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Coupling and thermal effects
in semiconductor devices

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Chapter 1

Introduction

In recent years, many research groups have started a systematic mathematical study of coupling effects arising in the transition from microelectronics to nanoelectronics. In this thesis we refer to effects which are especially relevant in integrated circuit modeling, and whose relevance increases with the decreasing of the scales, like the ones due to electrothermal coupling [17, 20, 22], electromagnetic coupling [23, 27], and electric network-device coupling [1, 2, 54].

We concentrate here on two main topics: coupling of devices ad electric networks, and heat effects in semiconductor devices. Both topics heave the common feature that they refer to high order effects, which can be neglected when microscopic scales scale are involved.

In the first part of this thesis, we focus on the electric network-device coupling.

Usually the components of an electric networks are described in terms of constitutive relations which link node voltages and branch current. In the case of components constituted by semiconductor devices, the representation of the physical device takes the form at an equivalent circuit, which captures the main features of the device itself. This is done by introducing a description in terms of non linear resistor, capacitors and inductors, with a set of fitting parameters which are recovered by measures. Coupling effects of devices and circuit are usually introduced by corrections in the equivalent circuit. In this approach, all quantities are lumped, without any distributed quantity.

Here we follow a different approach. We consider an electric network which contains semiconductor devices, and we model the devices by multidimensional, steady-state, drift-diffusion equations.

In this case, the lumped variables are the node potentials of the network and the fluxes through branches with inductances or with independent voltage sources. The network equations which describe these variables come from Modified Nodal Analysis, and consists of Kirchhoff's current law, with some constitutive laws for the basic components of the network. The distributed equations enter the definition of the currents which cross the Ohmic contact of the devices in the network. These currents show up in the network equations, and are defined by means of surface integrals of some fluxes of the distributed variables. In turn, the distributed variables are described by a set of multi-dimensional, nonlinear, elliptic

equations, and the boundary data are related to the network's node potentials, which are part of the lumped variables.

Thus, it is generally possible to view the coupled model as a set of lumped equations with additional components modeled by complicated input/output relations, which involve partial differential equations, or as a set of distributed equations with additional differential-algebraic constraints. The first viewpoint is usually followed in the numerical simulation realms, while the second approach is generally preferable for an analysis of the coupled model. Here, the two viewpoints will be used alternatively one with the other. In fact, the analysis of the coupled is based on the analysis of the device equation, but the main existence result is established by using a fixed-point map for the network equations.

This kind of coupled model was considered in [29] from the point of view of abstract differential-algebraic systems, and the modeling of the coupling was discussed in [54]. An existence result was proved in [1] for a network containing one-dimensional devices modeled by steady-state drift diffusion equations, and a uniqueness result for the same model was established in [3], assuming that the system is close enough to an equilibrium state. We also mention [2], where it is established the well-posedness of the coupled model of the network equations and the time-dependent, one-dimensional, drift-diffusion equations, and [18], which deals with the perturbation analysis.

The first result presented in this thesis is directly related to [1], extending its results to general multi-dimensional, steady-state, drift-diffusion equations, when the coupled problem is index-1. This is the first existence result for the fully nonlinear model of the network equation coupled with multidimensional semiconductor devices. A second result is established for a special class of index-2 coupled problems, defined by means of some technical conditions. This is the first existence result for index-2 elliptic partial-differential-algebraic equations in microelectronics.

The second part of the thesis, which consists of the last chapter, deals with thermal effects in semiconductor devices. We propose a general framework to derive energy-transport model from the Bloch-Boltzmann-Peierl equations, which describe the evolution of the distribution functions of electrons and phonon in a semiconductor. Starting from an hydrodynamic model with closure relations obtained by application of the maximum entropy principle, we introduce a diffusive scaling, and derive formally the limit system. The resulting system is an energy-transport model with no fitting parameters.

The thesis is organized as follows. In chapter 2 we introduce the modified nodal analysis formalism, to deal with the circuit variables, and we set a general framework for the coupling with semiconductor devices. In chapter 3 we derive the semiconductor equations, starting from basic physical considerations. In the next chapter we prove an existence result for the semiconductor equations, introducing an iteration map which will be used in the existence proof for the coupled problem. Also, we derive some basic properties of this iteration map. Chapter 5 contain the two main results concerning coupled problems, the existence results for index-

1 and index-2 elliptic partial-differential-algebraic equations for semiconductor devices and electric networks. Finally, in chapter 6 we present the results on the derivation of the energy-transport model.

Chapter 2

Mathematical modeling in chip design in nanoelectronics

2.1 Circuit modeling

In microelectronics, an integrated circuit is usually described as an electric network. This is a simplified description, but it captures the main features of the electric behavior of the integrated circuit, at least when second order coupling effects between the active and passive components and the substrate can be neglected. Moreover, it is a very efficient description, because it leads to a system of differential-algebraic equations (DAEs) which can be efficiently solved numerically. For this reason, even when previously neglected secondary effects started to become important, they were introduced in the network framework by adding appropriate sub-networks and more and more refined equivalent circuits.

From a mathematical point of view, an electric circuit is a directed multigraph, that is, a set of n_v vertices (or nodes) connected by n_a arcs (or branches) with a direction. Two vertices may be connected by more than one arc. Each arc contains a basic component, and is labeled according to the component it contains. The electric behavior of the network is given by a set of time-dependent variables associated to its nodes and branches. An applied potential is associated to each node, $e_k(t)$, $k = 1, \ldots, n_v$, to each branch is associated a voltage drop $v_h(t)$ and a current $i_h(t)$, $j = 1, \ldots, n_a$, with $t \in [t_0, t_1]$. We denote by $\boldsymbol{e}(t) \in \mathbb{R}^{n_v}$, $\boldsymbol{v}(t) \in \mathbb{R}^{n_a}$ and $\boldsymbol{i}(t) \in \mathbb{R}^{n_a}$, the vectors comprising node potentials, voltage drops and currents, respectively.

The connections of the branch-node of the network graph can be described by an incidence matrix $\boldsymbol{A} = (a_{hk}) \in \mathbb{R}^{n_v \times n_a}$ defined by

$$a_{hk} = \begin{cases} -1 & \text{if the branch } k \text{ leaves the node } h, \\ 1 & \text{if the branch } k \text{ enters the node } h, \\ 0 & \text{otherwise.} \end{cases} \qquad (2.1)$$

This description applies also to networks with multi-terminal elements. In this case, the network can be appropriately described by an hypergraph, that is,

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a generalization of the concept of graph where a branch can connect more than two nodes. In practice, we can retrieve the incidence matrix formalism by identifying branches with ordered couples of terminals within the same multi-terminal element. We will provide more details when dealing with elements consisting of semiconductor devices.

The composition of the basic elements is ruled by the following two Kirchhoff's laws, which can be derived by applying Maxwell's equations.

- *Kirchhoff's voltage law (KVL)*: The algebraic sum of voltage along each loop of the network must be equal to zero at every istant of time. From this law we can derive an expression that links the node potentials $\boldsymbol{e}(t)$ to the voltage drops $\boldsymbol{v}(t)$

$$\boldsymbol{A}^\top \boldsymbol{e}(t) = \boldsymbol{v}(t), \quad \forall\, t \in [t_0, t_1]. \tag{2.2}$$

- *Kirchhoff's current law (KCL)*: The algebraic sum of current traversing each cut set of the network must be equal to zero at every istant of time

$$\boldsymbol{A}\boldsymbol{i}(t) = 0, \quad \forall\, t \in [t_0, t_1]. \tag{2.3}$$

2.1.1 Modified Nodal Analysis

In order to describe the behavior of the network quantities we chose to use one of the most common approaches for network analysis that is the Modified Nodal Analysis (MNA). This method represents a systematic way to derive equations for circuits. The main idea of MNA is:

1. Write node equations applying Kinchhoff's current law (2.3) to each node except for the reference node, corresponding to the zero reference potential.

2. In equation (2.3), replace the currents of voltage-controlled elements by the voltage-current relations of these elements.

3. Add the current-voltage relations for all current-controlled elements.

We consider RLC networks, that is, electric networks containing only resistances (labeled by R), inductances (labeled by L), and conductances (labeled by C). In addition, we need to allow also for branches with independent current and voltage sources, labeled with $\boldsymbol{i}_I(t) \in \mathbb{R}^{n_V}$, $\boldsymbol{v}_V(t) \in \mathbb{R}^{n_I}$, respectively. To keep detailed informations about the structure of the equations arising from the MNA, we make the splitting of the incidence matrix $\boldsymbol{A}$, with components described in (2.1), into the element-related incidence matrices

$$\boldsymbol{A} = (\boldsymbol{A}_R, \boldsymbol{A}_C, \boldsymbol{A}_L, \boldsymbol{A}_I, \boldsymbol{A}_V) \in \mathbb{R}^{n_v \times (n_R + n_C + n_L + n_I + n_V)} \equiv \mathbb{R}^{n_v \times n_a},$$

where $\boldsymbol{A}_R, \boldsymbol{A}_C, \boldsymbol{A}_L, \boldsymbol{A}_I$ and $\boldsymbol{A}_V$ describe the branch-current relations for resistive, capacitive, inductive branches and branches of current sources and voltage sources

respectively. To keep track of the different labels, we write

$$
\boldsymbol{v} = \begin{bmatrix} \boldsymbol{v}_R \\ \boldsymbol{v}_C \\ \boldsymbol{v}_L \\ \boldsymbol{v}_I \\ \boldsymbol{v}_V \end{bmatrix}, \qquad \boldsymbol{i} = \begin{bmatrix} \boldsymbol{i}_R \\ \boldsymbol{i}_C \\ \boldsymbol{i}_L \\ \boldsymbol{i}_I \\ \boldsymbol{i}_V \end{bmatrix},
$$

for voltage and current respectively. The direction of each branch coincides with the positive direction of the voltage drop and the current through the branch. To the above relations, (2.2) and (2.3), we need to add constitutive relations for the RLC components:

$$
\boldsymbol{i}_R = \boldsymbol{i}_R(\boldsymbol{v}_R), \qquad \boldsymbol{i}_C = \frac{\mathrm{d}\boldsymbol{q}_C(\boldsymbol{v}_C)}{\mathrm{d}t}, \qquad \boldsymbol{v}_L = \frac{\mathrm{d}\boldsymbol{\phi}_L(\boldsymbol{i}_L)}{\mathrm{d}t}, \tag{2.4}
$$

where $\boldsymbol{q}_C$ collects the charges inside the capacitors, and $\boldsymbol{\phi}_L$ is a flux term for the inductors. We also need to consider relations for the branches with sources:

$$
\boldsymbol{i}_L = \boldsymbol{I}, \qquad \boldsymbol{v}_V = \boldsymbol{V}. \tag{2.5}
$$

Following the formalism of Modified Nodal Analysis (MNA), we use the relations (2.4) and (2.5) in Kirchhoff's current law equation (2.3),to obtain the DAE equation for the unknowns $\boldsymbol{q}_C$, $\boldsymbol{\phi}_L$, $\boldsymbol{e}$, $\boldsymbol{i}_L$, $\boldsymbol{i}_V$. Sometimes it is convenient to reduce the number of variables, eliminating $\boldsymbol{q}_C$ and $\boldsymbol{\phi}_L$. This leads to the following form of the MNA equations, for the unknowns $\boldsymbol{e}$, $\boldsymbol{i}_L$, $\boldsymbol{i}_V$:

$$
\begin{aligned}
\boldsymbol{A}_C \frac{\mathrm{d}\boldsymbol{q}_C(\boldsymbol{A}_C^\top \boldsymbol{e})}{\mathrm{d}t} + \boldsymbol{A}_R \boldsymbol{i}_R(\boldsymbol{A}_R^\top \boldsymbol{e}) + \boldsymbol{A}_L \boldsymbol{i}_L + \boldsymbol{A}_V \boldsymbol{i}_V + \boldsymbol{A}_I \boldsymbol{I} &= 0, \\
\frac{\mathrm{d}\boldsymbol{\phi}_L(\boldsymbol{i}_L)}{\mathrm{d}t} - \boldsymbol{A}_L^\top \boldsymbol{e} &= 0, \\
\boldsymbol{A}_V^\top \boldsymbol{e} - \boldsymbol{V} &= 0.
\end{aligned} \tag{2.6}
$$

We notice that the constitutive relations $\boldsymbol{q}_C(\boldsymbol{v})$, $\boldsymbol{i}_R(\boldsymbol{v})$, $\boldsymbol{\phi}_L(\boldsymbol{i}_L)$, depend on the specific components present in the network.

We will restrict ourselves to linear RLC networks, that is, such that the constitutive relations for $\boldsymbol{q}_C$, $\boldsymbol{i}_R$, $\boldsymbol{\phi}_L$, are linear:

$$
\boldsymbol{q}_C(\boldsymbol{v}) = \boldsymbol{C}\boldsymbol{v}, \quad \boldsymbol{i}_R(\boldsymbol{v}) = \boldsymbol{G}\boldsymbol{v}, \quad \boldsymbol{\phi}_L(\boldsymbol{i}_L) = \boldsymbol{L}\boldsymbol{i}_L. \tag{2.7}
$$

The capacitance, inductance and conductance matrices $\boldsymbol{C} \in \mathbb{R}^{n_C \times n_C}$, $\boldsymbol{G} \in \mathbb{R}^{n_G \times n_G}$ and $\boldsymbol{L} \in \mathbb{R}^{n_L \times n_L}$, appearing in the previous relations, are assumed to be symmetric and positive definite.

For linear RLC networks the system (2.6) can be written in the following compact form:

$$
\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t), \tag{2.8}
$$

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where we have introduced the unknowns vector

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{e} \\ \boldsymbol{i}_L \\ \boldsymbol{i}_V \end{bmatrix},$$

and the matrices

$$\boldsymbol{E} = \begin{bmatrix} \boldsymbol{A}_C \boldsymbol{C} \boldsymbol{A}_C^\top & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{L} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \end{bmatrix}, \; \boldsymbol{A} = - \begin{bmatrix} \boldsymbol{A}_R \boldsymbol{G} \boldsymbol{A}_R^\top & \boldsymbol{A}_L & \boldsymbol{A}_V \\ -\boldsymbol{A}_L^\top & \boldsymbol{O} & \boldsymbol{O} \\ -\boldsymbol{A}_V^\top & \boldsymbol{O} & \boldsymbol{O} \end{bmatrix},$$

$$\boldsymbol{B} = - \begin{bmatrix} \boldsymbol{A}_I & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}, \quad \boldsymbol{u}(t) = \begin{bmatrix} \boldsymbol{I}(t) \\ \boldsymbol{V}(t) \end{bmatrix}.$$

Here, and in what follows, $\boldsymbol{O}$ denotes the generic zero matrix and $\boldsymbol{I}$ the generic identity matrix.

2.1.2 Charge-oriented Modified Nodal Analysis

The MNA approach presented in the previous subsection leads to the conventional MNA equations (2.6), for the unknowns $\boldsymbol{e}$, $\boldsymbol{i}_L$, $\boldsymbol{i}_V$. It is possible to choose an alternative approach, called charge-oriented MNA, in which we consider two additional unknowns: the charge of capacitances $\boldsymbol{q}$, and the flux of inductances $\boldsymbol{\phi}$ [34]. The charge-oriented MNA equations are:

$$
\begin{aligned}
\boldsymbol{A}_C \frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} + \boldsymbol{A}_R \boldsymbol{i}_R(\boldsymbol{A}_R^\top \boldsymbol{e}) + \boldsymbol{A}_L \boldsymbol{i}_L + \boldsymbol{A}_V \boldsymbol{i}_V + \boldsymbol{A}_I \boldsymbol{I} &= 0, \\
\frac{\mathrm{d}\boldsymbol{\phi}}{\mathrm{d}t} - \boldsymbol{A}_L^\top \boldsymbol{e} &= 0, \\
\boldsymbol{A}_V^\top \boldsymbol{e} - \boldsymbol{V} &= 0, \\
\boldsymbol{q} - \boldsymbol{q}_C(\boldsymbol{A}_C^\top \boldsymbol{e}) &= 0, \\
\boldsymbol{\phi} - \boldsymbol{\phi}_L(\boldsymbol{i}_L) &= 0.
\end{aligned}
\tag{2.9}
$$

We mention another approach to derive equations for electric network, which is the *stamping* approach. We consider Kirchhoff's current law (2.3), for each of the n_v electrical nodes of the network, writing that

$$\sum_{k=1}^{n_a} i_{kh} = 0 \qquad h = 1, \ldots, n_v \tag{2.10}$$

where $i_{kh} \equiv a_{hk} i_k$ denotes the current flowing from node h into element k.

The currents in (2.10) can be expressed in terms of the vector of electrical state variables $\boldsymbol{s} = [s_1, \ldots, s_{n_v}]^\top$ plus a set of additional (vector valued) variables $\boldsymbol{r}_k$ each of dimension I_k

$$i_{kh} = \boldsymbol{A}_{kh}\dot{\boldsymbol{r}}_k + J_{kh}(\boldsymbol{s}, \boldsymbol{r}_k), \quad h = 1, \ldots, n_a, \quad h = 1, \ldots, n_v, \tag{2.11}$$

where $\boldsymbol{A}_{kh} \in \mathbb{R}^{1 \times I_k}$, and I_k, $k = 1, \ldots, n_a$ being a set of non negative integers. As the variables $\boldsymbol{r}_k$ only appear in the equations defining the fluxes relative to the k-th element, they will henceforth be referred to as *internal variables* of the k-th element. The MNA model is completed by a suitable number I_k of constitutive relations for the internal variables of each element

$$\boldsymbol{B}_{ki}\dot{\boldsymbol{r}}_k + Q_{ki}(\boldsymbol{s}, \boldsymbol{r}_k) = 0, \quad k = 1, \ldots, n_a, \quad i = 1, \ldots, I_k, \tag{2.12}$$

where $\boldsymbol{B}_{ki} \in \mathbb{R}^{1 \times I_k}$. Notice that, although only time derivatives of internal variables appear in (2.12) and the terms involving such derivatives are linear, no restriction on the practical applicability of the model has been introduced so far.

2.2 General framework for device models

In this section we provide a general framework for the description of a semiconductor device, which is consistent with the MNA description of a network.

A semiconductor device can be model by means of a domain $\Omega \in \mathbb{R}^d$, with $d = 1, 2$, or 3, it is characterized by an electric potential $\phi(\mathbf{x}, t)$, and by a vector variable $\boldsymbol{U}(\mathbf{x}, t)$, with $\mathbf{x} \in \Omega$. The variable $\boldsymbol{U}(\mathbf{x}, t)$ collects the other macroscopic variables for the device, such as carrier density, flux density, energy, and so on. Many mathematical models can be used to describe semiconductor devices, these models have some common features.

The first common feature is that the electric potential ϕ is generated by the built-in charge, $\rho_{\text{bi}}(\mathbf{x})$, due to the dopants embedded in the semiconductor, and by the charge density $\rho(\boldsymbol{U})$, due to the carriers, so that it satisfies the Poisson equation:

$$-\nabla \cdot (\epsilon_s \nabla \phi) = \rho_{\text{bi}} + \rho(\boldsymbol{U}), \tag{2.13}$$

where $\epsilon_s(\mathbf{x})$ is the dielectric constant.

The second common feature in the semiconductor mathematical models, is that the device variable $\boldsymbol{U}$ satisfies a system of partial differential equations, which is coupled to the electric potential only through the electric field

$$\mathbf{E} = -\nabla \phi. \tag{2.14}$$

Symbolically, we can write

$$\mathcal{F}(\boldsymbol{U}, \tfrac{\partial}{\partial t}\boldsymbol{U}, \nabla \cdot \boldsymbol{U}, \ldots; \mathbf{E}) = 0. \tag{2.15}$$

The last common feature is that the previous equation is consistent with the conservation of the charge density:

$$\frac{\partial \rho(\boldsymbol{U})}{\partial t} + \nabla \cdot \boldsymbol{J}(\boldsymbol{U}) = 0. \tag{2.16}$$

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in which we have indicated with $\boldsymbol{J}(\boldsymbol{U})$ the electric current. It is also possible to include this variable $\boldsymbol{J}(\boldsymbol{U})$ as a component of the variable $\boldsymbol{U}$, or can be evaluated as a functional of the said variable.

The equation (2.13) must be supplemented by appropriate boundary conditions. We assume that the boundary $\partial\Omega$ is the union of two disjoint parts Γ_D and Γ_N. The first part of the boundary is the union of all the Ohmic contacts

$$\Gamma_D = \bigcup_{k=0}^{K} \Gamma_{D,k},$$

that is, the union of the terminals $\Gamma_{D,k}$, Here, we assign conditions of Dirichlet type:

$$\phi = \phi_{\text{bi}}(\rho_{\text{bi}}) + e_{D,k}, \qquad \text{on } \Gamma_{D,k}, \ k = 0, 1, \ldots, K, \tag{2.17}$$

where $\phi_{\text{bi}}(\rho_{\text{bi}})$ is the built-in potential, $e_{D,k}, \ k = 0, 1, \ldots, K$, are the applied potentials at the Ohmic contacts of the device considered. For later use, we denote by $\boldsymbol{e}_D$ the vector comprising the applied potentials.

The second part of the boundary, Γ_N, is the union of all the insulated portions of the boundary, $\Gamma_N = \partial\Omega \setminus \Gamma_D$. Here we assign Neumann conditions:

$$\boldsymbol{\nu} \cdot \nabla\phi = 0, \qquad \text{on } \Gamma_N, \tag{2.18}$$

where $\boldsymbol{\nu}$ denotes the external unit normal to $\partial\Omega$.

