie group of transformations (6.11). The one-parameter Lie group of transformations (6.11) acts on the space (\mathbf{x}, \mathbf{u}) , while the extended group acts, more in general, on the space $(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \dots, \mathbf{u}_{(s)})$.

Definition 12 *The one parameter Lie group of point transformations (6.11) leaves invariant the system (6.9), i.e. is a point symmetry admitted by system (6.9), if its sth extension, leaves invariant the surfaces*

$$\mathbf{F}(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \dots, \mathbf{u}_{(s)}) = 0.$$

All the information about the one-parameter Lie group of transformations (6.11) is contained in its infinitesimal generator (6.6) that, for system under consideration, is written in the form

$$X = \sum_{i=1}^n \xi_i(\mathbf{x}, \mathbf{u}) \frac{\partial}{\partial x_i} + \sum_{i=k}^m \eta_i^k(\mathbf{x}, \mathbf{u}) \frac{\partial}{\partial u_i^k}. \quad (6.12)$$

About the extended group we take in account its extended infinitesimal generator.

We write recursively the sth extension of generator (6.12). We start with the first order prolongation

$$X^{(1)} = X + \sum_{k=1}^m \sum_{i=1}^n \eta_i^k \frac{\partial}{\partial u_i^k}$$

where $u_i^k = \frac{\partial u^k}{\partial x_i}$ and

$$\eta_i^k = D_i \eta^k - \sum_{j=1}^n u_j^k D_i \xi_j$$

with D_i the total derivatives with respect to x_i .

Then the general s th extension of generator (6.12) ($s > 1$) recursively defined by

$$X^{(s)} = X^{s-1} + \sum_{k=1}^m \sum_{i_1=1}^n \cdots \sum_{i_s=1}^n \eta_{i_1 \dots i_s}^k \frac{\partial}{\partial u_{i_1 \dots i_s}^k}$$

where $u_{i_1 \dots i_s}^k = \frac{\partial^s u^k}{\partial x_{i_1} \dots \partial x_{i_s}}$ and

$$\eta_{i_1 \dots i_s}^k = D_{i_s} \eta_{i_1 \dots i_{s-1}}^k - \sum_{j=1}^n u_{i_1 \dots i_{s-1} j}^k D_{i_s} \xi_j. \quad (6.13)$$

Theorem 5 *Infinitesimal criterion for differential equations.*

Let

$$X = \sum_{i=1}^n \xi_i(\mathbf{x}, \mathbf{u}) \frac{\partial}{\partial x_i} + \sum_{k=1}^m \eta^k(\mathbf{x}, \mathbf{u}) \frac{\partial}{\partial u^k},$$

be the infinitesimal generator of the Lie group of point transformation (6.11) and let $X^{(s)}$ be its s th extension. Then the one-parameter Lie group of point transformations (6.11) is admitted by system (6.9), i.e. it is a point symmetry of system (6.9), if and only if

$$X^{(s)} \mathbf{F}(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \dots, \mathbf{u}_{(s)}) = 0 \quad \text{when} \quad \mathbf{F}(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \dots, \mathbf{u}_{(s)}) = 0.$$

The infinitesimal criterion for the invariance of a system of partial differential equations leads directly to an algorithm to determine the infinitesimal generators of the Lie group of point transformations admitted by a given system of partial differential equations.

The equations (6.9) can be splitted with respect to the components of the remaining derivatives of \mathbf{u} , that can be arbitrarily varied. We put on equal to zero the coefficients of these partial derivatives and obtain a system, called *system of the determining equations* or *simply determining system*, that therefore is often an overdetermined system of linear differential equations for the infinitesimal. The integration of equations of this system leads to the infinitesimal group. The infinitesimal involves arbitrary constants and in some cases arbitrary functions.

Invariant solutions of partial differential equations.

The function $\mathbf{u} = \boldsymbol{\theta}(\mathbf{x})$ with components $u^A = \theta^A(\mathbf{x})$ ($A = 1, 2, \dots, m$) is said to be *invariant solution* of (6.9) if $\mathbf{u} = \boldsymbol{\theta}(\mathbf{x})$ is an invariant surface of transformation (6.11), and a solution of (6.9), i.e. a solution is invariant if and only if

$$X(u^A - \theta^A(\mathbf{x})) = 0 \quad \text{for} \quad u^A = \theta^A(\mathbf{x}) \quad (A = 1, 2, \dots, m) \quad (6.14)$$

$$\mathbf{F}(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \dots, \mathbf{u}_{(s)}) = \mathbf{0} \quad (6.15)$$

The equations (6.14), known as *invariant surface conditions*, have the form

$$\xi_1(\mathbf{x}, \mathbf{u}) \frac{\partial u^A}{\partial x_1} + \dots + \xi_n(\mathbf{x}, \mathbf{u}) \frac{\partial u^A}{\partial x_n} = \eta^A(\mathbf{x}, \mathbf{u}) \quad (A = 1, 2, \dots, m) \quad (6.16)$$

and can be solved by introducing the corresponding characteristic equations

$$\frac{dx_1}{\xi_1(\mathbf{x}, \mathbf{u})} = \dots = \frac{dx_n}{\xi_n(\mathbf{x}, \mathbf{u})} = \frac{du^1}{\eta^1(\mathbf{x}, \mathbf{u})} = \frac{du^m}{\eta^m(\mathbf{x}, \mathbf{u})}. \quad (6.17)$$

This allows to express the function $\mathbf{u} = \boldsymbol{\theta}(\mathbf{x})$ as

$$u^A = \theta^A(I_1(\mathbf{x}, \mathbf{u}), \dots, I_{n-1}(\mathbf{x}, \mathbf{u})) \quad (A = 1, 2, \dots, m). \quad (6.18)$$

By substituting this form of $\mathbf{u} = \boldsymbol{\theta}(\mathbf{x})$ into (6.15), we obtain a *reduced system* of differential equations, that involves $(n - 1)$ independent variables $I_k(\mathbf{x}, \mathbf{u})$, $k = 1, 2, \dots, n-1$, called *similarity variables*. The name *similarity variables* is due to the fact that the scaling invariance, i.e. the invariance under similarity transformations, was one of the first example where this procedure has been used. Solutions of the reduced system are the invariant solutions.

Chapter 7

Thermal lattice effects and Energy

Transport model

The heating of the charge carriers and crystal lattice may strongly influence the behavior of semiconductor devices and even lower their performance. For the decreasing feature sizes, a very great number of basic elements and a careful adjustment of fitting parameter must satisfy the required accuracy [11]. We explained as in Hydrodynamic model, Bløtekaer introduced as closure relation the heat flux by Fourier's law. This equation has been widely and successfully used in conventional problems, when the characteristic dimensions of the physical system are much greater than the mean-free path and the time scale of interest is much longer than the mean-free time of the energy carriers, but it can not be used to study the heat conduction in micro and nano-scale and ultra-fast processes. To overcome the drawback of the Fourier's law, others constitutive heat transport equations were proposed for mathematical models. They describe the thermal effects in semiconductor devices, in which at small scales, the thermal transport is explained through the concept of quantized lattice vibrations. The heat carriers in the crystal lattice are the electrons and phonons, that have characteristic wavelengths in the order of a few nanometres at room temperature. Non-

isothermal device models were already considered in the 1970s [50], employing drift-diffusion and heat flow models for the lattice temperature. A thermodynamic approach to extend the drift-diffusion equations was developed by Wachutka in [54] and later it was generalized, including also charge carriers temperature, in [1], using Maximum Entropy Principle.