The electric current $\boldsymbol{J}$ depends also on the applied potentials $e_{D,k}, \ k = 0, 1, \ldots, K$, due to the coupling of (2.15) with the Poisson's equation (2.13), through the electric field $\mathbf{E}$.

Using equation (2.13) in equation (2.16), taking into account (2.14), we obtain

$$\nabla \cdot \left(\epsilon_s \frac{\partial}{\partial t} \mathbf{E} + \boldsymbol{J}(\boldsymbol{U}) \right) = 0 \tag{2.19}$$

The term $\epsilon_s \frac{\partial}{\partial t}\mathbf{E}$ is the displacement current, and represents the current induced by time-variations of the electric field. Then, the total current in the device is given by

$$\boldsymbol{j} := \epsilon_s \frac{\partial}{\partial t}\mathbf{E} + \boldsymbol{J}(\boldsymbol{U}). \tag{2.20}$$

The current $j_{D,k}$ through the k-th contact of the device, is defined by:

$$j_{D,k} = - \int_{\Gamma_{D,k}} \boldsymbol{j} \cdot \boldsymbol{\nu} \, \mathrm{d}\sigma(\mathbf{x}), \tag{2.21}$$

with $k = 0, 1, \ldots, K$, and we denote by $\boldsymbol{j}_D$ the vector of these currents.

When connected to an electric network, a semiconductor device with $K+1$ Ohmic contacts can be regarded as a multi-terminal element. We have mentioned that, in presence of multi-terminal elements, the multigraph description of an

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electric network should be replaced by a hypergraph description. In practice, we can avoid this complication by introducing internal branches of a multi-terminal element, as appropriate pairs of terminals.

For a semiconductor device, the simplest way to do so, is by identifying the node labeled by 0 with the reference potential. Then, the internal branches will be given by the pairs $(0, 1), \ldots, (0, K)$, and we can define the internal incidence matrix

$$\widehat{\boldsymbol{A}} = \begin{bmatrix} -1 & \cdots & -1 \\ 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}. \tag{2.22}$$

The corresponding voltage drops through the internal branches are given by $v_{D,k} = e_{D,k} - e_{D,0}$. If we introduce the vector $\boldsymbol{v}_D$ of the voltage drops, it is immediate to verify that

$$\boldsymbol{v}_D = \widehat{\boldsymbol{A}}^\top \boldsymbol{e}_D. \tag{2.23}$$

Moreover, introducing the vector

$$\boldsymbol{i}_D = \begin{bmatrix} j_{D,1} \\ \vdots \\ j_{D,K} \end{bmatrix}, \tag{2.24}$$

it is possible to verify that

$$\boldsymbol{j}_D = \widehat{\boldsymbol{A}} \boldsymbol{i}_D. \tag{2.25}$$

In fact, integrating (2.19) over Ω, we find

$$\sum_{k=0}^{K} j_{D,k} = 0, \tag{2.26}$$

so the current $j_{D,0}$ can be expressed as the opposite of the sum of the other currents. For this reason, we can use the vector $\boldsymbol{i}_D$ instead of $\boldsymbol{j}_D$.

Recalling (2.15), the variable $\boldsymbol{U}$ is coupled to the Poisson equation only through the electric field $\mathbf{E}$, and so are the components of the electric current $\boldsymbol{J}(\boldsymbol{U})$, and the components of $\boldsymbol{j}$, which appear in (2.21). Since the electric field is not affected by a time-dependent translation of the electric potential,

$$\phi_D \to \phi_D + e_{D,0}(t),$$

we can conclude that $\boldsymbol{j}$, and thus $\boldsymbol{i}_D$, depends on the voltage drops $\boldsymbol{v}_D$ rather than on the applied potentials $\boldsymbol{e}_D$.

2.3 Coupled problem

Now we consider an RLC electric network that contains n_D semiconductor devices, described as in the previous section. That is: each i-th device is modeled

by a domain Ω^i, of dimension $d = 1, 2$ or 3. This i-th device has $K_i + 1$ contacts and we assume that the boundary $\partial\Omega^i$ is made of a Dirichlet part Γ_D^i, union of $K_i + 1$ disjoint parts, which represent Ohmic contacts, and of a Neumann part Γ_N^i, which represents insulating boundaries (for $d > 1$),

$$\Gamma_D^i = \bigcup_{j=0}^{K_i} \Gamma_{D,j}^i, \quad \Gamma_N^i = \partial\Omega^i \setminus \Gamma_D^i, \quad i = 1, \dots, n_D.$$

In total, the devices contain n_{vD} terminals (Ohmic contacts) and n_{aD} internal branches, with

$$n_{vD} := n_D + \sum_{j=1}^{n_D} K_j, \qquad n_{aD} := \sum_{j=1}^{n_D} K_j.$$

Following the definition of the applied potential vectors, voltage drop vectors and current vectors of the previous section, we define:

$$\boldsymbol{e}_D^i = \begin{bmatrix} e_{D,0}^i \\ \vdots \\ e_{D,K_i}^i \end{bmatrix} \in \mathbb{R}^{K_i+1}, \qquad \boldsymbol{e}_D = \begin{bmatrix} \boldsymbol{e}_D^{n_D} \\ \vdots \\ \boldsymbol{e}_D^{n_D} \end{bmatrix} \in \mathbb{R}^{n_{vD}}, \qquad (2.27)$$

$$\boldsymbol{v}_D^i = \begin{bmatrix} v_{D,1}^i \\ \vdots \\ v_{D,K_i}^i \end{bmatrix} \in \mathbb{R}^{K_i}, \qquad \boldsymbol{v}_D = \begin{bmatrix} \boldsymbol{v}_D^1 \\ \vdots \\ \boldsymbol{v}_D^{n_D} \end{bmatrix} \in \mathbb{R}^{n_{aD}}, \qquad (2.28)$$

$$\boldsymbol{i}_D^i = \begin{bmatrix} j_{D,1}^i \\ \vdots \\ j_{D,K_i}^i \end{bmatrix} \in \mathbb{R}^{K_i}, \qquad \boldsymbol{i}_D = \begin{bmatrix} \boldsymbol{i}_D^1 \\ \vdots \\ \boldsymbol{i}_D^{n_D} \end{bmatrix} \in \mathbb{R}^{n_{aD}}. \qquad (2.29)$$

Moreover, we have internal incidence matrices

$$\widehat{\boldsymbol{A}}^i \in \mathbb{R}^{(K_i+1)\times K_i}, \quad \widehat{\boldsymbol{A}} = \mathrm{diag}\left(\widehat{\boldsymbol{A}}^1, \dots, \widehat{\boldsymbol{A}}^{n_D}\right) \in \mathbb{R}^{n_{vD}\times n_{aD}}$$

where $\widehat{\boldsymbol{A}}^i$ is defined as in (2.22).

Each contact must be connected to a node of the electric network. To relate the contacts of the devices to the nodes of the network, we need to introduce a contact-to-node selection matrix, $\boldsymbol{S}_D = (s_{D,ij}) \in \mathbb{R}^{n_v \times n_{vD}}$, defined by:

$$s_{D,ij} = \begin{cases} 1, & \text{if the contact } j \text{ is connected to the node } i, \\ 0, & \text{otherwise.} \end{cases} \qquad (2.30)$$

By using this matrix, we can define an incidence matrix for the internal branches of the devices:

$$\boldsymbol{A}_D = \boldsymbol{S}_D \widehat{\boldsymbol{A}}. \qquad (2.31)$$

Now we are ready to apply the formalism of MNA to derive equations for the network variables. We consider an incidence matrix $\boldsymbol{A}$ that comprises the semiconductor incidence matrix that is

$$\boldsymbol{A} = (\boldsymbol{A}_R, \boldsymbol{A}_C, \boldsymbol{A}_L, \boldsymbol{A}_I, \boldsymbol{A}_V, \boldsymbol{A}_D) \in \mathbb{R}^{n_v \times (n_R + n_C + n_L + n_I + n_V + n_{aD})} \equiv \mathbb{R}^{n_v \times n_a}.$$

To keep track of the different branches, we write

$$\boldsymbol{v} = \begin{bmatrix} \boldsymbol{v}_R \\ \boldsymbol{v}_C \\ \boldsymbol{v}_L \\ \boldsymbol{v}_I \\ \boldsymbol{v}_V \\ \boldsymbol{v}_D \end{bmatrix}, \quad \boldsymbol{i} = \begin{bmatrix} \boldsymbol{i}_R \\ \boldsymbol{i}_C \\ \boldsymbol{i}_L \\ \boldsymbol{i}_I \\ \boldsymbol{i}_V \\ \boldsymbol{i}_D \end{bmatrix}.$$

We notice that in this decomposition, the vectors $\boldsymbol{v}_D$ and $\boldsymbol{i}_D$ appears, which have been defined above. The presence of the voltage drop vector $\boldsymbol{v}_D$ is justified by the identification

$$\boldsymbol{e}_D = \boldsymbol{S}_D^\top \boldsymbol{e}. \tag{2.32}$$

In fact, recalling the definition of $\boldsymbol{v}_D$ in terms of $\boldsymbol{e}_D$, we have

$$\boldsymbol{v}_D = \widehat{\boldsymbol{A}}^\top \boldsymbol{e}_D = \widehat{\boldsymbol{A}}^\top \boldsymbol{S}_D^\top \boldsymbol{e} = \boldsymbol{A}_D^\top \boldsymbol{e}, \tag{2.33}$$

consistently with the MNA formalism. We will refer to (2.32) as network-to-device coupling relation, since it relates the network variables $\boldsymbol{e}$ to the device variables $\boldsymbol{e}_D$.

As for the presence of the current vector $\boldsymbol{i}_D$, we observe that

$$\boldsymbol{A}_D \boldsymbol{i}_D = \boldsymbol{S}_D \widehat{\boldsymbol{A}} \boldsymbol{i}_D = \boldsymbol{S}_D \boldsymbol{j}_D,$$

which is consistent with the interpretation of the term $\boldsymbol{A}_D \boldsymbol{i}_D$. The current vector $\boldsymbol{i}_D$ is defined by the device equations, through the relations

$$\boldsymbol{i}_D = \begin{bmatrix} \boldsymbol{i}_D^1 \\ \vdots \\ \boldsymbol{i}_D^{n_D} \end{bmatrix}, \quad \boldsymbol{i}_D^i = \begin{bmatrix} j_{D,1}^i \\ \vdots \\ j_{D,K_i}^i \end{bmatrix}, \quad j_{D,k}^i = - \int_{\Gamma_{D,k}^i} \boldsymbol{j}^i \cdot \boldsymbol{\nu} \, d\sigma(\mathbf{x}). \tag{2.34}$$

We will refer to (2.34) as device-to-network coupling relation, since it relates the device quantities $\boldsymbol{j}^i$ to the network variable $\boldsymbol{i}_D$.

With the above formalism, it is possible to derive, from the Kirchhoff current law, MNA equations formally equivalent to the ones obtained in the previous section, both the conventional form (2.6) and the charge-oriented form (2.9). The conventional form of the MNA equations is:

$$\boldsymbol{A}_C \frac{d\boldsymbol{q}_C(\boldsymbol{A}_C^\top)}{dt} + \boldsymbol{A}_R \boldsymbol{i}_R(\boldsymbol{A}_R^\top \boldsymbol{e}) + \boldsymbol{A}_L \boldsymbol{i}_L + \boldsymbol{A}_V \boldsymbol{i}_V + \boldsymbol{A}_I \boldsymbol{I} + \boldsymbol{A}_D \boldsymbol{i}_D = 0,$$

$$\frac{d\boldsymbol{\phi}_L(\boldsymbol{i}_L)}{dt} - \boldsymbol{A}_L^\top \boldsymbol{e} = 0, \tag{2.35}$$

$$\boldsymbol{A}_V^\top \boldsymbol{e} - \boldsymbol{V} = 0.$$

The equations (2.35) need to be coupled with the semiconductor equations, to express the constitutive relations for the currents $\boldsymbol{i}_D$. We will discuss more extensively this problem in a subsequent chapter.

For a linear RLC network, we can write system (2.35) in compact form, similarly to what done for system (2.6). By using the same notation as in (2.8), we can write (2.35) in the form

$$\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x}). \tag{2.36}$$

The term $\boldsymbol{\sigma}(\boldsymbol{x})$, that represent the currents through the devices, is given by

$$\boldsymbol{\sigma}(\boldsymbol{x}) = -\boldsymbol{\mathcal{A}}\boldsymbol{i}_D(\boldsymbol{\mathcal{A}}^\top \boldsymbol{x}) \tag{2.37}$$

with

$$\boldsymbol{\mathcal{A}} = \begin{bmatrix} \boldsymbol{A}_D \\ \boldsymbol{O} \\ \boldsymbol{O} \end{bmatrix}. \tag{2.38}$$

If there are no semiconductor devices, the matrix $\boldsymbol{\mathcal{A}}$ is identically zero, and (2.36) reduces to (2.8).

We note explicitly the identity

$$\boldsymbol{\mathcal{A}}^\top \boldsymbol{x} = \boldsymbol{A}_D^\top \boldsymbol{e} = \boldsymbol{v}_D. \tag{2.39}$$

For later use, we introduce also the matrix

$$\boldsymbol{\mathcal{S}} = \begin{bmatrix} \boldsymbol{S}_D \\ \boldsymbol{O} \\ \boldsymbol{O} \end{bmatrix}. \tag{2.40}$$

The matrices $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{S}}$ are related by

$$\boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{S}}\widehat{\boldsymbol{A}}. \tag{2.41}$$

We have also the identity

$$\boldsymbol{\mathcal{S}}^\top \boldsymbol{x} = \boldsymbol{S}_D^\top \boldsymbol{e} = \boldsymbol{e}_D. \tag{2.42}$$

2.4 Tractability index for linear systems

To study the index concept of the DAE equation (2.36), we adopt a perturbative approach, studying first the equations without the nonlinear term, that is the equation (2.8). Then we will write down additional conditions depending on the matrix $\boldsymbol{\mathcal{A}}$ that appears in the nonlinear term $\boldsymbol{\sigma}(\boldsymbol{x})$, such that the structure of the system is preserved.

We consider equation (2.8), that we rewrite here for convenience:

$$\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t). \tag{2.43}$$

To define the tractability index of (2.43) we need the notion of projector [51].

Definition 2.4.1 *(1) A matrix $\boldsymbol{Q} \in \mathbb{R}^{m \times m}$ is a projector onto $\boldsymbol{T}_1$ if and only if $\boldsymbol{Q}^2 = \boldsymbol{Q}$ and $\operatorname{im} \boldsymbol{Q} = \boldsymbol{T}_1$.*

(2) A matrix $\boldsymbol{Q} \in \mathbb{R}^{m \times m}$ is a projector along $\boldsymbol{T}_2$ if and only if $\boldsymbol{Q}^2 = \boldsymbol{Q}$ and $\ker \boldsymbol{Q} = \boldsymbol{T}_2$.

(3) For $\mathbb{R}^m = \boldsymbol{T}_1 \bigoplus \boldsymbol{T}_2$ a matrix $\boldsymbol{Q} \in \mathbb{R}^{m \times m}$ is the uniquely defined projector onto $\boldsymbol{T}_1$ along $\boldsymbol{T}_2$ if and only if $\boldsymbol{Q}^2 = \boldsymbol{Q}$, $\operatorname{im} \boldsymbol{Q} = \boldsymbol{T}_1$ and $\ker \boldsymbol{Q} = \boldsymbol{T}_2$.

We set

$$\boldsymbol{E}_0 = \boldsymbol{E}, \qquad \boldsymbol{A}_0 = \boldsymbol{A}.$$

We define $\boldsymbol{Q}_0$ projector onto $\ker \boldsymbol{E}_0$, that is

$$\boldsymbol{E}_0 \boldsymbol{Q}_0 = \boldsymbol{O} \qquad \boldsymbol{Q}_0^2 = \boldsymbol{Q}_0. \tag{2.44}$$

and $\boldsymbol{P}_0$ complementary projector of $\boldsymbol{Q}_0$, that is

$$\boldsymbol{P}_0 = \boldsymbol{I} - \boldsymbol{Q}_0. \tag{2.45}$$

Let $\boldsymbol{E}_i$, $\boldsymbol{A}_i$ $i = 1, \ldots, k$, and we consider $\boldsymbol{Q}_i$ projector onto the $\ker \boldsymbol{E}_i$, such that[1]

$$\boldsymbol{E}_i \boldsymbol{Q}_i \;=\; \boldsymbol{O}, \qquad \boldsymbol{Q}_i^2 = \boldsymbol{Q}_i, \tag{2.46}$$
$$\boldsymbol{Q}_i \boldsymbol{Q}_j \;=\; \boldsymbol{O}, \quad \forall j < i, \quad i = 1, \ldots, k. \tag{2.47}$$

We set

$$\boldsymbol{P}_i = \boldsymbol{I} - \boldsymbol{Q}_i. \tag{2.48}$$

We define iteratively the matrices $\boldsymbol{E}_k$, $\boldsymbol{A}_k$, $k \geq 0$, in the following way:

$$\boldsymbol{E}_0 = \boldsymbol{E}, \qquad \boldsymbol{A}_0 = \boldsymbol{A}, \tag{2.49}$$
$$\boldsymbol{E}_k \;=\; \boldsymbol{E}_{k-1} - \boldsymbol{A}_{k-1} \boldsymbol{Q}_{k-1}, \quad k \geq 1, \tag{2.50}$$
$$\boldsymbol{A}_k \;=\; \boldsymbol{A}_{k-1} \boldsymbol{P}_{k-1}, \qquad k \geq 1. \tag{2.51}$$

Lemma 2.4.1 *The sequences of matrices defined iteratively in (2.49)-(2.51) using the projectors defined in (2.46),(2.48), and having the property (2.47), are such that equation*

$$\boldsymbol{E}_k(\boldsymbol{P}_{k-1} \cdots \boldsymbol{P}_0 \dot{\boldsymbol{x}} + \boldsymbol{Q}_0 \boldsymbol{x} + \cdots + \boldsymbol{Q}_{k-1} \boldsymbol{x}) = \boldsymbol{A}_k \boldsymbol{x} + \boldsymbol{B} \boldsymbol{u}(t), \tag{2.52}$$

is equivalent to (2.43) for any $k \geq 1$.

Proof. We argument by induction on k.

For $k = 1$, equation (2.52) becomes

$$\boldsymbol{E}_1(\boldsymbol{P}_0 \dot{\boldsymbol{x}} + \boldsymbol{Q}_0 \boldsymbol{x}) = \boldsymbol{A}_1 \boldsymbol{x} + \boldsymbol{B} \boldsymbol{u}(t). \tag{2.53}$$

---

[1]It is always possible to choose a projector satisfying these additional conditions.

Using the identities

$$\begin{aligned}
\boldsymbol{E}_1\boldsymbol{P}_0 &= (\boldsymbol{E}_0 - \boldsymbol{A}_0\boldsymbol{Q}_0)\boldsymbol{P}_0 = \boldsymbol{E}_0\boldsymbol{P}_0 = \boldsymbol{E}_0, \\
\boldsymbol{E}_1\boldsymbol{Q}_0 &= (\boldsymbol{E}_0 - \boldsymbol{A}_0\boldsymbol{Q}_0)\boldsymbol{Q}_0 = -\boldsymbol{A}_0\boldsymbol{Q}_0,
\end{aligned}$$

and the definition of $\boldsymbol{A}_1$, equation (2.53) reduces to

$$\boldsymbol{E}_0\dot{\boldsymbol{x}} - \boldsymbol{A}_0\boldsymbol{Q}_0\boldsymbol{x} = \boldsymbol{A}_0\boldsymbol{P}_0 + \boldsymbol{B}\boldsymbol{u}(t), \tag{2.54}$$

which is equivalent to (2.43), since $\boldsymbol{Q}_0 + \boldsymbol{P}_0 = \mathbf{I}$.

Next, for $k > 1$, we assume that

$$\boldsymbol{E}_{k-1}(\boldsymbol{P}_{k-2}\cdots\boldsymbol{P}_0\dot{\boldsymbol{x}} + \boldsymbol{Q}_0\boldsymbol{x} + \cdots + \boldsymbol{Q}_{k-2}\boldsymbol{x}) = \boldsymbol{A}_{k-1}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) \tag{2.55}$$

is equivalent to (2.43), and prove the same equivalence for the subsequent integer. To do so, using $\boldsymbol{E}_{k-1}\boldsymbol{P}_{k-1} = \boldsymbol{E}_{k-1}$, we compute

$$\begin{aligned}
\boldsymbol{E}_k\boldsymbol{P}_{k-1}\cdots\boldsymbol{P}_0 &= (\boldsymbol{E}_{k-1} - \boldsymbol{A}_{k-1}\boldsymbol{Q}_{k-1})\boldsymbol{P}_{k-1}\cdots\boldsymbol{P}_0 \\
&= \boldsymbol{E}_{k-1}\boldsymbol{P}_{k-2}\cdots\boldsymbol{P}_0
\end{aligned}$$

and considering (2.46)-(2.47)

$$\begin{aligned}
\boldsymbol{E}_k\boldsymbol{Q}_j &= (\boldsymbol{E}_{k-1} - \boldsymbol{A}_{k-1}\boldsymbol{Q}_{k-1})\boldsymbol{Q}_j = \boldsymbol{E}_{k-1}\boldsymbol{Q}_j, \qquad j < k-1, \\
\boldsymbol{E}_k\boldsymbol{Q}_{k-1} &= (\boldsymbol{E}_{k-1} - \boldsymbol{A}_{k-1}\boldsymbol{Q}_{k-1})\boldsymbol{Q}_{k-1} = -\boldsymbol{A}_{k-1}\boldsymbol{Q}_{k-1}.
\end{aligned}$$

Then, using the definition of $\boldsymbol{A}_k$, equation (2.52) reduces to

$$\boldsymbol{E}_k(\boldsymbol{P}_{k-1}\cdots\boldsymbol{P}_0\dot{\boldsymbol{x}} + \boldsymbol{Q}_0\boldsymbol{x} + \cdots + \boldsymbol{Q}_{k-1}\boldsymbol{x}) - \boldsymbol{A}_{k-1}\boldsymbol{Q}_{k-1}\boldsymbol{x} = \boldsymbol{A}_{k-1}\boldsymbol{P}_{k-1}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t),$$

which is equivalent to (2.55), since $\boldsymbol{Q}_{k-1} + \boldsymbol{P}_{k-1} = \mathbf{I}$. Using the inductive hypothesis concludes the proof of the Lemma. ∎

The procedure to construct the sequences (2.50)-(2.51) can be continued indefinitely, but after a finite number of iterations, we will end up with a non singular matrix $\boldsymbol{E}_\mu$, with $\boldsymbol{E}_k$ singular for $k < \mu$. Then we will have $\boldsymbol{E}_{\mu+i} = \boldsymbol{E}_\mu$, $\boldsymbol{A}_{\mu+i} = \boldsymbol{A}_\mu$ for all $i \geq 0$. The index μ is called index of the system (2.8).

For $k = \mu$, the form (2.52) of (2.8) becomes:

$$\boldsymbol{E}_\mu(\boldsymbol{P}_{\mu-1}\cdots\boldsymbol{P}_0\dot{\boldsymbol{x}} + \boldsymbol{Q}_0\boldsymbol{x} + \cdots + \boldsymbol{Q}_{\mu-1}\boldsymbol{x}) = \boldsymbol{A}_\mu\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t), \tag{2.56}$$

since $\boldsymbol{E}_\mu$ is nonsingular, we have

$$\boldsymbol{P}_{\mu-1}\cdots\boldsymbol{P}_0\dot{\boldsymbol{x}} + \boldsymbol{Q}_0\boldsymbol{x} + \cdots + \boldsymbol{Q}_{\mu-1}\boldsymbol{x} = \boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t)). \tag{2.57}$$

The matrices appearing on the left-hand side of (2.57) are projectors and consitute a decomposition of the identity matrix,

$$\mathbf{I} = \boldsymbol{P}_{\mu-1}\cdots\boldsymbol{P}_0 + \boldsymbol{Q}_0 + \cdots + \boldsymbol{Q}_{\mu-1}, \tag{2.58}$$

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as we can see from the definition of the projectors $\boldsymbol{Q}_i$, and condition (2.47).

Using the theory of projectors it is possible to decouple the equation (2.8) following the strategy that we will introduce. By definition of projector, using (2.58), we can prove that the following multiplicative table holds:

	$\boldsymbol{P}_{\mu-1}\cdots\boldsymbol{P}_0$	$\boldsymbol{Q}_0$	$\boldsymbol{Q}_1$	$\ldots$	$\boldsymbol{Q}_{\mu-1}$
$\boldsymbol{P}_0\boldsymbol{P}_1\cdots\boldsymbol{P}_{\mu-1}$	$\boldsymbol{P}_0\boldsymbol{P}_1\cdots\boldsymbol{P}_{\mu-1}$	$\boldsymbol{O}$	$\boldsymbol{O}$	$\ldots$	$\boldsymbol{O}$
$\boldsymbol{Q}_0\boldsymbol{P}_1\cdots\boldsymbol{P}_{\mu-1}$	$-\boldsymbol{Q}_0\boldsymbol{Q}_1$	$\boldsymbol{Q}_0$	$\boldsymbol{O}$	$\ldots$	$\boldsymbol{O}$
$\boldsymbol{P}_0\boldsymbol{Q}_1\cdots\boldsymbol{P}_{\mu-1}$	$-\boldsymbol{P}_0\boldsymbol{Q}_1\boldsymbol{Q}_2$	$\boldsymbol{O}$	$\boldsymbol{P}_0\boldsymbol{Q}_1$	$\ldots$	$\boldsymbol{O}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\boldsymbol{P}_0\boldsymbol{P}_1\cdots\boldsymbol{Q}_{\mu-1}$	$\boldsymbol{O}$	$\boldsymbol{O}$	$\boldsymbol{O}$	$\ldots$	$\boldsymbol{P}_0\boldsymbol{P}_1\cdots\boldsymbol{Q}_{\mu-1}$

In fact
$$\boldsymbol{P}_i\cdots\boldsymbol{P}_{\mu-1}\boldsymbol{Q}_j = \begin{cases} \boldsymbol{Q}_j & \text{if} \quad j < i \le \mu-1, \\ \boldsymbol{O} & \text{if} \quad i \le j \le \mu-1, \end{cases} \tag{2.59}$$

$$\boldsymbol{P}_0\cdots\boldsymbol{P}_{i-2}\boldsymbol{P}_i\cdots\boldsymbol{P}_{\mu-1}\boldsymbol{Q}_j = \begin{cases} \boldsymbol{Q}_j & \text{if} \quad j < i \le \mu-1, \\ \boldsymbol{O} & \text{if} \quad i \le j \le \mu-1. \end{cases} \tag{2.60}$$

Then it is possible to write

$$\begin{cases} \boldsymbol{P}_0\cdots\boldsymbol{P}_{\mu-1}\dot{\boldsymbol{x}} = \boldsymbol{P}_0\cdots\boldsymbol{P}_{\mu-1}\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{x}+\boldsymbol{B}\boldsymbol{u}), \\ -\boldsymbol{Q}_0\boldsymbol{Q}_1\dot{\boldsymbol{x}}+\boldsymbol{Q}_0\boldsymbol{x} = \boldsymbol{Q}_0\boldsymbol{P}_1\cdots\boldsymbol{P}_{\mu-1}\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{x}+\boldsymbol{B}\boldsymbol{u}), \\ \vdots \\ -\boldsymbol{P}_0\cdots\boldsymbol{P}_{i-1}\boldsymbol{Q}_i\boldsymbol{Q}_{i+1}\dot{\boldsymbol{x}}+\boldsymbol{P}_0\cdots\boldsymbol{P}_{i-1}\boldsymbol{Q}_i\boldsymbol{x} \\ \quad = \boldsymbol{P}_0\cdots\boldsymbol{P}_{i-1}\boldsymbol{Q}_i\boldsymbol{P}_{i+1}\cdots\boldsymbol{P}\mu-1\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{x}+\boldsymbol{B}\boldsymbol{u}), \\ \vdots \\ -\boldsymbol{P}_0\boldsymbol{P}_1\cdots\boldsymbol{P}_{\mu-2}\boldsymbol{Q}_{\mu-1}\boldsymbol{x} = \boldsymbol{P}_0\cdots\boldsymbol{P}_{\mu-2}\boldsymbol{Q}_{\mu-1}\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{x}+\boldsymbol{B}\boldsymbol{u}), \end{cases} \tag{2.61}$$

with $0 < i < \mu-1$. Using the system (2.61) we decouple the equation (2.8) in the following $\mu+1$ equations:

$$\begin{cases} \dot{\boldsymbol{y}} = \boldsymbol{P}_0\cdots\boldsymbol{P}_{\mu-1}\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{y}+\boldsymbol{B}\boldsymbol{u}), \\ \boldsymbol{z}_0 = \boldsymbol{Q}_0\boldsymbol{Q}_1\dot{\boldsymbol{x}}+\boldsymbol{Q}_0\boldsymbol{P}_1\cdots\boldsymbol{P}_{\mu-1}\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{y}+\boldsymbol{B}\boldsymbol{u}), \\ \vdots \\ \boldsymbol{z}_i = \boldsymbol{P}_0\cdots\boldsymbol{P}_{i-1}\boldsymbol{Q}_i\boldsymbol{Q}_{i+1}\dot{\boldsymbol{x}}+\boldsymbol{P}_0\cdots\boldsymbol{P}_{i-1}\boldsymbol{Q}_i\boldsymbol{P}_{i+1}\cdots\boldsymbol{P}_{\mu-1}\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{x}+\boldsymbol{B}\boldsymbol{u}), \\ \vdots \\ \boldsymbol{z}_{\mu-1} = \boldsymbol{P}_0\cdots\boldsymbol{P}_{\mu-2}\boldsymbol{Q}_{\mu-1}\boldsymbol{E}_\mu^{-1}(\boldsymbol{A}_\mu\boldsymbol{y}+\boldsymbol{B}\boldsymbol{u}), \end{cases}$$
$$\tag{2.62}$$

with $0 < i < \mu-1$.

2.5 Tractability index for linear MNA equations

In the previous section we have defined the tractability index in an abstract way. In this section we specialize the tractability index to the equation of linear Modified Nodal Analysis. Due to the special structure of MNA equations, following

[51], we will be able to show that the index can be at most 2, giving topological conditions for index-1 and index-2 linear MNA equations.

We need some preliminary results.

Lemma 2.5.1 *If the capacitance and inductance matrices, $\boldsymbol{C}$ and $\boldsymbol{G}$ respectively, of all capacitances and inductance are positive definite then the following relations are satisfied*

$$\ker \boldsymbol{E} = \ker \boldsymbol{A}_C^\top \times \{\boldsymbol{0}\} \times \mathbb{R}^{n_V}, \qquad \text{and} \qquad \mathrm{im}\boldsymbol{E} = \mathrm{im}\boldsymbol{A}_C \times \mathbb{R}^{n_L} \times \{\boldsymbol{0}\}, \quad (2.63)$$

where n_L and n_V denote the number of inductance branches and voltage sources respectively.

To prove this lemma we need the following result.

Lemma 2.5.2 *If $\boldsymbol{M}$ is a positive definite $m \times m$-matrix and $\boldsymbol{N}$ is a rectangular matrix of dimension $k \times m$, then it holds that*

$$\ker \boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top = \ker \boldsymbol{N}^\top \quad and \quad \mathrm{im}\,\boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top = \mathrm{im}\,\boldsymbol{N}.$$

Proof. (Lemma 2.5.2) We consider the first assumption about the null space of the matrix $\boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top$. Obviously, $\ker \boldsymbol{N}^\top \subseteq \ker \boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top$. Now we assume that $\boldsymbol{z} \in \ker \boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top$, then we have

$$\boldsymbol{z}^\top \boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top = 0, \quad \text{equivalent to} \quad (\boldsymbol{N}^\top\boldsymbol{z})^\top \boldsymbol{M}(\boldsymbol{N}^\top\boldsymbol{z}) = 0, \qquad (2.64)$$

being $\boldsymbol{M}$ positive definite, we have $\boldsymbol{N}^\top\boldsymbol{z} = 0$. This implies the first statement of the thesis of the lemma. For the image space we know that $\mathrm{im}\,\boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top \subseteq \mathrm{im}\,\boldsymbol{N}$, and because of relation (2.64) we have

$$\mathrm{rank}\,\boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top = \mathrm{rank}\,\boldsymbol{N}^\top = \mathrm{rank}\,\boldsymbol{N},$$

that is $\dim(\mathrm{im}\,\boldsymbol{N}\boldsymbol{M}\boldsymbol{N}^\top) = \dim(\mathrm{im}\,\boldsymbol{N})$. This implies second statements of the thesis of the and complete the proof. ■

Proof. (Lemma 2.5.1) The matrices $\boldsymbol{C}$ and $\boldsymbol{L}$ are positive definite since all capacitances and inductances have positive definite capacitance and inductance matrices, respectively. Consider the nullspace of $\boldsymbol{E}$. Obviously

$$\ker \boldsymbol{E} = \ker(\boldsymbol{A}_C\boldsymbol{C}\boldsymbol{A}_C^\top) \times \ker \boldsymbol{L} \times \mathbb{R}^{n_V}.$$

Lemma 2.5.2 implies that $\ker \boldsymbol{A}_C\boldsymbol{C}\boldsymbol{A}_C^\top = \ker \boldsymbol{A}_C^\top$, and the regularity of $\boldsymbol{L}$ implies $\ker \boldsymbol{L} = \{\boldsymbol{0}\}$, hence the first part of the thesis.

For the image space of $\boldsymbol{E}$ we can write

$$\mathrm{im}\boldsymbol{E} = \mathrm{im}(\boldsymbol{A}_C\boldsymbol{C}\boldsymbol{A}_C^\top) \times \mathrm{im}\boldsymbol{L} \times \{\boldsymbol{0}\}. \qquad (2.65)$$

Applying again Lemma 2.5.2, we have $\mathrm{im}(\boldsymbol{A}_C\boldsymbol{C}\boldsymbol{A}_C^\top) = \mathrm{im}\boldsymbol{A}_C$, and since $\boldsymbol{L}$ is regular it follows $\mathrm{im}\boldsymbol{L} = \mathbb{R}^{n_L}$, and thus the thesis. ■

Definition 2.5.1 *An L-I cutset is a cutset consisting of inductances and/or current sources only.*

Definition 2.5.2 *A C-V loop is a loop consisting of capacitances voltage sources only.*

Theorem 2.5.3 *Let the capacitance, inductance and resistance matrices of all capacitances, inductances and resistances, respectively be positive definite. If the network contains neither L-I cutsets nor controlled C-V loops except for capacitance-only loops, then the MNA leads to an index-1 DAE.*

Proof. Let $\boldsymbol{E}_0 \equiv \boldsymbol{E}$, $\boldsymbol{A}_0 \equiv \boldsymbol{A}$, and we define a projector $\boldsymbol{Q}_0$ onto the nullspace of $\boldsymbol{E}_0$ in the following way

$$\boldsymbol{Q}_0 = \begin{bmatrix} \boldsymbol{Q}_C & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{I} \end{bmatrix}, \tag{2.66}$$

where $\boldsymbol{Q}_C$ is a constant projector onto the ker $\boldsymbol{A}_C^\top$. We will show that the equation (2.8) is index-1-tractable, that is the matrix

$$\boldsymbol{E}_1 = \boldsymbol{E}_0 - \boldsymbol{A}_0 \boldsymbol{Q}_0,$$

is non singular. The matrix $\boldsymbol{E}_1$ is given by

$$\boldsymbol{E} = \begin{bmatrix} \boldsymbol{A}_C \boldsymbol{C} \boldsymbol{A}_C^\top + \boldsymbol{A}_R \boldsymbol{G} \boldsymbol{A}_R^\top \boldsymbol{Q}_C & \mathbf{O} & \boldsymbol{A}_V \\ -\boldsymbol{A}_L^\top \boldsymbol{Q}_C & \boldsymbol{L} & \mathbf{O} \\ -\boldsymbol{A}_V^\top \boldsymbol{Q}_C & \mathbf{O} & \mathbf{O} \end{bmatrix}.$$

Let $\boldsymbol{x}^* = [\boldsymbol{e}^* \ \ \boldsymbol{i}_L^* \ \ \boldsymbol{i}_V^*]$ be a vector of the nullspace of $\boldsymbol{E}_1$ then $\boldsymbol{x}^*$ occurs the following system

$$\boldsymbol{A}_C \boldsymbol{C} \boldsymbol{A}_C^\top \boldsymbol{e}^* + \boldsymbol{A}_R \boldsymbol{G} \boldsymbol{A}_R^\top \boldsymbol{Q}_C \boldsymbol{e}^* + \boldsymbol{A}_V \boldsymbol{i}_V^* = 0, \tag{2.67}$$

$$-\boldsymbol{A}_L^\top \boldsymbol{Q}_C \boldsymbol{e}^* + \boldsymbol{L} \boldsymbol{i}_L^* = 0, \tag{2.68}$$

$$-\boldsymbol{A}_V^\top \boldsymbol{Q}_C \boldsymbol{e}^* = 0. \tag{2.69}$$

Multiplying (2.67) by $\boldsymbol{Q}_C^\top$ and whereas $\boldsymbol{Q}_C^\top \boldsymbol{A}_C = (\boldsymbol{A}_C^\top \boldsymbol{Q}_C)^\top = 0$, we obtain

$$\boldsymbol{Q}_C^\top \boldsymbol{A}_R \boldsymbol{G} \boldsymbol{A}_R^\top \boldsymbol{Q}_C \boldsymbol{e}^* + \boldsymbol{Q}_C^\top \boldsymbol{A}_V \boldsymbol{i}_V^* = 0. \tag{2.70}$$

Let $\boldsymbol{Q}_{VC}$ be a projector onto ker $\boldsymbol{A}_V^\top \boldsymbol{Q}_C$, then $\boldsymbol{Q}_{VC}^\top \boldsymbol{Q}_C^\top \boldsymbol{A}_V = 0$. Multiplying the previous equation by $\boldsymbol{Q}_{VC}^\top$ we have

$$\boldsymbol{Q}_{VC}^\top \boldsymbol{Q}_C^\top \boldsymbol{A}_R \boldsymbol{G} \boldsymbol{A}_R^\top \boldsymbol{Q}_C \boldsymbol{e}^* = 0. \tag{2.71}$$

We notice that we can write the equation (2.71) in the following way

$$\boldsymbol{Q}_{VC}^\top \boldsymbol{Q}_C^\top \boldsymbol{A}_R \boldsymbol{G} \boldsymbol{A}_R^\top \boldsymbol{Q}_C \boldsymbol{Q}_{VC} \boldsymbol{e}^* = (\boldsymbol{Q}_{VC}^\top \boldsymbol{Q}_C^\top \boldsymbol{A}_R) \boldsymbol{G} (\boldsymbol{Q}_{VC}^\top \boldsymbol{Q}_C^\top \boldsymbol{A}_R)^\top \boldsymbol{e}^* = 0, \tag{2.72}$$

since from (2.69), $\boldsymbol{e}^* \in \ker \boldsymbol{A}_V^\top \boldsymbol{Q}_C$, that is

$$\boldsymbol{e}^* = \boldsymbol{Q}_{VC} \boldsymbol{e}^*. \tag{2.73}$$

Applying the Lemma 2.5.1 and since $\boldsymbol{G}$ is positive definite, we can conclude

$$\boldsymbol{A}_R^\top \boldsymbol{Q}_C \boldsymbol{Q}_{VC} \boldsymbol{e}^* = 0, \tag{2.74}$$

and considering (2.73), we have

$$\boldsymbol{A}_R^\top \boldsymbol{Q}_C \boldsymbol{e}^* = 0. \tag{2.75}$$

Taking into account that $\boldsymbol{Q}_C$ is a projector onto the ker $\boldsymbol{A}_C^\top$, considering equations (2.69) and (2.75), we obtain

$$(\boldsymbol{A}_V \boldsymbol{A}_R \boldsymbol{A}_C)^\top \boldsymbol{Q}_C \boldsymbol{e}^* = 0. \tag{2.76}$$

The matrix $(\boldsymbol{A}_V \boldsymbol{A}_R \boldsymbol{A}_C)^\top$ has full rank since by assumption the network does not contain an L-I cutset, then we have

$$\boldsymbol{Q}_C \boldsymbol{e}^* = 0. \tag{2.77}$$

and by (2.70) we obtain $\boldsymbol{Q}_C^\top \boldsymbol{A}_V \boldsymbol{i}_V^* = 0$. Moreover we know that if the network does not contain a C-V loop except for capacitance-only loops, the matrix $\boldsymbol{A}_V^\top \boldsymbol{Q}_C$ has full rank than the nullspace of its transpose is only the zero vector, that is $\boldsymbol{i}_V^* = 0$. Hence by (2.67) and (2.77) we can deduce

$$\boldsymbol{A}_C \boldsymbol{C} \boldsymbol{A}_C^\top \boldsymbol{e}^* = 0,$$

and being $\boldsymbol{C}$ positive definite, since Lemma 2.5.1, we have $\boldsymbol{A}_C^\top \boldsymbol{e}^* = 0$, that implies $\boldsymbol{e}^* \in \text{im } \boldsymbol{Q}_C$. Regarding equation (2.77) we can conclude that

$$\boldsymbol{e}^* = \boldsymbol{Q}_C \boldsymbol{e}^* = 0,$$

then the matrix $\boldsymbol{E}_1$ is non singular and the network equation system is of index 1. ∎

For a system of index-2 it is possible to prove the following theorem.

Theorem 2.5.4 *If the network contains L-I cutsets or C-V loops except for capacitance-only loops, then the MNA leads to an index-2 DAE.*

For the proof of this Theorem we refer to [51].

2.6 Index concept for the nonlinear MNA equations

In this section we propose index conditions for the MNA system (2.36), that we rewrite here for convenience

$$\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x}). \tag{2.78}$$

This equation is nonlinear, due to the coupling term with the semiconductor device $\boldsymbol{\sigma}(\boldsymbol{x})$, definited in (2.37). Anyway, due to the special structure of $\boldsymbol{\sigma}(\boldsymbol{x})$, we can extend the method applies for decoupling linear DAEs [40]-[51], described above, to the specific case by assuming some additional structural conditions.

Following this idea we will assume that the system (2.78) has a given index when the coupling term $\boldsymbol{\sigma}$ is not present:

$$\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t). \tag{2.79}$$

Then we write additional conditions which ensure the same index for the coupled system (2.78).

In the next subsections we will treat in details the cases of index-1 and index-2 systems.