7.1 An Energy Transport model with crystal heating

Here we introduce a unipolar energy transport model with crystal heating. The equations of this model involve temperatures of the electrons and the crystal lattice. The temperature of the crystal lattice is modeled by the heat flux equation. This is given by [11]

$$\rho_L c_L \theta_t - \nabla \cdot (k_L \nabla \theta) = H \quad (7.1)$$

where θ is the lattice temperature, k_L is the heat conductivity of the lattice, ρ_L is the material density and c_L is the heat capacity, while the source term H represents the crystal energy production, derived under thermodynamical and phenomenological considerations of energy fluxes. It generally includes energy relaxation, recombination heat, and radiation effects. In the literature several expressions of term H have been proposed (more details can be found in [49], [18], [11], [54], [7]). Assuming non degenerate semiconductors, we can suppose that energy bands do not depend on the space and that the dependency of the energy bands on the lattice temperature is rather small, so that it is neglected. We assume that the crystal energy production has the following form

$$H = -nC_W - S_L (\theta - T_{en}) \quad (7.2)$$

where the second term is a phenomenological radiation one, depending on the environment temperature T_{en} and on the transmission coefficient S_L . Under assumptions of unipolar device, in the source term H there are not generation and recombination processes.

The resulting energy transport model involves four equations: the continuity and the energy

balance equations for the electrons, the thermal diffusion equation for lattice and the Poisson equation for the electrical potential. These partial differential equations are given by

$$\left\{ \begin{array}{l} \partial_t n + \nabla \cdot J = 0 \\ \partial_t \left(\frac{3}{2} n T \right) + \nabla \cdot \left(\frac{5}{2} T J - k_0 \nabla T \right) = J E - \frac{3}{2 \tau_0} n (T - \theta) \\ \partial_t (\rho_L c_L \theta) - \nabla \cdot (k_L \theta) = \frac{3}{2 \tau_0} n (T - \theta) - \frac{1}{\tau_L} (\theta - T_{en}) \\ -\nabla E = n - D \end{array} \right. \quad (7.3)$$

with $J = n \nabla \phi - \nabla (n T)$, k_0 and k_L the electron and lattice thermal conductivities, τ_0 and τ_L the electron energy and lattice thermal relaxation times. In the heat equation we assumed $S_L = \frac{1}{\tau_L}$ and T_{en} constant. The physical parameters k_0 , k_L , τ_0 and τ_L depend on the temperature T and the lattice temperature θ , while the material density ρ_L and the heat capacity c_L are constant. Finally the doping D is a function of the position x .

7.2 The symmetry classification in the one-dimensional case

For the model, introduced in the previous section, we perform a symmetry classification by the infinitesimal Lie method. In one-dimensional case, the system becomes

$$\left\{ \begin{array}{l} n_t + J_x = 0 \\ \frac{3}{2} (n_t T + n T_t) + \frac{5}{2} (T_x J + T J_x) - (k_0 T_x)_x = J E - \frac{3}{2 \tau_0} n (T - \theta) \\ \rho_L c_L \theta_t - (k_L \theta_x)_x = \frac{3}{2 \tau_0} n (T - \theta) - \frac{1}{\tau_L} (\theta - T_{en}) \\ -E_x = n - D(x) \end{array} \right. \quad (7.4)$$

with $J = -n E - (n T)_x$.

In the follow, when it will be necessary, in order to avoid long formulas, we will use the following notation

$$\mathbf{x} = (x^1, x^2) \equiv (t, x), \quad \mathbf{u} = (u_1, u_2, u_3, u_4) \equiv (n, T, \theta, E),$$

$$u_{i_j} = \frac{\partial u_i}{\partial x^j}, \quad u_{i_{jk}} = \frac{\partial^2 u_i}{\partial x^j \partial x^k}, \quad i = 1, \dots, 4, \quad j, k = 1, 2.$$

Then we look for symmetry operators in the form

$$X = \sum_{i=1}^2 \xi^i(\mathbf{x}, \mathbf{u}) \frac{\partial}{\partial x^i} + \sum_{i=1}^4 \eta^i(\mathbf{x}, \mathbf{u}) \frac{\partial}{\partial u_i}, \quad (7.5)$$

corresponding to the one-parameter Lie group of infinitesimal transformations in the (\mathbf{x}, \mathbf{u}) -space given by:

$$\tilde{x}^i = x^i + \varepsilon \xi^i(\mathbf{x}, \mathbf{u}) + O(\varepsilon^2), \quad i = 1, 2,$$

$$\tilde{u}_j = u_j + \varepsilon \eta^j(\mathbf{x}, \mathbf{u}) + O(\varepsilon^2), \quad j = 1, 2, 3, 4,$$

where ε is the group parameter.

Taking into account the structure of system (7.4), we need the following second order prolongation of the infinitesimal generator (7.5)

$$\tilde{X} = X + \sum_{i=1}^4 \sum_{j=1}^2 \zeta_j^i \frac{\partial}{\partial u_{i_j}} + \sum_{i=1}^4 \zeta_{22}^i \frac{\partial}{\partial u_{i_{22}}} \quad (7.6)$$

where the coefficients ζ_j^i and ζ_{22}^i ($i = 1, \dots, 4, \quad j = 1, 2$) are given by

$$\zeta_j^i = D_j \eta^i - u_{i_1} D_j \xi^1 - u_{i_2} D_j \xi^2, \quad \zeta_{22}^i = D_2 \zeta_2^i - u_{i_{12}} D_2 \xi^1 - u_{i_{22}} D_2 \xi^2,$$

and D_i represent the total derivatives with respect to x^i ($i = 1, 2$).

The corresponding determining system arises from the following invariance conditions

$$\tilde{X}(n_t + J_x) = 0 \quad (7.7)$$

$$\tilde{X} \left(\frac{3}{2} (n_t + nT_t) + \frac{5}{2} (T_x J + T J_x) - (k_0 T_x)_x + J E + \frac{3}{2\tau_0} n (T - \theta) \right) = 0 \quad (7.8)$$

$$\tilde{X} \left(\rho_{LC_L} \theta_t - (k_L \theta_x)_x - \frac{3}{2\tau_0} n (T - \theta) + \frac{1}{\tau_L} (\theta - T_{en}) \right) = 0 \quad (7.9)$$

$$\tilde{X}(-E_x - n + D) = 0 \quad (7.10)$$

under the constraints that the variables n , T , θ and E have to satisfy system (7.4).

We write eq. (7.7)-(7.10) as polynomial in the partial derivatives of dependent variables. Since the coefficients ξ^1, ξ^2 and η^i do not depend on these variables, the equations of system are satisfied identically only if all coefficients of the polynomial are equal to zero. We obtain a set of differential equations, that represents the determining system. The presence of the constitutive functions $k_0(T, \theta)$, $k_L(T, \theta)$, $\tau_0(T, \theta)$, $\tau_L(T, \theta)$ and $D(x)$ makes the equations very complicated to solve. This system involved many equations, but after a first simplification, taking into account that we assume $k_0 k_L \tau_0 \tau_L D \neq 0$, the invariance conditions lead to the following results

$$\xi^1 = -a_1 t + a_2$$

$$\xi^2 = x a_3 + a_0$$

$$\eta^1 = a_1 u_1$$

$$\eta^2 = u_2 (2a_3 + a_1)$$

$$\eta^3 = 2u_3 (a_1 + a_3) + g(t, x)$$

$$\eta^4 = u_4 (a_1 + a_3)$$

where the constants a_0, a_1, a_2, a_3 and the function g must satisfy the following equations