2.6.1 Index-1 conditions for nonlinear systems

Let us assume that the system (2.79) is index-1. In this case $\boldsymbol{E}_0$ is singular and we can define the projector $\boldsymbol{Q}_0$ and $\boldsymbol{P}_0$, as in (2.44), (2.45), respectively. We introduce the new matrices

$$\boldsymbol{E}_1 = \boldsymbol{E}_0 - \boldsymbol{A}_0\boldsymbol{Q}_0, \quad \boldsymbol{A}_1 = \boldsymbol{A}_0\boldsymbol{P}_0, \tag{2.80}$$

thus, using Lemma 2.4.1, equation (2.43) can be written in the form

$$\boldsymbol{E}_1\left(\boldsymbol{P}_0\dot{x} + \boldsymbol{Q}_0x\right) = \boldsymbol{A}_1\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}. \tag{2.81}$$

In conclusion, system (2.79) is index-1 if we have

$$\boldsymbol{E}_0 \text{ is singular}, \quad \boldsymbol{E}_1 \text{ is nonsingular}. \tag{2.82}$$

In this case the projected equations (2.62) become

$$\dot{\boldsymbol{y}} = \boldsymbol{P}_0\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t)\right], \tag{2.83}$$
$$\boldsymbol{z} = \boldsymbol{Q}_0\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t)\right], \tag{2.84}$$

with

$$\boldsymbol{y} = \boldsymbol{P}_0\boldsymbol{x}, \quad \boldsymbol{z} = \boldsymbol{Q}_0\boldsymbol{x}. \tag{2.85}$$

Notice that $\boldsymbol{y}$ and $\boldsymbol{z}$ are differential and algebraic components of $\boldsymbol{x}$. In this way we have obtained a decomposition of the original DAE in a differential equation and an algebraic equation [5, 52].

If we we apply the same decomposition procedure to equation (2.78), we get the following projected equations:

$$\dot{\boldsymbol{y}} = \boldsymbol{P}_0\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x})\right], \tag{2.86}$$
$$\boldsymbol{z} = \boldsymbol{Q}_0\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x})\right]. \tag{2.87}$$

As we can see, equations (2.86)-(2.87), are coupled through the nonlinear term. To decoupled these equations we assume that this term depend only on the differential part of $\boldsymbol{x}$, that is,

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{y}). \tag{2.88}$$

Then, we can still use the decomposition (2.85), derived without coupling, also in the nonlinear case. In fact we have then

$$\dot{\boldsymbol{y}} = \boldsymbol{P}_0 \boldsymbol{E}_1^{-1} [\boldsymbol{A}_1 \boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{y})], \tag{2.89}$$

$$\boldsymbol{z} = \boldsymbol{Q}_0 \boldsymbol{E}_1^{-1} [\boldsymbol{A}_1 \boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{y})]. \tag{2.90}$$

If we have that $\boldsymbol{\sigma}(\boldsymbol{y})$ is Lipschitz continuous, equation (2.89) can be solved for $\boldsymbol{y}$ and (2.90) gives $\boldsymbol{z}$ as function of $\boldsymbol{y}$.

Proposition 2.6.1 *If $\boldsymbol{A}^\top \boldsymbol{Q}_0 = \mathbf{O}$, then we have*

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{y}), \tag{2.91}$$

$$\boldsymbol{Q}_0 \boldsymbol{E}_1^{-1} \boldsymbol{\sigma} = \mathbf{0}, \tag{2.92}$$

where $\boldsymbol{E}_1$ is defined in (2.80).

Proof. First we prove (2.91). Considering the decomposition

$$\boldsymbol{x} = \boldsymbol{P}_0 \boldsymbol{x} + \boldsymbol{Q}_0 \boldsymbol{x} = \boldsymbol{y} + \boldsymbol{z},$$

we find immediately

$$\begin{aligned}
\boldsymbol{\sigma}(\boldsymbol{x}) &= -\boldsymbol{\mathcal{A}}\boldsymbol{i}_D(\boldsymbol{\mathcal{A}}^\top \boldsymbol{x}) \\
&= -\boldsymbol{\mathcal{A}}\boldsymbol{i}_D(\boldsymbol{\mathcal{A}}^\top (\boldsymbol{P}_0 \boldsymbol{x} + \boldsymbol{Q}_0 \boldsymbol{x})) \\
&= -\boldsymbol{\mathcal{A}}\boldsymbol{i}_D(\boldsymbol{\mathcal{A}}^\top \boldsymbol{P}_0 \boldsymbol{x}) \\
&= \boldsymbol{\sigma}(\boldsymbol{y}).
\end{aligned}$$

The second statement, (2.92), is immediate if we consider the identity

$$\boldsymbol{Q}_0 \boldsymbol{E}_1^{-1} \equiv \boldsymbol{Q}_0 (\boldsymbol{E}_0 + \boldsymbol{Q}_0^\top \boldsymbol{A}_0 \boldsymbol{Q}_0)^{-1} \boldsymbol{Q}_0^\top. \tag{2.93}$$

in fact we have

$$\begin{aligned}
\boldsymbol{Q}_0 \boldsymbol{E}_1^{-1} \boldsymbol{\sigma} &= -\boldsymbol{Q}_0 (\boldsymbol{E}_0 + \boldsymbol{Q}_0^\top \boldsymbol{A}_0 \boldsymbol{Q}_0)^{-1} \boldsymbol{Q}_0^\top \boldsymbol{\mathcal{A}}\boldsymbol{i}_D \\
&= \mathbf{0},
\end{aligned}$$

since $\boldsymbol{Q}_0^\top \boldsymbol{\mathcal{A}} = \mathbf{O}$. ∎

The previous proposition shows that system (2.78) has index-1 if conditions (2.82) hold together with the additional condition

$$\boldsymbol{\mathcal{A}}\boldsymbol{Q}_0^\top = \mathbf{O}. \tag{2.94}$$

Remark 2.6.1 *Condition (2.94) has a simple topological interpretation. In fact, using the explicit representation (2.66), we find*

$$\boldsymbol{\mathcal{A}}^{\top}\boldsymbol{Q}_0 = \begin{bmatrix} \boldsymbol{A}_D^{\top}\boldsymbol{Q}_C \\ \mathbf{O} \\ \mathbf{O} \end{bmatrix}.$$

Thus condition (2.94) is equivalent to

$$\boldsymbol{A}_D^{\top}\boldsymbol{Q}_C = \mathbf{O},$$

which holds, if any device terminal is connected to ground by a path of capacitors.

Equation (2.78), which is equivalent to (2.89)–(2.90), is considered for $t \in [t_0, t_1]$, and must be supplemented with consistent initial data

$$\boldsymbol{x}(t_0) = \boldsymbol{x}_0. \tag{2.95}$$

The consistency of the initial data is related to the decomposition (2.85) of $\boldsymbol{x}$. Namely we can supplemented the equation (2.78) with the initial data

$$\boldsymbol{y}(t_0) = \boldsymbol{y}_0 = \boldsymbol{P}_0\boldsymbol{x}_0. \tag{2.96}$$

Then, we can evaluate the component $\boldsymbol{z}(t_0)$ by using the equation (2.90).

2.6.2 Index-2 conditions for nonlinear systems

Let us assume that the system (2.79) is index-2. In this case we can follow the same procedure used in the previous subsection, defining $\boldsymbol{Q}_0$, $\boldsymbol{P}_0$ and $\boldsymbol{E}_1$, $\boldsymbol{A}_1$. At this point we have that $\boldsymbol{E}_1$ is also singular so we need to continue the procedure.

We consider a projector $\boldsymbol{Q}_1$ onto the null space of $\boldsymbol{E}_1$, satisfying the additional condition

$$\boldsymbol{Q}_1\boldsymbol{Q}_0 = \mathbf{O}, \tag{2.97}$$

and introduce its complementary projector, $\boldsymbol{P}_1 = \boldsymbol{I} - \boldsymbol{Q}_1$. Then we can define the new matrices

$$\boldsymbol{E}_2 = \boldsymbol{E}_1 - \boldsymbol{A}_1\boldsymbol{Q}_1, \quad \boldsymbol{A}_2 = \boldsymbol{A}_1\boldsymbol{P}_1. \tag{2.98}$$

Using 2.4.1, equation (2.79), equation (2.81) is equivalent to

$$\boldsymbol{E}_2\left(\boldsymbol{P}_1\boldsymbol{P}_0\dot{\boldsymbol{x}} + \boldsymbol{Q}_1\boldsymbol{x} + \boldsymbol{Q}_0\boldsymbol{x}\right) = \boldsymbol{A}_2\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t). \tag{2.99}$$

Since we assume that (2.79) is index-2, we have that the matrix $\boldsymbol{E}_2$ is nonsingular. In conclusion the index-2 conditions for (2.79) are:

$$\boldsymbol{E}_0, \boldsymbol{E}_1 \text{ are singular}, \tag{2.100}$$

$$\boldsymbol{E}_2 \quad \text{is nonsingular}. \tag{2.101}$$

Then using the multiplicative table

	P_1P_0	Q_0	Q_1
P_0P_1	P_0P_1	O	O
Q_0P_1	$-Q_0Q_1$	Q_0	O
P_0Q_1	O	O	P_0Q_1

we obtain the index-2 version of the projected equations (2.62):

$$\dot{y} = P_0P_1E_2^{-1}\left[A_2y + Bu(t)\right], \tag{2.102}$$
$$z = Q_0Q_1\dot{w} + Q_0P_1E_2^{-1}\left[A_2y + Bu(t)\right], \tag{2.103}$$
$$w = P_0Q_1E_2^{-1}\left[A_2y + Bu(t)\right], \tag{2.104}$$

with

$$y = P_0P_1x, \qquad z = Q_0x, \qquad w = P_0Q_1x. \tag{2.105}$$

Notice that P_0P_1 is a projector $((P_0P_1)^2 = P_0P_1)$ such that $A_2x = A_2y$.

In this way we have obtained a decomposition of the original DAE in a differential equation and two algebraic equations. We can solve the equation (2.102) for y, then we compute w by (2.104), and finally z by (2.103). We see that in the solution appears the time derivative of the source term $u(t)$.

Now, we include also the nonlinear term $\boldsymbol{\sigma}(x)$. We can still define the projectors Q_0, Q_1, and write the system (2.78) in the form

$$\dot{y} = P_0P_1E_2^{-1}\left[A_2y + Bu(t) + \boldsymbol{\sigma}(x)\right], \tag{2.106}$$
$$z = Q_0Q_1\dot{w} + Q_0P_1E_2^{-1}\left[A_2y + Bu(t) + \boldsymbol{\sigma}(x)\right], \tag{2.107}$$
$$w = P_0Q_1E_2^{-1}\left[A_2y + Bu(t) + \boldsymbol{\sigma}(x)\right]. \tag{2.108}$$

We would like to identify additional conditions so that the above nonlinear system still exhibits an index-2 structure by means of the above decomposition. We will propose two different strategy to do so.

1. Recalling the structure of $\boldsymbol{\sigma}(x)$, we have

$$\boldsymbol{\sigma}(x) = -\boldsymbol{A}i_D(\boldsymbol{A}^\top x) = -\boldsymbol{A}i_D(\boldsymbol{A}^\top(P_0P_1x + Q_0x + P_0Q_1x)).$$

If we assume the additional conditions

$$\boldsymbol{A}^\top P_0Q_1 = O, \qquad \boldsymbol{A}^\top Q_0 = O, \tag{2.109}$$

we have

$$\boldsymbol{\sigma}(x) = -\boldsymbol{A}i_D(\boldsymbol{A}^\top P_0P_1x) = \boldsymbol{\sigma}(y),$$

and the resulting equations have the same structure as in (2.102)-(2.103):

$$\dot{y} = P_0P_1E_2^{-1}\left[A_2y + Bu(t) + \boldsymbol{\sigma}(y)\right], \tag{2.110}$$
$$z = Q_0Q_1\dot{w} + Q_0P_1E_2^{-1}\left[A_2y + Bu(t) + \boldsymbol{\sigma}(y)\right]. \tag{2.111}$$
$$w = P_0Q_1E_2^{-1}\left[A_2y + Bu(t) + \boldsymbol{\sigma}(y)\right], \tag{2.112}$$

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2. A second strategy is to allow the function $\boldsymbol{\sigma}$ to depend on $\boldsymbol{y}$ and $\boldsymbol{w}$ but not on $\boldsymbol{z}$. This can be done by assuming the condition

$$\mathcal{A}^\top \boldsymbol{Q}_0 = \boldsymbol{O}. \tag{2.113}$$

Moreover, we assume that it is possible to choose $\boldsymbol{Q}_1$ so that the following additional conditions are satisfied:

$$\boldsymbol{P}_0 \boldsymbol{Q}_1 \boldsymbol{E}_2^{-1} \mathcal{A} = \boldsymbol{O}, \quad \boldsymbol{Q}_0 \boldsymbol{E}_2^{-1} \mathcal{A} = \boldsymbol{O}. \tag{2.114}$$

This amounts to imposing that the components $\boldsymbol{w}$ and $\boldsymbol{z}$ of the solution do not depend on the nonlinear term $\boldsymbol{\sigma}(\boldsymbol{x}) = -\mathcal{A} i_D(\mathcal{A}^\top \boldsymbol{x})$. Then we obtain:

$$
\begin{aligned}
\dot{\boldsymbol{y}} &= \boldsymbol{P}_0 \boldsymbol{P}_1 \boldsymbol{E}_2^{-1} \left[\boldsymbol{A}_2 \boldsymbol{y} + \boldsymbol{B} \boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{y} + \boldsymbol{w}) \right], & (2.115) \\
\boldsymbol{z} &= \boldsymbol{Q}_0 \boldsymbol{Q}_1 \dot{\boldsymbol{w}} + \boldsymbol{Q}_0 \boldsymbol{P}_1 \boldsymbol{E}_2^{-1} \left[\boldsymbol{A}_2 \boldsymbol{y} + \boldsymbol{B} \boldsymbol{u}(t) \right], & (2.116) \\
\boldsymbol{w} &= \boldsymbol{P}_0 \boldsymbol{Q}_1 \boldsymbol{E}_2^{-1} \left[\boldsymbol{A}_2 \boldsymbol{y} + \boldsymbol{B} \boldsymbol{u}(t) \right]. & (2.117)
\end{aligned}
$$

In this decomposition, we see that the system is still index-2, since we can solve $\boldsymbol{w}$ in terms of $\boldsymbol{y}$ by using (2.117), and then solving (2.115) for $\boldsymbol{y}$. Finally, $\boldsymbol{z}$ can be reconstructed by (2.116).

The second strategy is slightly more general and will be considered in the following. Therefore we will consider index-2 system which satisfy conditions (2.100), (2.101), together with the additional conditions (2.114).

Remark 2.6.2 *The additional conditions* (2.113), (2.114) *define a non empty class of index-2 differential-algebraic systems. We can show this by exhibiting an explicit example. We consider the circuit shown in Fig. 2.1.*
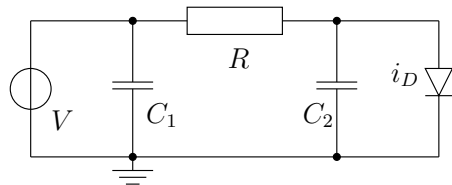

Fig. 2.1 Simple circuit schematic.

The respective incidence matrices read:

$$\boldsymbol{A}_C = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \boldsymbol{A}_R = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad \boldsymbol{A}_V = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \boldsymbol{A}_D = \begin{bmatrix} 0 \\ -1 \end{bmatrix}.$$

The MNA equations for this circuit are:

$$
\begin{aligned}
C_1 \dot{e}_1 &= 1/R(e_2 - e_1) - i_V, \\
C_2 \dot{e}_2 &= -1/R(e_2 - e_1) - i_D, & (2.118) \\
0 &= V - e_1.
\end{aligned}
$$

For $C_1, C_2, R \neq 0$, $\boldsymbol{i}_D = \boldsymbol{i}_D(e_2)$, $\boldsymbol{u}(t) = \boldsymbol{V}(t)$ and

$$\boldsymbol{x} = \begin{bmatrix} e_1 \\ e_2 \\ i_V \end{bmatrix},$$

we can recast the MNA equations (2.118) in the above matrix form (2.78) using

$$\boldsymbol{E}_0 = \begin{bmatrix} C_1 & 0 & 0 \\ 0 & C_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{A}_0 = \begin{bmatrix} -1/R & 1/R & -1 \\ 1/R & -1/R & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

$$\boldsymbol{B} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \boldsymbol{\mathcal{A}} = \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix}.$$

For this example we find for the matrix chain:

$$\boldsymbol{Q}_0 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \boldsymbol{P}_0 = \mathbf{I} - \boldsymbol{Q}_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{2.119}$$

consequently

$$\boldsymbol{E}_1 = \begin{bmatrix} C_1 & 0 & 1 \\ 0 & C_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{A}_1 = \begin{bmatrix} -1/R & -1/R & 0 \\ 1/R & -1/R & 0 \\ -1 & 0 & 0 \end{bmatrix}. \tag{2.120}$$

From this we deduce the general form of the projector $\boldsymbol{Q}_1$ (characterized by $\boldsymbol{Q}_1^2 = \boldsymbol{Q}_1$, $\boldsymbol{E}_1 \boldsymbol{Q}_1 = O$) which satisfies condition (2.97), with free parameter $\alpha \in \mathbb{R}$, and consequentely the matrix $\boldsymbol{E}_2$:

$$\boldsymbol{Q}_1 = \begin{bmatrix} 1 & \alpha & 0 \\ 0 & 0 & 0 \\ -C_1 & -\alpha C_1 & 0 \end{bmatrix}, \quad \boldsymbol{E}_2 = \boldsymbol{E}_1 - \boldsymbol{A}_1 \boldsymbol{Q}_1 = \begin{bmatrix} C_1 + 1/R & \alpha/R & 1 \\ -1/R & C_2 - \alpha/R & 0 \\ 1 & \alpha & 0 \end{bmatrix}.$$

If we check the additional conditions (2.113) and (2.114) we will see that

$$\boldsymbol{\mathcal{A}}^\top \boldsymbol{Q}_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{P}_0 \boldsymbol{Q}_1 \boldsymbol{E}_2^{-1} \boldsymbol{\mathcal{A}} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{Q}_0 \boldsymbol{E}_2^{-1} \boldsymbol{\mathcal{A}} = \begin{bmatrix} 0 \\ 0 \\ -\frac{\alpha C_1}{C_2} \end{bmatrix}. \tag{2.121}$$

Choosing $\alpha = 0$, which is allowed, the additional conditions are satisfied.

Equation (2.78), which is equivalent to (2.115)–(2.116), is considered for $t \in [t_0, t_1]$, and must be supplemented with consistent initial data

$$\boldsymbol{x}(t_0) = \boldsymbol{x}_0. \tag{2.122}$$

The consistency of the initial data is related to the decomposition (2.105) of $\boldsymbol{x}$. Namely we can supplemented the equation (2.78) with the initial data

$$\boldsymbol{y}(t_0) = \boldsymbol{y}_0 = \boldsymbol{P}_0\boldsymbol{P}_1\boldsymbol{x}_0. \tag{2.123}$$

Then, we can evaluate the components $\boldsymbol{w}(t_0)$, $\boldsymbol{z}(t_0)$ by using the equations (2.115)-(2.116).

Chapter 3

Basic semiconductor equations

3.1 Outline of semiconductor physics

In literature, the term *semiconductor* has been introduced to denote solid materials with a much higher conductivity than insulators, but a much lower conductivity than metals measured at room temperature. Usually, a semiconductor device can be considered as a device which needs an input and produces an output. The device is connected to the outside world by contacts at which a voltage (potential difference) is applied. Depending on the device structure, the main transport phenomena of the electrons may be very different, for instance, due to drift, diffusion, convection, or quantum mechanical effects. For this reason, we have to devise different mathematical models which are able to describe the main physical phenomena for a particular situation or for a particular device. This leads to a hierarchy of semiconductor models. We can divide semiconductor models in three classes: *quantum models*, *kinetic models* and *fluiddynamical (macroscopic) models*. However we can say that it is possible to derive all other descriptions for the evolution of the electron and in particular the fluiddynamical and kinetic models, from the Schrödinger equation. For this reason we introduce only this quantum view-point.

We consider the vector quantity $\mathbf{p} = m\boldsymbol{v}$ called momentum. The space of all states $(\mathbf{x}, \mathbf{p}) \in \mathbb{R}^3 \times \mathbb{R}^3$ is the phase space. A path $\mathbf{x} = \mathbf{x}(t)$ in the phisical space identifies a curve $(\mathbf{x}, \mathbf{p}) = (\mathbf{x}(t), m\dot{\mathbf{x}}(t))$ in the phase space.

As is well known to a path in phisical space is associated a total energy of the particle. Also in the phase space to each curve in this space is related a total energy. To explain this report we introduce the Hamiltonian function

$$\mathcal{H}(\mathbf{x}, \mathbf{p}) := \frac{|\mathbf{p}|^2}{2m} - q\phi(\mathbf{x}). \tag{3.1}$$

where m is the mass of the particle and ϕ is the electric potential. Using the Hamiltonian function we can write the equations of the motion in the form

$$\dot{\mathbf{x}} = \nabla_{\mathbf{p}}\mathcal{H}, \qquad \dot{\mathbf{p}} = -\nabla_{\mathbf{x}}\mathcal{H}. \tag{3.2}$$

We have to add also the relation that between the Hamiltonian function and the energy

$$\mathcal{H}(\mathbf{x}, \mathbf{p}) = \mathcal{E}. \tag{3.3}$$

that is to every path $\mathbf{x}(t)$ is related an energy $\mathcal{E}(t)$, given by

$$\mathcal{E}(t) = \mathcal{H}\left(\mathbf{x}(t), \mathbf{p}(t)\right). \tag{3.4}$$

In quantum mechanics every elementary particle is associated to a material wave. Related to this wave there are the concepts of wave vector $\mathbf{k}$ and pulsation ω. The wave vector indicates the direction of propagation of the wave front. The carrier wave and pulse wave associated with a material particle are related to the impulse and energy of the particle through the law of de Broglie,

$$\mathbf{p} = \hbar\mathbf{k}, \tag{3.5}$$

and the Planck-Einstein relation

$$\mathcal{E} = \hbar\omega, \tag{3.6}$$

where $\hbar = h/2\pi$ is the reduced Planck constant.

In general the dynamics of an elementary particle is described by a wave complex function $\psi(\mathbf{x}, t)$, related to the Probability that the particle occupies the position $\mathbf{x}$ at time t. We consider now the most simple wave function, that is a plane wave with wave vactor $\mathbf{k}$ and pulsation ω

$$\psi(\mathbf{x}, t) = e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}, \tag{3.7}$$

where i is such that $i^2 = -1$. This wave function is related to a free electron under the action of a constant potential ϕ_0, that in classical mechanics is described by the Hamiltonian function.

$$\mathcal{H}(\mathbf{x}, \mathbf{p}) = \frac{|\mathbf{p}|^2}{2m} - q\phi_0.$$

Then, from equation (3.7),

$$\frac{\partial \psi}{\partial t} = -i\omega\psi, \qquad \Delta_{\mathbf{x}}\psi = -|\mathbf{k}|^2\psi.$$

Hence, using the law of de Broglie and the Planck-Einstein relation, we can write

$$i\hbar\frac{\partial \psi}{\partial t} = \mathcal{E}\psi, \tag{3.8}$$

$$-\frac{\hbar^2}{2m}\Delta_{\mathbf{x}}\psi - q\phi_0\psi = \mathcal{H}(\mathbf{x}, \mathbf{p})\psi. \tag{3.9}$$

Introducing the following Hemiltonian

$$H := -\frac{\hbar^2}{2m}\Delta_{\mathbf{x}} - q\phi_0,$$

equation (3.9) can be written as

$$H\psi = \mathcal{H}(\mathbf{x}, \mathbf{p})\psi. \tag{3.10}$$

we can find the expression for the operator H form the Hemiltonian function $\mathcal{H}$, usng the substitution

$$\mathbf{x} \rightarrow \mathbf{x}, \qquad \mathbf{p} \rightarrow -i\hbar\nabla_{\mathbf{x}}. \tag{3.11}$$

Remembering that there is a correspondence between a trajectory total energy of the physical space of the particle. From equation (3.4), using equations (3.8) and (3.10), we have

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi. \tag{3.12}$$

This equation, obtained in this case, is called Schrödinger equation, its validity is postulated in the description of the behavior of matter at the atomic scale or lower. Finally we have to add the boundary conditions for the wave function

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}). \tag{3.13}$$

Considering a single electron of mass m_e and elementary charge q moving in a vacuum under the action of an electric field $\mathbf{E} = \mathbf{E}(\mathbf{x}, t)$, its motion is governed by the single-particle *Schrödinger equation*, as we have said,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_e}\Delta\psi - q\phi(\mathbf{x}, t)\psi, \quad \mathbf{x} \in \mathbb{R}^d, \, d = 1, 2, 3, \, t > 0, \tag{3.14}$$

with initial condition

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d.$$

A more precise definition of semiconductor is that a semiconductor is a solid with an energy gap larger than zero and smaller than about $4eV$. Metals have no energy gap, whereas this gap is usually larger than $4eV$ in insulators. Therefore it is necessary to introduce the concept of *energy gap* $\mathcal{E}_g$, and for this aim we have to explain the crystal structure of solids. A solid is made of an infinite three-dimensional array of atoms arranged according to a lattice. A lattice L is a countable subset of $\mathbb{R}^d$, generated by d independent vectors $a_1, \ldots a_d$. We can write

$$L = \left\{ \mathbf{a} \in \mathbb{R}^d \mid \mathbf{a} = n_1 a_1 + \cdots + n_d a_d, \, n_1, \ldots, n_d \in \mathbb{Z} \right\}.$$

where $a_1, \ldots, a_d$ are the basis vectors of L. The choice of the basis for the lattice can be done in infinite number of ways by d independent vectors just choosing a d-tuple $a'_1, \ldots a'_d$ with

$$a'_i = \sum_{j=1}^{d} m_{ij} a_j, \quad m_{ij} \in \mathbb{Z}, \quad \det(m_{ij}) = 1.$$

Usually chooses a basis consisting of vectors of minimum length.

We define the *primitive cell* of L in $\mathbb{R}^d$ a subset D in $\mathbb{R}^d$ that contains a unique element of L (usually the origin) and that its translated form a partition of $\mathbb{R}^d$. There are infinite choices of primitive cells of the same lattice. Among them, the one defined by the basis vectors of minimal length is called the *unit cell*. Explicitly, the unit cell of a lattice is the set

$$D = \{\mathbf{x} = \alpha_1 a_1 + \cdots + \alpha_d a_d, \text{ with } \alpha_1, \ldots, \alpha_d \in [0, 1[\}.$$

We say that the *Wigner-Seitz primitive cell* is the region D_{WS} around the origin, whose points are closest to the origin than to any other lattice point, that is

$$D_{WS} = \{\mathbf{x} \in \mathbb{R}^d : |\mathbf{x}| \le |\mathbf{x} + \mathbf{a}|, \forall \mathbf{a} \in L\}.$$

In the following, we consider for simplicity $d = 3$. Each lattice is translation invariant if and only if it is traslated with respect one of its element. It is possible to see that there exists a finite number of traslation lattice called *Bravais lattice*. To any lattice L, generated by the vector $\{a_1, a_2, a_3\}$, we can associate a *reciprocal lattice* L^*,

$$L^* = \{n_1 a_1^* + n_2 a_2^* + n_3 a_3^*, \ n_1, n_2, n_3 \in \mathbb{Z}\}. \tag{3.15}$$

where the basis vectors $\{a_1^*, a_2^*, a_3^*\}$, satisfy the relation

$$a_i^* \cdot a_j = 2\pi \delta_{ij}, \tag{3.16}$$

where δ_{ij} is the Kronecker delta, equal to 1 if $i = j$, 0 otherwise. Explicitly

$$a_i^* = 2\pi \frac{a_j \wedge a_k}{a_1 \cdot a_2 \wedge a_3}, \quad (i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2).$$

From (3.16) we can derive

$$e^{i\mathbf{a}^* \cdot \mathbf{a}} = 1, \quad \forall \mathbf{a} \in L, \mathbf{a}^* \in L^*.$$

The reciprocal lattice of any Bravais lattice is still a Bravais lattice. If we indicate with $|D_L|$ the volume of the primitive cell D_L of L it is possible to see that the volume of the primitive cell D_{L^*} of the reciprocal lattice L^* is given by

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

The Wigner-Seitz primitive cell of the reciprocal lattice

$$\mathscr{B} := \{\mathbf{k} \in \mathbb{R}^3 : |\mathbf{k}| \le |\mathbf{k} + \mathbf{a}^*|, \forall \mathbf{a}^* \in L^*\}$$

is called (first) *Brillouin zone*, that is the Brillouin zone $\mathscr{B}$ 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^*.

If the atoms of the solid are arranged in a lattice L, the potential, ϕ_L, generated by them, will be a periodic with the same lattice periodicity, that is will be invariant with respect to a translation for each element of L:

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

As we have seen the energy states that can be filled by an electron are determined by the solution of the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m_e}\Delta\psi - q\phi_L(\mathbf{x}, t)\psi = \mathcal{E}\psi, \quad \mathbf{x} \in \mathbb{R}^3, \tag{3.17}$$

where $\mathcal{E}$ is the total energy. The equation (3.17) is an eigenvalue problem and we have to find eigenfunction-eigenvalue pairs $(\psi, \mathcal{E})$.

Now we can apply the *Bloch Theorem* that says that the Schrödinger equation is equivalent to the system of Schrödinger equations

$$-\frac{\hbar^2}{2m_e}\Delta\psi_\mathbf{k} - q\phi_L(\mathbf{x}, t)\psi_\mathbf{k} = \mathcal{E}(\mathbf{k})\psi_\mathbf{k}, \quad \mathbf{x} \in D_L, \tag{3.18}$$

indexed by $\mathbf{k} \in \mathscr{B}$, with pseudo-periodic boundary conditions

$$\psi_\mathbf{k}(\mathbf{x} + \mathbf{y}) = \psi_\mathbf{k}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{y}}, \quad \mathbf{x}, \mathbf{x} + \mathbf{y} \in \partial D_L, \tag{3.19}$$

where D_L is a primitive cell of L. It is possible to prove that the wave function $\psi_\mathbf{k}$ and the energy state $\mathcal{E}_\mathbf{k}$, seen as functions of $\mathbf{k}$, are periodic with respect to the reciprocal lattice L^* that is

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

The eigenvalue problem (3.18)-(3.19), for any $\mathbf{k} \in \mathscr{B}$ has 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

$$\psi_\mathbf{k}(\mathbf{x}) = \sum_{\ell \in L} e^{-i\mathbf{k}\cdot\boldsymbol{\ell}}\psi(\mathbf{x} + \boldsymbol{\ell}).$$

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

$$\psi_\mathbf{k}^m = u_\mathbf{k}^m(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{3.20}$$

where

$$u_\mathbf{k}^m(\mathbf{x}) = \sum_{\boldsymbol{\ell} \in L} e^{-i\mathbf{k}\cdot(\mathbf{x}+\boldsymbol{\ell})}\psi(\mathbf{x} + \boldsymbol{\ell})$$

is periodic in L. It is possible to see the functions $\psi_\mathbf{k}^m$ as the plane waves $e^{i\mathbf{k}\cdot\mathbf{x}}$ which are modulated by a periodic function $u_\mathbf{k}^m$ called *Bloch waves*. The function $\mathbf{k} \mapsto \mathcal{E}_m(\mathbf{k})$ is called the *dispersion relation* or the m-th *energy band*. It shows how the energy of the n-th band depends on the wave vector $\mathbf{k}$. The union of the ranges of $\mathcal{E}_m$ over $m \in \mathbb{N}$ is not necessarily the whole set $\mathbb{R}$, i.e., there may exist

energies $\mathcal{E}^*$ for which there is no $m \in \mathbb{N}$ and no $\mathbf{k} \in \mathscr{B}$ such that $\mathcal{E}_m(\mathbf{k}) = \mathcal{E}^*$. The connected components of the set of energies with this non-existence property are called *energy gaps*. The energy gap separates two energy bands. The nearest energy band below the energy gap is called *valence band*; the nearest energy band above the energy gap is termed *conduction band*. Now we are able to state the definition of a semiconductor: It is a solid with an energy gap whose value is positive and smaller than about $4eV$. In other words we can say that at absolute zero the electrons occupy the states available to more low energy in the energy bands of the crystal. There may be two very different situations. Some bands can be completely filled, while all others remain completely empty. In this case it is called the energy gap $\mathcal{E}_g$, the maximum difference between the highest (in energy) filled band and the minimum of the most low empty band. These bands are called respectively valence band $\mathcal{E}_v(\mathbf{k})$ and conduction band $\mathcal{E}_c(\mathbf{k})$. The energy is given by

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

Depending on how big is the energy gap the crystals are insulators or semiconductors. Typically the value of $\mathcal{E}_g$ is from 1 to several eV in the case of insulators, for semiconductors is between 0.1 and 0.5 eV. Examples of semiconductors are silicon (Si), germanium (Ge) and gallium arsenide (GaAs). The second situation that can occur is one in which at absolute zero some bands are only partially filled, in this case, we say that the crystal is a conductor.

It is possible to show that the *group velocity* of the wave packet in the n-th band is given by

$$\boldsymbol{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}_n \tag{3.21}$$

Differentiantig (3.21) we have

$$\frac{\partial \boldsymbol{v}_n}{\partial t} = \frac{1}{\hbar}\frac{\mathrm{d}^2\mathcal{E}_n}{\mathrm{d}\mathbf{k}^2}\frac{\partial \mathbf{k}}{\partial t} = \frac{1}{\hbar^2}\frac{\mathrm{d}^2\mathcal{E}_n}{\mathrm{d}\mathbf{k}^2}F,$$

where F indicates the force. Using the Newton's law

$$\mathbf{F} = \frac{\partial \mathbf{p}}{\partial t} = m^*\frac{\partial \boldsymbol{v}_n}{\partial t},$$

in wich m^* is the effective mass and p is the momentum, we obtain

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

We consider this equation as a definition of the *effective mass m^**. The second derivative of $\mathcal{E}_n$ with respect to $\mathbf{k}$ is a 3×3 matrix, so the symbol $(m^*)^1$ is also a matrix. If we evaluate the Hessian of $\mathcal{E}_n$ near a local minimum, i.e. $\nabla_{\mathbf{k}}\mathcal{E}_n(\mathbf{k}_0) = 0$, then $\mathrm{d}^2 E_n(\mathbf{k}_0)/\mathrm{d}\mathbf{k}^2$ is a symmetric positive matrix which can be diagonalized and the diagonal elements are positive:

$$\begin{bmatrix} 1/m_x^* & 0 & 0 \\ 0 & 1/m_y^* & 0 \\ 0 & 0 & 1/m_z^* \end{bmatrix} = \frac{1}{\hbar^2}\frac{\mathrm{d}^2\mathcal{E}_n}{\mathrm{d}\mathbf{k}^2}(\mathbf{k}_0).$$

Assume that the energy values are shifted in such a way that the energy vanishes at the local minimum $\mathbf{k}_0$. For wave vectors $\mathbf{k}$ "close" to $\mathbf{k}_0$, we have from Taylor's formula and

$$
\begin{aligned}
\mathcal{E}_n(\mathbf{k}) &= \mathcal{E}_n(\mathbf{k}_0) + \nabla_{\mathbf{k}}\mathcal{E}_n(\mathbf{k}_0) \cdot \mathbf{k} + \frac{1}{2}\mathbf{k}^\top \frac{\mathrm{d}^2 \mathcal{E}_n}{\mathrm{d}\mathbf{k}^2}(k_0)\mathbf{k} + O(|\mathbf{k} - \mathbf{k}_0|^3) \\
&= \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x^*} + \frac{k_y^2}{m_y^*} + \frac{k_z^2}{m_z^*}\right) + O(|\mathbf{k} - \mathbf{k}_0|^3),
\end{aligned}
$$

where $\mathbf{k} = (k_x, k_y, k_z)^\top$. If the effective masses are equal in all directions, i.e. $m^* = m_x^* = m_y^* = m_z^*$, we can write, neglecting higher-order terms,

$$
\mathcal{E}_n(k) = \frac{\hbar^2}{2m^*}|\mathbf{k}|^2, \tag{3.22}
$$

for wave vectors k "close" to a local band minimum. In this situation, m^* is called the *isotropic effective mass*. We conclude that the energy of an electron near a band minimum equals the energy of a free electron in vacuum where the (rest) mass of the electron is replaced by the effective mass. The effects of the crystal potential are represented by the effective mass. The expression (3.22) is referred to as the parabolic band approximation and usually, the range of wave vectors k is extended to the whole space. In order to account for non-parabolic effects, the following non-parabolic band approximation in the sense of Kane is used

$$
\mathcal{E}_n(1 + \alpha \mathcal{E}_n) = \frac{\hbar^2}{2m^*}|\mathbf{k}|^2, \tag{3.23}
$$

where $\alpha > 0$ is a non-parabolicity parameter.

When we consider the effective mass near a band maximum, we find that the Hessian of $\mathcal{E}_n$ is negative definite which would lead to a negative effective mass. Using a positive charge leads to a positive effective mass. The corresponding particles are calles *holes*. Physically, a hole is a vacant orbital in an otherwise filled (valence) band. Thus, the current flow in a semiconductor crystal comes from two sources: the flow of electrons in the conduction band and the flow of holes in the valence band. It is a convention to consider rather the motion of the valence band vacancies that the motion of the electrons moving from one vacant orbital to the next.

3.2 Physics of equilibrium of semiconductors

It is possible to describe a statistical ensemble of particles in equilibrium using three thermodynamic quantities, such as the density of the number of particles, the temperature and the chemical potential. These quantities do not are independent of the another, but it is possible to express each of them in function of the other two with a relationship called the equation of state. In this section we determine the equation of state for the density of the number electrons in conduction band, and the density of the number hole in valence band. The starting

point is that in equilibrium the probability of employment of an electronic state depends only on the energy state and is given by the Fermi-Dirac distribution

$$F_{\text{FD}}(\mathcal{E}) = \frac{1}{\exp\left(\frac{\mathcal{E}-\mu}{k_B T}\right) + 1},$$
(3.24)

where k_B is the Boltzmann constant, T is the absolute temperature and μ is the chemical potential. This chemical potential represent the energy required to increase by one the number of particles, at constant temperature and constant volume. When the energy $\mathcal{E}$ is equal to the chemical potential μ, obviously the distribution function F_{FD} is equal to $1/2$, this value for the energy is called energy Fermi level $\mathcal{E}_F$.

Now we are able to determine the number of electrons in the conduction band and the number of holes in the valence band per unit volume. We use statistical methods, and we make two assumption:

- the electrons cannot be distinguished from one another and

- the Pauli exclusion principle that says that each level of a band can be occupied by not more than two electrons with opposite spin.

At the first we calculate the number of possible states within all energy bands per unit volume $(2\pi)^3$, this number is

$$g_c(\mathcal{E}) = \frac{2}{(2\pi)^3} \sum_\nu \int_{\mathscr{B}} \delta(\mathcal{E} - \mathcal{E}_\nu(\mathbf{k}))\, d\mathbf{k}.$$
(3.25)

this quantity is called *density of states*. In this equation $\mathscr{B}$ is the Brillouin zone and the function δ is the delta distribution defined by

$$\int_{-\infty}^{\infty} \delta(\mathcal{E}_0 - \mathcal{E})\varphi(\mathcal{E})d\mathcal{E} = \varphi(\mathcal{E}_0)$$
(3.26)

of all appropriate function φ. The electron density, that is the integral of the probability density occupancy of the energy state per unit volume

$$n_c = \frac{2}{(2\pi)^3} \sum_\nu \int_{\mathscr{B}} f_{\text{FD}}(\mathcal{E}_\nu(\mathbf{k}))\, d\mathbf{k}.$$
(3.27)

Using the (3.26), the definition of the density of states $g_c(\mathcal{E})$, and the properties of the delta function, we have

$$
\begin{aligned}
n_c &= \frac{1}{4\pi^3} \sum_\nu \int_{\mathscr{B}} \int_{-\infty}^{\infty} \delta(\mathcal{E} - \mathcal{E}_\nu(\mathbf{k})) f_{\text{FD}}(\mathcal{E})\, d\mathbf{k}, \\
&= \int_{\mathcal{E}_c}^{\infty} g_c(\mathcal{E}) f_{\text{FD}}(\mathcal{E}) d\mathcal{E},
\end{aligned}
$$
(3.28)

in wich $\mathcal{E}_c$ is the minimum of the conduction band $\mathcal{E}_c(\mathbf{k})$. Thus using the definition of the Fermi-Dirac distribution we have the following expression for the electron density

$$n_c = \int_{\mathcal{E}_c}^{\infty} \frac{g_c(\mathcal{E})\mathrm{d}\mathcal{E}}{1 + \exp((\mathcal{E} - \mathcal{E}_F)/k_B T)}. \tag{3.29}$$

In a similar way for the hole density p_v, we obtain the following expression

$$
\begin{aligned}
p_v &= \int_{-\infty}^{\infty} g_c(\mathcal{E}) \left(1 - \frac{1}{1 + \exp((\mathcal{E} - \mathcal{E}_F)/k_B T)}\right) \mathrm{d}\mathcal{E} \\
&= \int_{-\infty}^{\mathcal{E}_v} \frac{g_c(\mathcal{E})\mathrm{d}\mathcal{E}}{1 + \exp((\mathcal{E}_F - \mathcal{E})/k_B T)},
\end{aligned}
\tag{3.30}
$$

where $\mathcal{E}_v$ is the maximum of the valence band $\mathcal{E}_v(\mathbf{k})$.