$$\begin{aligned}
& [(k_L g_{xx} - \rho_L c_L g_t) \tau_L - g - (3a_1 + 2a_3) T_{en} + a_1 u_3] \tau_L + (u_3 - T_{en}) (g + 2(a_1 + a_3) u_3) \tau_{L u_3} + \\
& (a_1 + 2a_3) u_2 (u_3 - T_{en}) \tau_{L u_2} = 0, \\
& (2(a_1 + a_3) u_3 + g) (u_2 - u_3) \tau_{0 u_3} + (a_1 + 2a_3) u_2 (u_2 - u_3) \tau_{0 u_2} + (g + a_1 u_2) \tau_0 = 0, \\
& (2(a_3 + a_1) u_3 + g) k_{0 u_3} + (a_1 + 2a_3) u_2 k_{0 u_2} - 2(a_1 + a_3) k_0 = 0, \\
& (2(a_3 + a_1) u_3 + g) k_{L u_3} + (a_1 + 2a_3) u_2 k_{L u_2} - (a_1 + 2a_3) k_L = 0, \\
& k_{L u_2} g_x = 0, \\
& a_1 D - D_x (x a_3 + a_0) = 0.
\end{aligned} \tag{7.11}$$

Solving this system we obtain the complete group classification of system (7.4).

The *principal Lie algebra* $\mathcal{L}_{\mathcal{P}}$ is obtained when we consider D, τ_0, τ_L, k_0 and k_L arbitrary functions. In this case we get $a_0 = a_1 = a_3 = g(t, x) = 0$, then $\mathcal{L}_{\mathcal{P}}$ is one dimensional and it is spanned by the operator

$$X_1 = \frac{\partial}{\partial x^1} \equiv \frac{\partial}{\partial t}. \tag{7.12}$$

Only for some special form of the functions D, τ_0, τ_L, k_0 and k_L the principal Lie algebra can be enlarged. Below we list these special cases and the additional generators to (7.12).

Case 1. If

$$k_0 = k_0(T, \theta), \quad k_L = k_L(T, \theta), \quad \tau_0 = \tau_0(T, \theta), \quad \tau_L = \tau_L(T, \theta), \quad D = D_0, \tag{7.13}$$

with k_0, k_L, τ_0 and τ_L arbitrary functions of their arguments, with D_0 arbitrary constant, we get $a_1 = a_3 = 0$ and $g(x, t) = 0$ and the following extension of $\mathcal{L}_{\mathcal{P}}$

$$X_0 = \frac{\partial}{\partial x}.$$

Case 2. If

$$k_0 = k_0(T), \quad k_L = k_L(T), \quad \tau_0 = (T - \theta) F_1(T), \quad \tau_L = \frac{T_{en} - \theta}{F_2(T) + b_0\theta}, \quad D = D(x), \quad (7.14)$$

with k_0, k_L, F_1, F_2 and D arbitrary functions of their arguments, with $k_{LT} \neq 0$, and b_0 arbitrary constant, and we get $a_0 = a_1 = a_3 = 0$ and $g(t, x) = a_4 e^{\frac{b_0 t}{\rho_L c_L}}$ and the following extension of \mathcal{L}_P

$$X_2 = e^{\frac{b_0 t}{\rho_L c_L}} \frac{\partial}{\partial \theta}.$$

Case 3. If

$$k_0 = k_0(T), \quad k_L = k_L, \quad \tau_0 = (T - \theta) F_1(T), \quad \tau_L = \frac{T_{en} - \theta}{F_2(T) + b_0\theta}, \quad D = D(x),$$

with k_0, F_1, F_2 and D arbitrary functions of their arguments, and b_0, k_L arbitrary constants, we get $g(x, t)$ solution the equation $\rho_L c_L g_t - k_L g_{xx} - b_0 g = 0$, $a_0 = a_1 = a_3 = 0$ and the following extension of \mathcal{L}_P

$$X_2 = g(t, x) \frac{\partial}{\partial \theta}.$$

Case 4. If

$$k_0 = G_1(T) (\theta + b_0), \quad k_L = G_2(T), \quad \tau_0 = \frac{\theta - T}{\theta + b_0} F_1(T), \quad \tau_L = \frac{T_{en} - \theta}{(\theta + b_0)^2} F_2(T),$$

$$D = (x + c_2)^{-2},$$

where G_1, G_2, F_1 and F_2 are arbitrary functions and b_0, c_2 constitutive constants, we get $a_0 = c_2 a_3, a_1 = -2a_3, g(x, t) = -2a_3$ and

$$X_2 = (x + c_2) \frac{\partial}{\partial x} + 2t \frac{\partial}{\partial t} - 2n \frac{\partial}{\partial n} - 2(\theta + b_0) \frac{\partial}{\partial \theta} - E \frac{\partial}{\partial E}.$$