For semiconductor we can consider the assumption of non degeneracy, that is

$$\mathcal{E}_c - \mathcal{E}_F \gg k_B T, \tag{3.31}$$
$$\mathcal{E}_F - \mathcal{E}_v \gg k_B T, \tag{3.32}$$

then for (3.31), for all $\mathcal{E} > \mathcal{E}_c$, we have that $\mathcal{E} - \mathcal{E}_F \gg k_B T$ and then the Fermi-Dirac distribution function in (3.28) can be approximated with the Maxwell-Boltzmann distribution function (for electron):

$$\frac{1}{1 + \exp\left(\frac{\mathcal{E} - \mathcal{E}_F}{k_B T}\right)} \approx \exp\left(-\frac{\mathcal{E} - \mathcal{E}_F}{k_B T}\right), \quad \forall \mathcal{E} < \mathcal{E}_c. \tag{3.33}$$

In similar way if we assume (3.32) for the hole we have the Maxwell-Boltzmann distribution function (for hole):

$$\frac{1}{1 + \exp\left(\frac{\mathcal{E}_F - \mathcal{E}}{k_B T}\right)} \approx \exp\left(-\frac{\mathcal{E}_F - \mathcal{E}}{k_B T}\right), \quad \forall \mathcal{E} < \mathcal{E}_v. \tag{3.34}$$

Using these approximations we can write

$$
\begin{aligned}
n_c &= \left\{\int_{\mathcal{E}_c}^{\infty} g_c(\mathcal{E}) \exp\left(-\frac{\mathcal{E} - \mathcal{E}_c}{k_B T}\right) d\mathcal{E}\right\} \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_F}{k_B T}\right), \\
p_v &= \left\{\int_{-\infty}^{\mathcal{E}_v} g_v(\mathcal{E}) \exp\left(-\frac{\mathcal{E}_v - \mathcal{E}}{k_B T}\right) d\mathcal{E}\right\} \exp\left(-\frac{\mathcal{E}_F - \mathcal{E}_v}{k_B T}\right).
\end{aligned}
$$

If we define the quantities

$$
\begin{aligned}
N_c(T) &:= \int_{\mathcal{E}_c}^{\infty} g_c(\mathcal{E}) \exp\left(-\frac{\mathcal{E} - \mathcal{E}_c}{k_B T}\right) d\mathcal{E}, \\
P_v(T) &:= \int_{-\infty}^{\mathcal{E}_v} g_v(\mathcal{E}) \exp\left(-\frac{\mathcal{E}_v - \mathcal{E}}{k_B T}\right) d\mathcal{E},
\end{aligned}
\tag{3.35}
$$

the electron density and the hole density have the form

$$n_c = N_c(T) \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_F}{k_B T}\right),$$
$$p_v = P_v(T) \exp\left(-\frac{\mathcal{E}_F - \mathcal{E}_v}{k_B T}\right). \tag{3.36}$$

Multiplying the last two expressions for n_c and p_v, we obtain the *law of mass action*

$$n_c p_v = n_i^2, \tag{3.37}$$

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

$$n_i^2 = N_c P_v \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_v}{k_B T}\right) \equiv N_c P_v \exp\left(-\frac{\mathcal{E}_g}{k_B T}\right). \tag{3.38}$$

A pure semiconductor crystal with no impurities is called *intrinsic semiconductor*. In this case the conduction band electrons can only have come from formerly occupied valence band levels leaving holes behind them. The number of conduction band electrons is therefore equal to the number of valence band holes:

$$n_c(T) = p_v(T) =: n_i(T). \tag{3.39}$$

Using this relation and (3.36), it is possible to determine the chemical potential (Fermi level) depending on the temperature,

$$N_c(T) \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_F}{k_B T}\right) = P_v(T) \exp\left(-\frac{\mathcal{E}_F - \mathcal{E}_v}{k_B T}\right). \tag{3.40}$$

Then, from (3.40), we have

$$\mathcal{E}_F = \mathcal{E}_{F,i}(T) \equiv \frac{1}{2}(\mathcal{E}_c + \mathcal{E}_v) + \frac{1}{2}k_B T \log\left(\frac{P_v(T)}{N_c(T)}\right). \tag{3.41}$$

Now using (3.39), we obtain the carrier density n_i,

$$n_i(T) = \sqrt{N_c(T) P_v(T)} \exp\left(-\frac{\mathcal{E}_g}{2k_B T}\right), \tag{3.42}$$

that is equivalent to (3.38). Then we can say that the "intrinsic concentration" is the concentration of the carrier for an intrinsic semiconductor in equilibrium state.

We notice that the expressions (3.36) are valide also in partial equilibrium, in which we have to replace the Fermi level $\mathcal{E}_F$ with $\mathcal{E}_{F,c}$ for the electrons in conduction band and with $\mathcal{E}_{F,v}$ for holes in valence band, then we have

$$n_c = N_c(T) \exp\left(-\frac{\mathcal{E}_c - \mathcal{E}_{F,c}}{k_B T}\right),$$
$$p_v = P_v(T) \exp\left(-\frac{\mathcal{E}_{F,v} - \mathcal{E}_v}{k_B T}\right). \tag{3.43}$$

These relations are equivalent to the following relations in which we consider the intrinsic concentratio ni and the Fermi level depending on temperature $\mathcal{E}_{F,\mathrm{i}}(T)$

$$N_c(T) = n_\mathrm{i} \exp\left(\frac{E_c - E_{F,\mathrm{i}}}{k_B T}\right), \quad P_v(T) = n_\mathrm{i} \exp\left(\frac{E_{F,\mathrm{i}} - E_v}{k_B T}\right). \tag{3.44}$$

Using these identities we can write the equations (3.43) as

$$n_c = n_\mathrm{i} \exp\left(\frac{\mathcal{E}_{F,c} - \mathcal{E}_{F,\mathrm{i}}}{k_B T}\right), \qquad p_v = n_\mathrm{i} \exp\left(\frac{\mathcal{E}_{F,\mathrm{i}} - \mathcal{E}_{F,v}}{k_B T}\right). \tag{3.45}$$

The relations (3.45) are the Maxwell-Boltzmann relations. From these equations we obtain also

$$\mathcal{E}_{F,c} = \mathcal{E}_{F,\mathrm{i}} + k_B T \ln\frac{n_c}{n_\mathrm{i}}, \qquad \mathcal{E}_{F,v} = \mathcal{E}_{F,\mathrm{i}} - k_B T \ln\frac{p_v}{n_\mathrm{i}}. \tag{3.46}$$

The intrinsic density is too small to result in a significant conductivity. However, it is possible to replace some atoms in a semiconductor crystal by atoms which provide free electrons in the conduction band or free holes in the valence band. This process is called *doping*. Impurities that contribute to the carrier density are called onors if they supply additional electrons to the conduction band, and acceptors if they supply additional holes to the valence band. A semiconductor which is doped with donors is termed n-type semiconductor, and a semiconductor doped with acceptors is called p-type semiconductor. Generally speaking, let $\mathcal{E}_d$ and $\mathcal{E}_a$ be the energy level of a donor electron and an acceptor hole, respectively. Then $\mathcal{E}_c - \mathcal{E}_d$ and $\mathcal{E}_a - \mathcal{E}_v$ are small compared to $k_B T$. This means that the additional particles contribute at room temperature to the electron and hole density.

3.3 Derivation of the drift-diffusion model from BTE equation

We introduce the phase space which is the space with seven coordinates: spatial coordinates $\mathbf{x} = (x_1, x_2, x_3)^\top$, momentum coordinates $\mathbf{k} = (k_1, k_2, k_3)^\top$ and time t. At the beginning we introduce the unipolar case. The electron concentration is described by a distribution function $f(\mathbf{x}, \mathbf{k}, t)$, we can find the carrier concentration per unit volume of phase space integranting the distribution function over the entire momentum volume $V_\mathbf{k}$, that is

$$\int_{V_\mathbf{k}} f(\mathbf{x}, \mathbf{k}, t) \, d\mathbf{k} = n(\mathbf{x}, t). \tag{3.47}$$

The distribution function has the property that in the entire phase space the derivative along a particle trajectory $\mathbf{x}(t)$, $\mathbf{k}(t)$ with respect to time vanishes,

when scattering events are not present that is the Boltzmann transport equation in implicit form. Expanding the total derivative we obtain

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} f \cdot \frac{d\mathbf{x}}{dt} + \nabla_{\mathbf{k}} f \cdot \frac{d\mathbf{k}}{dt} = 0,$$

clearly $\nabla_{\mathbf{k}}$ and $\nabla_{\mathbf{x}}$ indicate the gradients operator with respect to the momentum coordinates $\mathbf{k}$, and the spatial coordinates $\mathbf{x}$, respectively.

In the presence of scattering, we have

$$\frac{\mathrm{d}}{\mathrm{d}t} f(\mathbf{x}(t), \mathbf{k}(t), t) = \mathcal{C}[f],$$

and then the Boltzmann transport equation becomes

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} f \cdot \frac{d\mathbf{x}}{dt} + \nabla_{\mathbf{k}} f \cdot \frac{d\mathbf{k}}{dt} = \mathcal{C}[f], \qquad (3.48)$$

where $\mathcal{C}[f]$ represents the scattering events due to the macroscopic external fields, internal forces and to internal localized crystal attributes like impurity atoms or ions, vacancies, and thermal lattice vibrations (phonons). Using statistical laws (Fermi's golden rule), and placing $f = f(\mathbf{x}, \mathbf{k}, t)$ and $f' = f(\mathbf{x}, \mathbf{k}', t)$ we can write

$$\mathcal{C}[f] = -\int_{V_{\mathbf{k}'}} [f(1 - f'/y)P(\mathbf{k}, \mathbf{k}') - f'(1 - f/y)P(\mathbf{k}', \mathbf{k})] \, \mathrm{d}\mathbf{k}'.$$

where $y = 1/(4\pi)^3$ is the density of the states, and $P(\mathbf{k}, \mathbf{k}') \, \mathrm{d}\mathbf{k}'$ represents the probability per unit time that a carrier in the state $\mathbf{k}$ will be scattered into the momentum volume $\mathrm{d}\mathbf{k}'$.

We must introduce some considerations about the collision term described above. In general, this term should also consider another type of particle or rather pseudo-particles called *phonons*. These quasi-particles correspond to the oscillations of the nuclei of the semiconductor around the equilibrium configuration which determine the lattice, they are bosons, that is, many phonons may occupu the same quantum state.

If we take into account the thermal effects we have to consider electrons and holes immersed in a thermal bath of phonons. We consider n_{ph} relevant families of phonons, then the phonon concentrations, that we indicate with g_i, with $i = 1, \dots, n_{\mathrm{ph}}$, depends only from the lattice temperature or rether from the internal energy.

In this section we consider the equilibrium state for phonons and this state is characterized by the fact that the number of occupancy, N_B, (average number of phonons which are in a given state quantum) is given by the Bose-Einstein distribution

$$N_B = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T_L}\right) - 1}, \qquad (3.49)$$

where $\hbar\omega$ is the energy of phonon.

For this reason in general we must write

$$\mathcal{C} = \mathcal{C}[f, g_i]$$

but in the Boltzmann description we neglect thermal effect and then we have

$$\mathcal{C} = \mathcal{C}[f].$$

Back to our derivation of the model, we notice that the derivative of $\mathbf{k}$ with respect to time, that appears in (3.48), multiplied times the Planck's constant $\hbar$ it's equal to the sum of all forces $\mathbf{F}$, and the derivative of $\mathbf{x}$ with respect to time is the velocity group of the carriers $\boldsymbol{v}(\mathbf{k})$, that is

$$\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = \frac{1}{\hbar}\mathbf{F}, \qquad \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \boldsymbol{v}(\mathbf{k}).$$

Thus the explicit form of the Boltzmann equation is

$$\frac{\partial f}{\partial t} + \boldsymbol{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}}f - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}}f = \mathcal{C}[f]. \tag{3.50}$$

If we consider the bipolar case we have that the Boltzmann transport equation comprise a scattering term which describe the collisions also between holes and electron, that is

$$\frac{\partial f_\nu}{\partial t} + \boldsymbol{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}}f_\nu - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}}f_\nu = \mathcal{C}_\nu[f_\nu, f_{\bar\nu}], \tag{3.51}$$

where ν stands for n or p in electron or hole case, respectively, and $\bar\nu$ the opposite of ν. The collision term has the form

$$\mathcal{C}_\nu[f_\nu, f_{\bar\nu}] = \mathcal{C}_{\nu\nu}[f_\nu] + \mathcal{C}_{\nu\bar\nu}[f_\nu, f_{\bar\nu}],$$

in this equality the first term represents the scattering between electron-electron or hole-hole, and the second term is the generation-recombination term.

Continue to investigate the unipolar case, we derive the first and simpler model for semiconductor device called *drift-diffusion model* from the Boltzmann equation (3.50). Integrating this equation with respect to the momentum space $\mathbf{k}$ on the Brillouin zone $\mathscr{B}$, and using the periodicity on the boundary of this region, we have

$$-\int_{\mathscr{B}} \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}}f \,\mathrm{d}\mathbf{k} = -\frac{q}{\hbar}\mathbf{E} \cdot \int_{\partial\mathscr{B}} f\boldsymbol{\nu}_{\mathscr{B}} \,\mathrm{d}\sigma(\mathbf{k}) = 0, \tag{3.52}$$

where $\boldsymbol{\nu}_{\mathscr{B}}(\mathbf{k})$ is the external unit normal on the boudary of $\mathscr{B}$. We have the same result with parabolic approximation (3.22) or with Kane approximation (3.23), if we assume that the distribution function for eletrons quickly vanish to infinity. It is possible to see that 1 is a collision invariant for $\mathcal{C}[f]$ because is a function that does not depend on $\mathbf{k}$, then

$$\int_{\mathscr{B}} \mathcal{C}[f] \,\mathrm{d}\mathbf{k} = 0. \tag{3.53}$$

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Apllying (3.52) and (3.53) in the Boltzmann equation (3.50), we obtain the continuity equation for the electron density,

$$\frac{\partial n}{\partial t} + \nabla_{\mathbf{x}} \cdot \boldsymbol{j}_n = 0, \tag{3.54}$$

where the current density for the electrons

$$\boldsymbol{j}_n = \int_{\mathcal{B}} f \boldsymbol{v}_n \, d\mathbf{k}. \tag{3.55}$$

Sometimes we write also $\boldsymbol{j}_n = n\boldsymbol{v}$, where

$$\boldsymbol{v}_n = \frac{1}{n} \int_{\mathcal{B}} f \boldsymbol{v} \, d\mathbf{k} \quad \text{is the average velocity.} \tag{3.56}$$

Equations (3.54) for electrons, coupled with the Poisson equation, forms the much simpler system that describes the carrier in semiconductor. To solve this system we need the closure relation for $\boldsymbol{j}_n$. In ather words we have to write $\boldsymbol{j}_n$ as function of n and ϕ_n. To have this closure relation from the semiclassical Boltzmann equation with elementary methods, is necessary to simplify the collision term $\mathcal{C}[f]$, replacing the integral operator representing the physical scattering with relaxation term. The basic concept is that the carriers, because of collisions with phonons and other carriers, tend to relax gradually to the state of global thermal equilibrium at the lattice temperature T_L and this relaxation takes place over a period relatively long. During the relaxation the system retain for a time comparable to that of interest simulations (at least nanoseconds) in a state of local thermodynamic equilibrium described by a Maxwellian with a carriers temperature T different from that of the lattice. With this phisical description we can replace the collision term with a relaxation term of the following form

$$\mathcal{C}[f] = -\frac{f - f_{\text{eq}}}{\tau(\mathcal{E})}, \tag{3.57}$$

where $\tau(\mathcal{E})$ is the relaxation time and f_{eq} is the distribution function at equilibrium that has the form

$$f_{\text{eq}}(\mathbf{x}, \mathbf{k}, t) = y F_{\text{M}}(\mathcal{E}(\mathbf{k})), \tag{3.58}$$

in which we have posed

$$F_{\text{M}}(\mathcal{E}) = \exp\left(-\frac{\mathcal{E} - \mathcal{E}_F}{k_B T_L}\right).$$

At global thermal equilibrium we have that the temperature in a constant value that is equal to lattice temperature $T = T_L$, and the quasi-Fermi level $\mathcal{E}_F$ is also a constant value with respect to space and time. We use now the Hilbert expansion, that is: we rescale the relaxation time in the following way

$$\tau(\mathcal{E}) \to \epsilon \tau(\mathcal{E}), \tag{3.59}$$

where τ denotes a typical value of the relaxation time, which is a measure of its size. The parameter τ is related to the time scale in which the equilibrium relaxation becomes important. To express it we rescale the time by introducing a rescaled time

$$t \rightarrow \frac{t}{\epsilon} \tag{3.60}$$

The derivative with respect to time is

$$\frac{\partial}{\partial t} \rightarrow \tau \frac{\partial}{\partial t}$$

Using this new time variable, the Boltzmann equation with BGK approximation (3.57) for the collision operator becames

$$\tau \frac{\partial f}{\partial t} + \boldsymbol{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f = -\frac{1}{\bar{\tau}} \frac{f - f_{\mathrm{eq}}}{\tau(\mathcal{E})}. \tag{3.61}$$

With the same scaling the electric field equation and the Poisson equation become

$$\mathbf{E} = -\nabla_{\mathbf{x}} \phi, \qquad -\nabla_{\mathbf{x}} \cdot (\epsilon_s \nabla_{\mathbf{x}} \phi) = q(N_D - n), \tag{3.62}$$

with

$$f(\mathbf{x}, \mathbf{k}, t) \rightarrow f(\mathbf{x}, \mathbf{k}, t/\tau), \quad \phi(\mathbf{x}, t) \rightarrow \phi(\mathbf{x}, t/\tau). \tag{3.63}$$

Then we introduce the following series expansion of the new distribution function f, writed with the new time t^* around the equilibrium distribution function f_{eq} with respect to the parameter τ

$$f = \sum_{k=0}^{\infty} \tau^k f_k \equiv f_0 + \tau f_1 + \tau^2 f_2 + \cdots, \qquad \mathrm{con} \quad f_0 = f_{\mathrm{eq}}. \tag{3.64}$$

Similarly we have for the electric potential

$$\phi = \sum_{k=0}^{\infty} \tau^k \phi_k \equiv \phi_0 + \tau \phi_1 + \tau^2 \phi_2 + \cdots. \tag{3.65}$$

Using the expansions (3.64)-(3.65) in the Boltzmann equation (3.61), we obtain

$$\boldsymbol{v} \cdot \nabla_{\mathbf{x}} f_0 - \frac{q}{\hbar} \mathbf{E}_0 \cdot \nabla_{\mathbf{k}} f_0$$

$$+ \sum_{k=1}^{\infty} \tau^k \left\{ \frac{\partial f_{k-1}}{\partial t} + \boldsymbol{v} \cdot \nabla_{\mathbf{x}} f_{\mathbf{k}} - \frac{q}{\hbar} \sum_{i=0}^{k} \mathbf{E}_i \cdot \nabla_{\mathbf{k}} f_{k-i} \right\}$$

$$= -\frac{1}{\tau(\mathcal{E})} f_1 - \frac{1}{\tau(\mathcal{E})} \sum_{k=1}^{\infty} \tau^k f_{k+1},$$

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from which, equating all the coefficients of τ in both sides of the equation, we have

$$f_0 = f_{\text{eq}}, \tag{3.66}$$

$$f_1 = -\tau(\mathcal{E})\left\{\boldsymbol{v}\cdot\nabla_\mathbf{x}f_0 - \frac{q}{\hbar}\mathcal{E}_0\cdot\nabla_\mathbf{k}f_0\right\}, \tag{3.67}$$

$$f_{k+1} = -\tau(\mathcal{E})\left\{\frac{\partial f_{k-1}}{\partial t'} + \boldsymbol{v}\cdot\nabla_\mathbf{x}f_k - \frac{q}{\hbar}\sum_{i=0}^{k}\mathbf{E}_i\cdot\nabla_\mathbf{k}f_{k-i}\right\}, \quad k = 1, 2, \ldots \tag{3.68}$$

Using the same expansion in the Poisson equation we find

$$-\nabla_\mathbf{x}\cdot(\epsilon_s\nabla_\mathbf{x}\phi_0) - \sum_{k=1}^{\infty}\tau^k\nabla_\mathbf{x}\cdot(\epsilon_s\nabla_\mathbf{x}\phi_k) = q(N_D - n_0) - \sum_{k=1}^{\infty}\tau^k q n_k,$$

then the electric potential ϕ_k satisfy the Poisson equations

$$-\nabla_\mathbf{x}\cdot(\epsilon\nabla_\mathbf{x}\phi_0) = q(N_D - n_0), \tag{3.69}$$

$$-\nabla_\mathbf{x}\cdot(\epsilon\nabla_\mathbf{x}\phi_k) = -q n_k, \quad k = 1, 2, \ldots \tag{3.70}$$

In the previous equations, we have

$$\mathbf{E}_k = -\nabla_\mathbf{x}\phi_k, \quad n_k = \int_{\mathscr{B}} f_k^n \, d\mathbf{k}. \tag{3.71}$$

Using this procedure iteratively we can obtain the approximation of f at the desired order of τ. At the first order of τ, we find

$$\begin{aligned} f &= f_0 + \tau f_1 \\ &= f_{\text{eq}} - \tau\tau(\mathcal{E})\left\{\boldsymbol{v}\cdot\nabla_\mathbf{x}f_{\text{eq}} - \frac{q}{\hbar}\mathbf{E}_0\cdot\nabla_\mathbf{k}f_{\text{eq}}\right\}, \end{aligned} \tag{3.72}$$

with

$$\mathbf{E}_0 = -\nabla_\mathbf{x}\phi_0, \quad -\nabla_\mathbf{x}\cdot(\epsilon\nabla_\mathbf{x}\phi_0) = q(N_D - n_0), \tag{3.73}$$

where

$$n_0 = \int_{\mathscr{B}} f_{\text{eq}} \, d\mathbf{k}.$$

Using the approximation (3.72) we can compute the rescaled n, $\boldsymbol{j}_n$

$$n = \int_{\mathscr{B}} f_{\text{eq}} \, d\mathbf{k} + \tau\int_{\mathscr{B}} f_1 d\mathbf{k}, \quad \boldsymbol{j}_n = \int_{\mathscr{B}} \boldsymbol{v} f_{\text{eq}} \, d\mathbf{k} + \tau\int_{\mathscr{B}} \boldsymbol{v} f_1 d\mathbf{k}. \tag{3.74}$$

Observing that f_{eq} and $\mathcal{E}$ are even function with respect to $\mathbf{k}$, while f_1 and $\boldsymbol{v}$ are odd function,

$$\begin{aligned} f_{\text{eq}}(\mathbf{x}, -\mathbf{k}, t) &= f_{\text{eq}}(\mathbf{x}, \mathbf{k}, t), \quad \mathcal{E}(-\mathbf{k}) = \mathcal{E}(\mathbf{k}), \\ f_1(\mathbf{x}, -\mathbf{k}, t) &= -f_1(\mathbf{x}, \mathbf{k}, t), \quad \boldsymbol{v}(-\mathbf{k}) = -\boldsymbol{v}(\mathbf{k}). \end{aligned}$$