Case 5. If

$$k_0 = G_1(\sigma), \quad k_L = TG_2(\sigma), \quad \tau_0 = (\theta - T)F_1(\sigma), \quad \tau_L = T(T_{en} - \theta)F_2(\sigma),$$

$$D = (x + c_2)^{-1},$$

where G_1, G_2, F_1 and F_2 are arbitrary functions of $\sigma \equiv \theta + b_0 \ln T$, with b_0 and c_2 constitutive constants, we get $a_0 = -c_2 a_1, a_3 = -a_1, g(t, x) = b_0 a_1$ and

$$X_2 = (x + c_2) \frac{\partial}{\partial x} + t \frac{\partial}{\partial t} - n \frac{\partial}{\partial n} + T \frac{\partial}{\partial T} - b_0 \frac{\partial}{\partial \theta}.$$

Case 6. If

$$k_0 = T^{\frac{2(c_1+1)}{c_1+2}} G_1(\sigma), \quad k_L = TG_2(\sigma),$$

$$\tau_0 = (T - \theta) T^{-\frac{2(c_1+1)}{c_1+2}} F_1(\sigma), \quad \tau_L = (T_{en} - \theta) T^{-\frac{2+3c_1}{c_1+2}} F_2(\sigma), \quad D(x) = (x + c_2)^{c_1},$$

where G_1, G_2, F_1 and F_2 are arbitrary functions of $\sigma \equiv (\theta + b_0) T^{-\frac{2(c_1+1)}{c_1+2}}$, and b_0, c_1, c_2 constitutive constants with $c_1 \neq -2$, we get $g(t, x) = 2b_0 a_3 (1 + c_1), a_0 = c_2 a_3, a_1 = c_1 a_3$ and

$$X_2 = (x + c_2) \frac{\partial}{\partial x} - c_1 t \frac{\partial}{\partial t} + c_1 n \frac{\partial}{\partial n} + (2 + c_1) T \frac{\partial}{\partial T} + 2(c_1 + 1)(\theta + b_0) \frac{\partial}{\partial \theta} \\ + (c_1 + 1) E \frac{\partial}{\partial E}.$$

Case 7. If

$$k_0 = b_1 T^{\frac{2(c_1+1)}{c_1+2}}, \quad k_L = b_2 T,$$

$$\tau_0 = b_3 (T - \theta) T^{-\frac{2(c_1+1)}{c_1+2}}, \quad \tau_L = \frac{(T_{en} - \theta)}{b_4 T^{\frac{2+3c_1}{c_1+2}} + b_5}, \quad D(x) = (x + c_2)^{c_1},$$

where $b_i (i = 1...5), c_1, c_2$ are constitutive constants with $c_1 \neq -2$, we obtain $a_0 = c_2 a_3,$

$a_1 = c_1 a_3$ and $g(t, x) = a_4 - \frac{b_5 a_3 (2 + 3c_1)}{\rho_L c_L} t$, with a_4 arbitrary constant, and then

$$\begin{aligned} X_2 &= (x + c_2) \frac{\partial}{\partial x} - c_1 t \frac{\partial}{\partial t} + c_1 n \frac{\partial}{\partial n} + (2 + c_1) T \frac{\partial}{\partial T} \\ &\quad + \left(2(c_1 + 1)\theta - (2 + 3c_1) \frac{b_5}{\rho_L c_L} t \right) \frac{\partial}{\partial \theta} + (c_1 + 1) E \frac{\partial}{\partial E}, \\ X_3 &= \frac{\partial}{\partial \theta}. \end{aligned}$$