Then in equations (3.74), because of the symmetry, are different from zero only the integrals of even functions

$$n = \int_{\mathscr{B}} f_{\mathrm{eq}} \mathrm{d}\mathbf{k}, \quad \boldsymbol{j}_n = \tau \int_{\mathscr{B}} \boldsymbol{v} f_1 \mathrm{d}\mathbf{k}. \tag{3.75}$$

Then the continuity equation (3.54), for electrons becomes

$$\tau \frac{\partial n}{\partial t} + \nabla_{\mathbf{x}} \cdot \boldsymbol{j}_n = 0. \tag{3.76}$$

Considering the previuos time t and the Poisson equation we obtain the system

$$\frac{\partial n}{\partial t} + \nabla_{\mathbf{x}} \cdot \boldsymbol{j}_n = 0, \tag{3.77}$$

$$\mathbf{E} = -\nabla_{\mathbf{x}} \phi, \quad -\nabla_{\mathbf{x}} \cdot (\epsilon_s \nabla_{\mathbf{x}} \phi) = q(N_D - n), \tag{3.78}$$

with

$$n = \int_{\mathscr{B}} f_{\mathrm{eq}} \mathrm{d}\mathbf{k}, \tag{3.79}$$

$$\boldsymbol{j}_n = -\int_{\mathscr{B}} \tau(\mathcal{E}) \boldsymbol{v} \left\{ \boldsymbol{v} \cdot \nabla_{\mathbf{x}} f_{\mathrm{eq}} - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_{\mathrm{eq}} \right\} \mathrm{d}\mathbf{k}. \tag{3.80}$$

To close the system we have to explicit the closure relation (3.79). To this aim we insert equation (3.58) in the expression for the electron density (3.77),

$$n = \int_{\mathscr{B}} f_{\mathrm{eq}} \mathrm{d}\mathbf{k} = \frac{1}{4\pi^3} \int_{\mathscr{B}} f_{\mathrm{M}}(\mathcal{E}(\mathbf{k})) \mathrm{d}\mathbf{k}$$

$$= \frac{1}{4\pi^3} \int_{\mathscr{B}} \exp\left(-\frac{\mathcal{E} - \mathcal{E}_F^c}{k_B T}\right) \mathrm{d}\mathbf{k},$$

from which,

$$n = N \exp\left(\frac{\mathcal{E}_F^c}{k_B T}\right), \quad N := \frac{1}{4\pi^3} \int_{\mathscr{B}} \exp\left(-\frac{\mathcal{E}}{k_B T}\right) \mathrm{d}\mathbf{k}. \tag{3.81}$$

and remembering the expression for the intrinsic concentration $n_{\mathrm{i}} = n_{\mathrm{i}}(T_L)$ we can identify the intrinsic Fermi level as

$$\mathcal{E}_{F,\mathrm{i}} = -k_B T \log \frac{N}{n_{\mathrm{i}}} \iff N = n_{\mathrm{i}} \exp\left(-\frac{\mathcal{E}_{F,\mathrm{i}}}{k_B T}\right).$$

and we can rewrite equation (3.81) in the form

$$n = n_{\mathrm{i}} \exp\left(\frac{\mathcal{E}_F^c - \mathcal{E}_{F,\mathrm{i}}}{k_B T}\right). \tag{3.82}$$

Now we compute the closure relation (3.79). Using the expression (3.58), and considering that, in this case, the temperature is constant and equal to lattice temperature $T = T_L$,

$$\nabla_{\mathbf{x}} f_{\mathrm{eq}} = f_{\mathrm{eq}} \frac{1}{k_B T} \nabla_{\mathbf{x}} \mathcal{E}_F^c$$

$$\nabla_{\mathbf{k}} f_{\mathrm{eq}} = -f_{\mathrm{eq}} \frac{\hbar}{k_B T} \boldsymbol{v}.$$

then we have,

$$\boldsymbol{v} \cdot \nabla_{\mathbf{x}} f_{\mathrm{eq}} - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_{\mathrm{eq}} = \frac{f_{\mathrm{eq}}}{k_B T} \boldsymbol{v} \cdot [\nabla_{\mathbf{x}}(\mathcal{E}_F^c - q\phi)] \tag{3.83}$$

Using this relation in equation (3.79) we obtain the following expression for the electron flux

$$\begin{aligned} \boldsymbol{j}_n &= -\int_{\mathcal{B}} \tau(\mathcal{E}) \boldsymbol{v} \left\{ \boldsymbol{v} \cdot \nabla_{\mathbf{x}} f_{\mathrm{eq}} - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_{\mathrm{eq}} \right\} \mathrm{d}\mathbf{k} \\ &= -\int_{\mathcal{B}} \tau(\mathcal{E}) \boldsymbol{v} \otimes \boldsymbol{v} f_{\mathrm{eq}} \, \mathrm{d}\mathbf{k} \cdot \left[\frac{1}{k_B T} \nabla_{\mathbf{x}}(\mathcal{E}_F^c - q\phi) \right] \end{aligned} \tag{3.84}$$

where $\otimes$ indicates the tonsorial product between vectors.

Remembering the Maxwell-Boltzmann relation, and that for the quasi-Fermi level $\mathcal{E}_F^c$ and the intrinsic Fermi level $\mathcal{E}_{F,\mathrm{i}}$ we can write the relation

$$\mathcal{E}_F^c - \mathcal{E}_{F,\mathrm{i}} = q(\phi - \phi_n), \tag{3.85}$$

that defines the quasi-Fermi potential ϕ_n. Then the closure relation (3.84) becomes

$$\begin{aligned} \boldsymbol{j}_n &= -\frac{1}{k_B T} \int_{\mathcal{B}} \tau(\mathcal{E}) \boldsymbol{v} \otimes \boldsymbol{v} f_{\mathrm{eq}} \, \mathrm{d}\mathbf{k} \cdot \nabla_{\mathbf{x}}(\mathcal{E}_{F,\mathrm{i}} - q\phi_n) \\ &= \frac{q}{k_B T} \int_{\mathcal{B}} \tau(\mathcal{E}) \boldsymbol{v} \otimes \boldsymbol{v} f_{\mathrm{eq}} \, \mathrm{d}\mathbf{k} \cdot \nabla_{\mathbf{x}} \phi_n. \end{aligned} \tag{3.86}$$

We have found a a linear dependence of $\boldsymbol{j}_n$ from $\nabla_{\mathbf{x}} \phi_n$.

Using phisical considerationit is also possible to write the current as a sum of two part, one that taking into account the drift of electron and other part that consider the diffusion of them that is

$$\boldsymbol{j}_n = \mu_n n \nabla_{\mathbf{x}} \phi_n - D_n \nabla_{\mathbf{x}} n, \tag{3.87}$$

where μ_n is the mobility and D_n is the diffusion coefficient

$$D_n = \phi_{\mathrm{th}} \mu_n = \frac{k_B T \mu_n}{q}.$$

From equation (3.86) we have

$$\boldsymbol{j}_n = \frac{1}{n} \frac{q}{k_B T} \int_{\mathcal{B}} \tau(\mathcal{E}) \boldsymbol{v} \otimes \boldsymbol{v} f_{\mathrm{eq}} \, \mathrm{d}\mathbf{k} \cdot \left[-\frac{k_B T}{q} \nabla_{\mathbf{x}} n + n \nabla_{\mathbf{x}} \phi \right],$$

that represents the fact that

$$\frac{1}{n}\frac{q}{k_B T}\int_{\mathscr{B}}\tau(\mathcal{E})\boldsymbol{v}\otimes\boldsymbol{v}f_{\text{eq}}\,\mathrm{d}\mathbf{k}$$

is the motility tensor.

Now we can write unipolar drift-diffusion model for electron is

$$\begin{cases} \dfrac{\partial n}{\partial t}+\nabla_{\mathbf{x}}\cdot\boldsymbol{j}_n=0,\\[2mm] \boldsymbol{j}_n=\mu_n\left(n\nabla\phi-\phi_{\text{th}}\nabla n\right),\\[2mm] \mathbf{E}=-\nabla_{\mathbf{x}}\phi,\quad -\nabla_{\mathbf{x}}\cdot(\epsilon_s\nabla_{\mathbf{x}}\phi)=q(N_D-n) \end{cases} \tag{3.88}$$

Similarly we can get a unipolar drift-diffusion model for holes in the valence band, and starting with a system of Boltzmann equations for electrons and holes, with a coupling term, we can get the following bipolar drift-diffusion model

$$\begin{cases} \dfrac{\partial n}{\partial t}+\nabla\cdot\boldsymbol{j}_n=H,\qquad \boldsymbol{j}_n=\mu_n\left(n\nabla\phi-\phi_{\text{th}}\nabla n\right),\\[2mm] \dfrac{\partial p}{\partial t}+\nabla\cdot\boldsymbol{j}_p=H,\qquad \boldsymbol{j}_p=-\mu_p\left(p\nabla\phi+\phi_{\text{th}}\nabla p\right).\\[2mm] \qquad\mathbf{E}=-\nabla_{\mathbf{x}}\phi,\qquad -\nabla_{\mathbf{x}}\cdot(\epsilon_s\nabla_{\mathbf{x}}\phi)=q(N_D-N_A+p-n). \end{cases} \tag{3.89}$$

The term H is the recombination-generation term that we will introduce in the following section.

3.4 Drift-diffusion model form Maxwell equations

In this section we give a first approach on building the equations that represent the mathematical models for the analysis of semiconductor devices. In the first chapter we gave a first idea on these equations, in this section, we show how to derive such equations from the following Maxwell's equations

$$\nabla\times\mathbf{H}=\boldsymbol{J}+\frac{\partial\mathbf{D}}{\partial t}, \tag{3.90}$$

$$\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}, \tag{3.91}$$

$$\nabla\cdot\mathbf{D}=\hat{\rho}, \tag{3.92}$$

$$\nabla\cdot\mathbf{B}=0. \tag{3.93}$$

The vectors $\mathbf{E}$ and $\mathbf{D}$ are the electric field and the displacement vector, $\mathbf{H}$ and $\mathbf{B}$ are the magnetic field and the induction vector respectively, $\boldsymbol{J}$ indicates the conduction current density and finally ρ is the electric charge density.

From the equation (3.92) we can derive the Poisson equation that we rewrite for convenience

$$-\nabla\cdot(\epsilon\nabla\phi)=\rho_{\text{bi}}+\rho. \tag{3.94}$$

We introduce the relation between the displacement vector $\mathbf{D}$ and the electric field $\mathbf{E}$

$$\mathbf{D} = \epsilon \mathbf{E}, \tag{3.95}$$

where ϵ denotes the dielectric constant considered time independent. We assume that the polarization by mechanical forces is neglected. These assumption are consistent with the semiconductor devices. Now we introduce a vector field $\mathbf{A}$, remembering that the operator $\nabla \cdot (\nabla \times \mathbf{u})$ applied to any vector $\mathbf{u}$ is zero and solving the equation(3.93) we obtain

$$\mathbf{B} = \nabla \times \mathbf{A} \quad \text{and} \quad \nabla \cdot \mathbf{A} = 0.$$

Using these identities in (3.91), assuming that the speed of light is large compared with to all velocities which are relevant for the device, we have

$$\nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0. \tag{3.96}$$

Then there exists a scalar field ϕ such that

$$-\nabla \phi = \mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}.$$

Finding the electric field E from the previous equality and substituting into (3.95) and the resulting vector D in (3.92) we obtain

$$-\nabla \cdot \left(\epsilon_s \frac{\partial \mathbf{A}}{\partial t} \right) - \nabla \cdot (\epsilon_s \nabla \phi) = \hat{\rho}. \tag{3.97}$$

We have obtained the Poisson equation (3.94) considering that the first term of the previous equation is zero if the dielectric constant ϵ can be considered homogenous. The term $\hat{\rho}$ includes the charge density due to the dopans embedded in semiconductor indicates with ρ_{bi} and the charge density due to the carriers ρ. We can express the charge density $\hat{\rho}$ as the product of the elementar charge q times the sum of the positively charged hole concentration p the negatively charged electron concentration n and an additional concentration N

$$\hat{\rho} = q(p - n + N). \tag{3.98}$$

As we will see later this is not only a substitution but we additional assumption are brought about by modeling the quantities n and p.

From the Maxwell equations we can derive also the continuity equations. Applying the divergence operator to equation (3.90) and considering (3.92), we have immediately

$$\nabla \cdot (\nabla \times \mathbf{H}) = \nabla \cdot \boldsymbol{J} + \frac{\partial \hat{\rho}}{\partial t} = 0, \tag{3.99}$$

The conduction current density $\boldsymbol{J}$ can be expressed as the sum of a component cuosed by holes $\boldsymbol{J}_p$ and a component due to the electrons $\boldsymbol{J}_n$. Assuming that all

charges in the semiconductor, except the mobile carriers electrons and holes, are time invariant, and using equation (3.98) in (3.99) we have

$$\nabla \cdot (\boldsymbol{J}_p + \boldsymbol{J}_n) + q\frac{\partial}{\partial t}(p - n) = 0. \tag{3.100}$$

This result just means that sources and sinks of the total conduction current are fully compensated by the time variation of the mobile charge.

Finally, to obtain the two continuity equations we have to define a quantity H using the following equation

$$\nabla \cdot \boldsymbol{J}_n - q\frac{\partial n}{\partial t} = qH, \tag{3.101}$$

thus we have from (3.100)

$$\nabla \cdot \boldsymbol{J}_p + q\frac{\partial p}{\partial t} = -qH. \tag{3.102}$$

The quantity H can be seen as a function that represents the net generation or recombination of electrons and holes. Positive H means recombination and negative H means generation. As we will see later this term has several different formulations depending on how one chooses to model it.

Finally, remembering (3.55) and (3.56), we can write that the current density of charged particles is the product of the charge constant per particle, the particle concentration and the average velocity (drift velocity) of the particles, so we have, respectively, for electrons

$$\boldsymbol{J}_n = -qn\boldsymbol{v}_n.$$

that is consistent with the description in prevous setcion noting that

$$\boldsymbol{J}_n = -q\boldsymbol{j}_n.$$

With same simple consideration we obtain similar thing for holes.

3.5 The recombination-generation term

In this section we describe the expression of the production term H in the drift-diffusion model. Usually we assume that H is a balance term in which there is a contribute to generation of electrons and holes, which cause an increase of the concentrations of particles, and there is also a contribute of recombination of electrons and holes, causing a decrease of the concentrations of particles. That is

$$H = G - R, \tag{3.103}$$

G and R stand for generation and recombination events respectively. The most basic recombination-generation processes, are described by Auger term and Shockley-Read-Hall term. We introduce at the first the Auger recombination-generation process. In this model we have two possible mechanisms of recombination

- Capture of an electron: an electron moves from the conduction band to the valence band and recombines with a hole in valence. The energy of this electron is transferred to another electron in the conduction band. The recombination rate for this mechanism is given by $C_n n^2 p$.

- Capture of a hole: an electron moves from the conduction band to the valence band and recombines with a hole in valence. The energy of the electron is transferred to another hole in the valence band. The recombination rate for this mechanism is given by $C_p \, np^2$.

There are also two possible mechanisms of generation

- Emission of an electron. The generation rate for this mechanism is given by $C_n n_{\mathrm{i}}^2 n$.

- Emission of a hole. The generation rate for this mechanism is given by $C_p n_{\mathrm{i}}^2 p$.

Then the recombination-generation term introduced by Auger is

$$
\begin{aligned}
G_{\mathrm{A}} - R_{\mathrm{A}} &= C_n n_{\mathrm{i}}^2 n + C_p n_{\mathrm{i}}^2 p - C_n n^2 p - C_p \, np^2 \\
&= -(C_n n + C_p \, p)(np - n_{\mathrm{i}}^2).
\end{aligned} \tag{3.104}
$$

The other model introduced by Shockley, Read and Hall, describes the effect of the presence of *traps*, that is additional levels of energy in the bandgap, due to the presence of impurities, accessible to electrons and holes. If we indicate with N_{tr} the traps density and with n_{tr} the occupied traps density, we have also in this description two mechanism of recombimation

- Capture of an electron. An electron moves from the conduction band to an unoccupied trap. The rate of this recombination mechanism is given by $C_a n(N_{\mathrm{tr}} - n_{\mathrm{tr}})$.

- Capture of a hole. An electron moves from an occupied trap to the valence band. A hole disappears. The rate of this recombination mechanism is given by $C_b p \, n_{\mathrm{tr}}$.

The following are possible mechanisms for generation.

- Emission of an electron. An electron moving from one trap to the conduction band occupied. The rate of this recombination mechanism is given by $C_c n_{\mathrm{tr}}$.

- Emission of a hole. An electron moves from the valence band to an unoccupied trap. A hole appears. The rate of this recombination mechanism is given by $C_d(N_{\mathrm{tr}} - n_{\mathrm{tr}})$.

Thus, the recombination-generation rate for electrons and holes are given, respectively, by

$$
\begin{aligned}
G_{\text{SRH}}^n - R_{\text{SRH}}^n &= C_c n_{\text{tr}} - C_a n (N_{\text{tr}} - n_{\text{tr}}), \\
G_{\text{SRH}}^p - R_{\text{SRH}}^p &= C_d (N_{\text{tr}} - n_{\text{tr}}) - C_b p\, n_{\text{tr}}.
\end{aligned}
$$

Moreover must be valid the balance equation for the occupied traps density

$$
\frac{\partial n_{\text{tr}}}{\partial t} = C_a n (N_{\text{tr}} - n_{\text{tr}}) - C_b p\, n_{\text{tr}} - C_c n_{\text{tr}} + C_d (N_{\text{tr}} - n_{\text{tr}}).
$$

Then we can assume that n_{tr} is in equilibrium and does not depend on time

$$
0 = C_a n (N_{\text{tr}} - n_{\text{tr}}) - C_b p\, n_{\text{tr}} - C_c n_{\text{tr}} + C_d (N_{\text{tr}} - n_{\text{tr}}).
$$

Requiring that two terms of recombination-generation terms are the same, we have

$$
n_{\text{tr}} = \frac{C_a n + C_d}{C_a n + C_b p + C_c + C_d}\, N_{\text{tr}},
$$

whence

$$
G_{\text{SRH}} - R_{\text{SRH}} = -\frac{C_a C_b\, np - C_c C_d}{C_a n + C_b p + C_c + C_d}\, N_{\text{tr}}.
$$

Dividing numerator and denominator of this expression by $C_a C_b$, introducing the idensities

$$
n_* = \frac{C_c}{C_a}, \qquad p_* = \frac{C_d}{C_b},
$$

and the electron and hole life-time

$$
\tau_n = \frac{1}{C_b N_{\text{tr}}}, \qquad \tau_p = \frac{1}{C_a N_{\text{tr}}},
$$

remembering that $n_* p_* = n_{\text{i}}^2$, we obtain the recombination-generation Shockley-Read-Hall term

$$
G_{\text{SRH}} - R_{\text{SRH}} = -\frac{np - n_{\text{i}}^2}{\tau_n (n + n_*) + \tau_p (p + p_*)}. \tag{3.105}
$$

Then we have the expression for the recombination-generation term

$$
H = G_{\text{A}} - R_{\text{A}} + G_{\text{SRH}} - R_{\text{SRH}} \equiv -F(n,p)(np - n_{\text{i}}^2), \tag{3.106}
$$

with

$$
F(n,p) = (C_n n + C_p p) + \frac{1}{\tau_n (n + n_*) + \tau_p (p + p_*)} \geq 0.
$$

3.6 Boundary conditions of the drift-diffusion model

As we have wrote in the previous chapter, the semiconductor is modeled by a doman Ω in $\mathbb{R}^d$, with $d = 1, 2$ or 3. The boundary of this region $\partial\Omega$ is divided in two parts Γ_D and Γ_N representing the ohmic contacts and the electrically isolated regions, respectively. Since the ohmic contacts are generally more than one, say n_D, we write

$$\Gamma_D = \bigcup_{i=1}^{n_D} \Gamma_{D,i}, \qquad \Gamma_N = \partial\Omega \setminus \Gamma_D.$$

At the first we consider the steady-state drift diffusion model

$$\begin{cases} -\nabla \cdot (\epsilon_s \nabla \phi) = q(N - n + p), \\ \qquad \nabla \cdot \boldsymbol{j}_n = H, \qquad \boldsymbol{j}_n = \mu_n \left(n\nabla\phi - \phi_{\text{th}}\nabla n \right), \\ \qquad \nabla \cdot \boldsymbol{j}_p = H, \qquad \boldsymbol{j}_p = -\mu_p \left(p\nabla\phi + \phi_{\text{th}}\nabla p \right), \end{cases} \tag{3.107}$$

where $N = N_D - N_A$. In this case we have the possibility to choose between different sets of variables. The first set of three variables consists of (ϕ, n, p). Ohmic contacts on the boundary conditions are found by requiring that the semiconductor is in equilibrium, the conditions of neutrality charge and the law of mass action are valid, moreover the quasi-Fermi potentials are equal to the applied potential,

$$N - n + p = 0, \quad np = n_{\text{i}}^2, \quad \phi_n = \phi_p = U_D, \qquad \text{su } \Gamma_D.$$