Case 8. If

$$k_0 = b_1 T, \quad k_L = b_2 T, \quad \tau_0 = \frac{\theta - T}{T} b_3, \quad \tau_L = \frac{T_{en} - \theta}{\theta + b_4 T + b_0}, \quad D = D_0,$$

where b_i ($i = 0 \dots 4$) and D_0 are constitutive constants, we get the following extensions of

$\mathcal{L}_{\mathcal{P}}$

$$\begin{aligned} X_0 &= \frac{\partial}{\partial x}, \\ X_2 &= x \frac{\partial}{\partial x} + 2T \frac{\partial}{\partial T} + 2(\theta + b_0) \frac{\partial}{\partial \theta} + E \frac{\partial}{\partial E}, \\ X_3 &= e^{\frac{t}{\rho_L c_L}} \frac{\partial}{\partial \theta}. \end{aligned}$$

7.3 Reduced system and exact solutions

One of the various applications of the symmetry analysis is to reduce a system in (1+1) dimension in a system of ordinary differential equations. This reduced system is obtained by using a special ansatzes determined from symmetry group admitted by the equations under consideration (for more details see, e.g., [37], [38]).

As example we consider system (7.4) with the doping D constant. This system falls in the case 2 of the previous section and it admits the two-dimensional algebra

$$X_0 = \frac{\partial}{\partial x}, \quad X_1 = \frac{\partial}{\partial t}.$$

We use the generator

$$X = X_1 + \lambda X_0 \equiv \frac{\partial}{\partial t} + \lambda \frac{\partial}{\partial x},$$

where λ is an arbitrary constant. The invariance conditions lead to traveling wave reduction. The similarity solution

$$n = v_1(z), \quad T = v_2(z), \quad \theta = v_3(z), \quad E = v_4(z), \quad \text{with } z = x - \lambda t,$$

are not zero functions solutions of the reduced system

$$\begin{aligned} (\lambda v_1 + v_1 v_4 + v_1' v_2 + v_1 v_2')' &= 0, \\ \frac{3}{2} \lambda (v_1 v_2)' + \frac{5}{2} (v_2 v_1 v_4 + v_2 (v_1 v_2)')' + (k_0 v_2')' + v_4 (v_1 v_4 + (v_1 v_2)') - \frac{3v_1}{2\tau_0} (v_2 - v_3) &= 0, \\ \rho_L c_L \lambda v_3' + (k_L v_3')' + \frac{3v_1}{2\tau_0} (v_2 - v_3) - \frac{1}{\tau_L} (v_3 - T_{en}) &= 0, \\ v_1 + v_4' - D &= 0, \end{aligned}$$

where the prime denotes differentiation with respect to the only variable z and k_0 , k_L , while τ_0 and τ_L depend on v_2 and v_3 .

In the case with τ_0 , τ_L , k_0 and k_L are constants, by setting

$$k_L = \frac{2(2\lambda^2 + k_0)(\lambda^2(4 + \rho_L c_L \tau_2 D) + 2k_0)}{\lambda^2 \tau_L D^2}$$

and

$$\lambda^2 = -\frac{5k_0}{12} + \frac{T_{en} D}{24} \pm \frac{\sqrt{4k_0^2 - 20k_0 T_{en} D + T_{en}^2 D^2}}{24}$$

we obtain the following solutions for the system (7.4)

$$\begin{aligned} n &= D + 2c_4 h^2 e^{h(x-\lambda t)} \\ T &= c_4 e^{h(x-\lambda t)} - \frac{\lambda}{h} + \frac{D}{2h^2} \\ \theta &= c_4 e^{h(x-\lambda t)} - \frac{\lambda}{h} + \frac{D}{2h^2} \\ E &= -2c_4 h e^{h(x-\lambda t)} \end{aligned}$$

where $h = -\frac{\lambda D}{2(2\lambda^2 + k_0)}$ and c_4 is an arbitrary constant.

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