Using the previous equations and the Maxwell-Boltzmann relations

$$n = n_{\text{i}} \exp\left(\frac{\phi - \phi_n}{\phi_{\text{th}}} \right), \quad p = n_{\text{i}} \exp\left(-\frac{\phi - \phi_p}{\phi_{\text{th}}} \right), \tag{3.108}$$

we find that on Γ_D must be valid:

$$\phi = e_D + \phi_{\text{bi}}, \quad n = n_D, \quad p = p_D, \tag{3.109}$$

with

$$\phi_{\text{bi}} := \phi_{\text{th}} \log \frac{n_D}{n_{\text{i}}}, \tag{3.110}$$

$$n_D := \frac{N(\mathbf{x})}{2} + \sqrt{\left(\frac{N(\mathbf{x})}{2} \right)^2 + n_{\text{i}}^2}, \tag{3.111}$$

$$p_D := -\frac{N(\mathbf{x})}{2} + \sqrt{\left(\frac{N(\mathbf{x})}{2} \right)^2 + n_{\text{i}}^2} \equiv \frac{n_D}{n_{\text{i}}^2}. \tag{3.112}$$

Usually the value of the applied potential is constant on each ohmic contact,

$$e_D(\mathbf{x}, t) = e_{D,i}(t), \quad \mathbf{x} \in \Gamma_{D,i}, \quad i = 1, \dots, n_D. \tag{3.113}$$

Another possible set of three variables for (3.107) is made up of (ϕ, ϕ_n, ϕ_p), with respect to which, using (3.108), the constitutive relations for the flows of carriers take the simplest form, $\boldsymbol{j}_n = \mu_n n \nabla \phi_n$, $\boldsymbol{j}_p = -\mu_p p \nabla \phi_p$, and system (3.107) becomes

$$\begin{cases} -\nabla \cdot (\epsilon_s \nabla \phi) = q(N + p - n), \\ \nabla \cdot \boldsymbol{j}_n = H \qquad \boldsymbol{j}_n = \mu_n n \nabla \phi_n, \qquad \text{in } \Omega. \\ \nabla \cdot \boldsymbol{j}_p = H \qquad \boldsymbol{j}_p = -\mu_p p \nabla \phi_p, \end{cases} \qquad (3.114)$$

For these variables, the boundary condition on Γ_D are:

$$\phi = e_D + \phi_{\text{bi}}, \quad \phi_n = e_D, \quad \phi_p = e_D. \qquad (3.115)$$

The last tern is that we consider is (ϕ, u, v), where u, v are the Slotboom variables, defined by:

$$u = n_{\text{i}} \exp \left(-\frac{\phi_n}{\phi_{\text{th}}} \right), \quad v = n_{\text{i}} \exp \left(\frac{\phi_p}{\phi_{\text{th}}} \right). \qquad (3.116)$$

With respect to this tern, the Maxwell-Boltzmann relations become

$$n = u \exp \left(\frac{\phi}{\phi_{\text{th}}} \right), \quad p = v \exp \left(-\frac{\phi}{\phi_{\text{th}}} \right), \qquad (3.117)$$

and the costitutive relations for the fluxes are

$$\boldsymbol{j}_n = -D_n \exp \left(\frac{\phi}{\phi_{\text{th}}} \right) \nabla u, \qquad \boldsymbol{j}_p = -D_p \exp \left(-\frac{\phi}{\phi_{\text{th}}} \right) \nabla v, \qquad (3.118)$$

with $D_n = \phi_{\text{th}} \mu_n$, $D_p = \phi_{\text{th}} \mu_p$. On Γ_D must be valid the boundary conditions

$$u = n_{\text{i}} \exp \left(-\frac{e_D}{\phi_{\text{th}}} \right), \quad v = n_{\text{i}} \exp \left(\frac{e_D}{\phi_{\text{th}}} \right). \qquad (3.119)$$

For each of the previous choices of variables, on Neumann region of the boundary Γ_N the conditions of isolation are valid

$$\boldsymbol{\nu} \cdot \mathbf{E} = 0, \quad \boldsymbol{\nu} \cdot \boldsymbol{j}_n = 0, \quad \boldsymbol{\nu} \cdot \boldsymbol{j}_p = 0, \qquad (3.120)$$

where $\boldsymbol{\nu}$ is the unit external normal on the boudary of Ω, and $\mathbf{E} = -\nabla \phi$. The above conditions for the three choices of variables became respectively

$$\frac{\partial \phi}{\partial \nu} = 0, \quad \frac{\partial n}{\partial \nu} = 0, \quad \frac{\partial p}{\partial \nu} = 0, \qquad (3.121)$$

$$\frac{\partial \phi}{\partial \nu} = 0, \quad \frac{\partial \phi_n}{\partial \nu} = 0, \quad \frac{\partial \phi_p}{\partial \nu} = 0, \qquad (3.122)$$

$$\frac{\partial \phi}{\partial \nu} = 0, \quad \frac{\partial u}{\partial \nu} = 0, \quad \frac{\partial v}{\partial \nu} = 0. \qquad (3.123)$$

Let us now consider the drift-diffusion equations depending on time:

$$\begin{cases} -\nabla \cdot (\epsilon_s \nabla \phi) = q(N - n + p), \\ \dfrac{\partial n}{\partial t} + \nabla \cdot \boldsymbol{j}_n = H, \qquad \boldsymbol{j}_n = \mu_n \left(n \nabla \phi - \phi_{\text{th}} \nabla n \right), \\ \dfrac{\partial p}{\partial t} + \nabla \cdot \boldsymbol{j}_p = H, \qquad \boldsymbol{j}_p = -\mu_p \left(p \nabla \phi + \phi_{\text{th}} \nabla p \right). \end{cases} \qquad (3.124)$$

In this case the choice of variables is of course the first (ϕ, n, p) then the boundary conditions are

$$\phi = \phi_{\text{bi}} + U_D, \quad n = n_D, \quad p = p_D, \qquad \text{on } \Gamma_D, \tag{3.125}$$

$$\frac{\partial \phi}{\partial \nu} = 0, \quad \frac{\partial n}{\partial \nu} = 0, \quad \frac{\partial p}{\partial \nu} = 0, \qquad \text{on } \Gamma_N. \tag{3.126}$$

In addition, we must impose the initial conditions for the main variables of the continuity equations, in which they appear derivative with respect to time:

$$n(\mathbf{x}, 0) = n_0(\mathbf{x}), \quad p(\mathbf{x}, 0) = p_0(\mathbf{x}), \qquad \text{on } \Omega. \tag{3.127}$$

Chapter 4

Analysis of the basic semiconductor device equations

4.1 The steady-state drift-diffusion model

We consider a semiconductor device with $n_D + 1$ terminals and model it by means of a domain $\Omega \subset \mathbb{R}^d$, characterized by a doping profile $N(\mathbf{x})$, with $\mathbf{x} \in \Omega$. We neglect all thermal effects, and assume that two carriers are responsible for the diode's output current, that is, electrons with negative charge $-q$, and holes with positive charge q. In the steady-state case we describe the behavior of the device in terms of number densities of electrons and holes, $n(\mathbf{x})$, $p(\mathbf{x})$, quasi-Fermi potentials for electron and holes, denoted by $\phi_n(\mathbf{x})$, $\phi_p(\mathbf{x})$, current densities for electrons and holes, denoted by $\boldsymbol{j}_n(\mathbf{x})$, $\boldsymbol{j}_p(\mathbf{x})$, and electrostatic potential, denoted by $\phi(\mathbf{x})$. As we have seen in the previous chapter, these variables satisfy the following drift-diffusion system:

$$\begin{cases} -\nabla \cdot (\epsilon_s \nabla \phi) = q(N + p - n), \\ \nabla \cdot \boldsymbol{j}_n = H \qquad \boldsymbol{j}_n = \mu_n n \nabla \phi_n, \qquad \text{in } \Omega. \\ \nabla \cdot \boldsymbol{j}_p = H \qquad \boldsymbol{j}_p = -\mu_p p \nabla \phi_p, \end{cases} \qquad (4.1)$$

In this section we write the steady-state drift diffusion system for electron and hole current density, that are related to electron and hole fluxes by the relations

$$\boldsymbol{J}_n = -q\boldsymbol{j}_n, \qquad \boldsymbol{J}_p = q\boldsymbol{j}_p, \qquad (4.2)$$

then the system (4.1) become

$$\begin{cases} -\nabla \cdot (\epsilon_s \nabla \phi) = q(N + p - n), \\ \nabla \cdot \boldsymbol{J}_n = -qH \qquad \boldsymbol{J}_n = -a_n \nabla \phi_n, \qquad \text{in } \Omega. \\ \nabla \cdot \boldsymbol{J}_p = qH \qquad \boldsymbol{J}_p = -a_p \nabla \phi_p, \end{cases} \qquad (4.3)$$

with

$$a_n = q\mu_n n, \qquad a_p = q\mu_p p, \qquad (4.4)$$

We choose as unknowns of the problem the electrostatic potential ϕ, and the quasi-Fermi potentials ϕ_n, ϕ_p. The densities n, p, are related to the quasi-Fermi potentials by the Maxwell-Boltzmann relations,

$$n = n_{\mathrm{i}} \exp\left(\frac{\phi - \phi_n}{\phi_{\mathrm{th}}}\right), \qquad p = n_{\mathrm{i}} \exp\left(-\frac{\phi - \phi_p}{\phi_{\mathrm{th}}}\right), \tag{4.5}$$

where n_{i} is the intrinsic concentration.

The system (4.3) is supplemented with mixed boundary conditions

$$\begin{cases} \phi - \phi_{\mathrm{bi}} = \phi_n = \phi_p = e_{D,i}, & \text{on } \Gamma_{D,i}, \ i = 0, 1, \ldots, n_D, \\ \dfrac{\partial \phi}{\partial \nu} = \dfrac{\partial \phi_n}{\partial \nu} = \dfrac{\partial \phi_p}{\partial \nu} = 0, & \text{on } \Gamma_N. \end{cases} \tag{4.6}$$

with $\partial \Omega = \Gamma_D \cup \Gamma_N$ with $\Gamma_D = \bigcup_{i=1}^{n_D} \Gamma_{D,i}$ and $\Gamma_N = \partial \Omega \setminus \Gamma_D$. In (4.6) we have indicate $\partial/\partial \nu = \nu \cdot \nabla$ the normal derivative along the external unit normal to the boundary, ν.

The built-in potential ϕ_{bi} is defined euquation (3.110) in chapter 3.

To prove an existence result for the steady-state drift-diffusion system (4.3) we need some assumption on the geometry, data and parameter models.

(**T.1**) Let Ω is a bounded domani in $\mathbb{R}^d$, with $d = 1, 2, 3$ of class $C^{0,1}$ and the $(k-1)$-dimensional Lebesgue measure of Γ_D is positive.

(**T.2**) The Dirichlet boundary data satisfy

$$e_{D,i}|_{\Gamma_D} \in L^\infty(\Gamma_D),$$

in particular they are constants on each $\Gamma_{D,i}$.

(**T.3**) The doping profiles satisfies $N \in L^\infty(\Omega)$. We denote with $\underline{N} := \inf_\Omega N(\mathbf{x})$ and $\overline{N} := \sup_\Omega N(\mathbf{x})$.

(**T.4**) We assume that ϵ_s is a bounded function, and there exists a positive constant $\underline{\epsilon}_s$ such that:
$$\epsilon_s(\mathbf{x}) \geq \underline{\epsilon}_s > 0.$$

(**T.5**) For the generation-recombination term $H = H(n, p)$ we assume

$$H(n, p) = -F(n, p)\left(\frac{np}{n_i^2} - 1\right) = F(n, p)\left(\exp\left(-\frac{\phi_n - \phi_p}{\phi_{\mathrm{th}}}\right) - 1\right), \tag{4.7}$$

with $F \geq 0$ and continuous with respect to the arguments. This expression for H comprises the Shockley-Read-Hall and the Auger recombination-generation terms.

(**T.6**) The electron and hole mobilities, that appear in equations (4.4) for a_n and a_p, will be assumed to be bounded, strictly positive functions of the space variable $\mathbf{x}$ and the densities n, p.

In this chapter we introduce the proof of the following main theorem for the existence of solution of the system

Theorem 4.1.1 *Under the assumption (T.1)-(T.6), the problem* (4.3) *has a weak solution* $(\phi, \phi_n, \phi_p) \in (H^1(\Omega) \cap L^\infty(\Omega))^3$, *which satisfies the L^∞-estimates:*

$$\inf_{\Gamma_D} \phi_{\text{bi}} + \min_i e_{D,i} \leq \phi \leq \sup_{\Gamma_D} \phi_{\text{bi}} + \max_i e_{D,i}, \tag{4.8}$$

$$\min_i e_{D,i} \leq \phi_n \leq \max_i e_{D,i}, \tag{4.9}$$

$$\min_i e_{D,i} \leq \phi_p \leq \max_i e_{D,i}. \tag{4.10}$$

The proof of this Theorem requires several step. For convenience, we introduce in the following section some preliminary results, which will be used in the subsequent sections to prove the existence theorem. The proof is based on an appropriate iteration map, which will be shown to be a fixed point map. The iteration map introduced here is more general than needed by the aim of the chapter, since this more general form will be used in the next chapter. In the last section we study some properties of the iteration map, for later use.

4.2 Some preliminary results

We start by introducing two basic lemmas. We will see later that these lemmas allow us to study the decoupled steady-state drift-diffusion system.

We introduce and prove these Lemmas in a more general case, that is comparising the time dependence because this is important in order to prove the results for the coupling with circuit.

Assumptions.

Let $f(\mathbf{x}, t, u)$ a continuous function with respect to $t \in [t_0, t_1]$ such that:

(**A.1**) $f(\mathbf{x}, t, u)$ is a non increasing function with respect to u, that is:

$$\frac{\partial f}{\partial u}(\mathbf{x}, t, u) \leq 0 \qquad \forall u \in \mathbb{R}, \quad \forall (\mathbf{x}, t) \in \Omega \times [0, T]. \tag{4.11}$$

(**A.2**) There exist two functions $\underline{f}(t, u)$ and $\overline{f}(t, u)$ such that:

$$\underline{f}(t, u) \leq f(\mathbf{x}, t, u) \leq \overline{f}(t, u) \qquad \forall u \in \mathbb{R}, \quad \forall (\mathbf{x}, t) \in \Omega \times [0, T]. \tag{4.12}$$

(**A.3**) There exist two functions $\underline{u}(t)$ and $\overline{u}(t)$ such that:

$$\underline{f}(t, \underline{u}(t)) = 0, \quad \text{and} \quad \overline{f}(t, \overline{u}(t)) = 0. \tag{4.13}$$

We consider the following problem:

$$\begin{cases} -\nabla \cdot (a(\mathbf{x},t)\nabla u) &= f(\mathbf{x},t,u), &\text{in } \Omega \times [t_0,t_1], \\ u &= u_D, &\text{on } \Gamma_D \times [t_0,t_1], \\ \dfrac{\partial u}{\partial \nu} &= 0, &\text{on } \Gamma_N \times [t_0,t_1], \end{cases} \qquad (4.14)$$

where $\Gamma_D \cup \Gamma_N = \partial\Omega$ and $\Gamma_D \cap \Gamma_N = \emptyset$ and $u_D(\mathbf{x},t)$ continuous with respect to $t \in [t_0,t_1]$.

For semplicity we introduce the notation

$$\underline{u}_D(t) = \min_{\Gamma_D} u_D(\cdot,t) \qquad \overline{u}_D(t) = \max_{\Gamma_D} u_D(\cdot,t). \qquad (4.15)$$

Lemma 4.2.1 *Let $a(\mathbf{x},t)$ is a bounded function and continuous with respect to $t \in [t_0,t_1]$, such that:*

$$a(\mathbf{x},t) \geq \underline{a} > 0, \ \text{for all } (\mathbf{x},t) \in \Omega \times [0,T], \qquad (4.16)$$

for a positive constant $\underline{a}$. Under the assumption (4.11)-(4.13), there exists a unique solution $u(\cdot,t) \in H^1(\Omega)$ of the problem (4.14), continuous with respect to $t \in [0,T]$. Moreover, this solution satisfies the following estimate:

$$\min\{\underline{u}_D(t), \underline{u}(t)\} \leq u(\mathbf{x},t) \leq \max\{\overline{u}_D(t), \overline{u}(t)\}. \qquad (4.17)$$

Proof. For convenience, we divide the proof of the Lemma in three parts.
1. A priori estimates.

We first prove the estimate (4.17). By (4.12) and (4.13) we have

$$-\nabla \cdot (a(\mathbf{x},t)\nabla\overline{u}) = 0 = \overline{f}(t,\overline{u}(t)) \geq f(\mathbf{x},t,\overline{u}(t)).$$

Then, if u is a solution to (4.14), we find

$$\begin{aligned} -\nabla \cdot (a(\mathbf{x},t)\nabla(u-\overline{u})) &\leq f(\mathbf{x},t,u) - f(\mathbf{x},t,\overline{u}) \\ &= \left\{ \int_0^1 \frac{\partial}{\partial u} f(\mathbf{x},t,\overline{u} + \theta(u-\overline{u}))\,d\theta \right\}(u-\overline{u}) \\ &= c(u-\overline{u}). \end{aligned}$$

where, from (4.11), we have $c = \int_0^1 \frac{\partial}{\partial u} f(\mathbf{x},t,\overline{u} + \theta(u-\overline{u}))\,d\theta \leq 0$. Then, we obtain

$$-\nabla \cdot (a(\mathbf{x},t)\nabla(u-\overline{u})) - c(u-\overline{u}) \leq 0. \qquad (4.18)$$

From the maximum principle, we have

$$\max_{\Omega}(u-\overline{u}) \leq \max_{\Gamma_D}(u-\overline{u})^+, \qquad (4.19)$$

where we use the notation $v^+ = \max(v,0)$ for any function v.

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Since $\overline{u}$ does not depend on $\mathbf{x}$, it follows that

$$\max_{\Omega}(u - \overline{u}) = \max_{\Omega} u - \overline{u}$$

and therefore

$$\max_{\Omega}(u) \le \overline{u} + \max_{\Gamma_D}(u - \overline{u})^+.$$

Now we observe that

$$\max_{\Gamma_D}(u - \overline{u})^+ \le \max\{\overline{u}_D(t) - \overline{u}, 0\}.$$

and consequently

$$u(\mathbf{x}, t) \le \max_{\Omega} u(\mathbf{x}, t) \le \max\{\overline{u}_D(t), \overline{u}(t)\}.$$

Then, since $\omega_i(-\mathbf{q})$ Similarly we obtain also

$$u(\mathbf{x}, t) \ge \min_{\Omega} u(\mathbf{x}, t) \ge \max\{\underline{u}_D(t), \underline{u}(t)\}.$$

then the estimate (4.17) is proved.

2. Uniqueness.

Let us assume that there exist two functions u' and u'', satisfying problem (4.14). Subtracting the equations obtained from (4.14) with $u = u'$ and $u = u''$, we find

$$-\nabla \cdot (a(\mathbf{x}, t)\nabla(u' - u'')) = f(u') - f(u'').$$

Multiplying by $(u' - u'')$ and integrating by part on Ω, we have

$$-\int_{\partial\Omega} (u' - u'')a(\mathbf{x}, t)\frac{\partial}{\partial\nu}(u' - u'')\, d\sigma(x)$$
$$+ \int_{\Omega} a(\mathbf{x}, t)|\nabla(u' - u'')|^2 dx = \int_{\Omega} (u' - u'')\,(f(u') - f(u''))\, dx. \quad (4.20)$$

Recalling assumption (4.11), the right-hand side is a negative quantity. Moreover, using the boundary conditions we obtain

$$\int_{\Omega} a(\mathbf{x}, t)\, |\nabla(u' - u'')|^2\, dx \le 0.$$

This inequality can hold if and only if

$$\nabla(u' - u'') = 0 \quad \text{a. e. in } \Omega, \quad (4.21)$$

because of the assumption (4.16). From (4.21), $u' - u''$ is a costant quantity but for the bonduary conditions this costant is necessarily zero.

3. Existence.

To prove the existence of solutions of the problem (4.14), we must define a fixed point map. Let $K > 0$. For $u' \in L^2(\Omega)$, we define, for all $\mathbf{x} \in \Omega$, the following cut function

$$u'_K(\mathbf{x}) = \begin{cases} K & \text{if} & u'(\mathbf{x}) \geq K, \\ u'(\mathbf{x}) & \text{if} & -K \leq u'(\mathbf{x}) \leq K, \\ -K & \text{if} & u'(\mathbf{x}) \leq K. \end{cases} \tag{4.22}$$

This function is in $L^\infty(\Omega)$, and if $u' \in H^1(\Omega)$ also $u'_K \in H^1(\Omega)$.

Now we choose $K = \max\left(|\overline{u}|, |\underline{u}|\right)$ and define an operator

$$M : L^2(\Omega) \times [0,1] \rightarrow L^2(\Omega) \quad \text{by} \quad M(u', \sigma) = u''$$

where u'' is the solution of the problem

$$\begin{cases} -\nabla \cdot (a(\mathbf{x}, t)\nabla u'') & = & \sigma f(\mathbf{x}, t, u'_K), & \text{in } \Omega \times [0, T]; \\ u'' & = & \sigma u_D, & \text{on } \Gamma_D \times [0, T], \\ \dfrac{\partial u''}{\partial \nu} & = & 0, & \text{on } \Gamma_N \times [0, T]. \end{cases} \tag{4.23}$$

Every fixed point u^* of $M(\cdot, 1)$ which satisfies $|u^*(\mathbf{x})| \leq K$ a.e. in Ω is a weak solution of (4.14). Let u^* be some fixed point of $M(., 1)$. A standard regularity result implies $u^* \in C^1(\Omega)$. Thus the set $\Omega_+ \subseteq \Omega$ of points $\mathbf{x}$ at which $u^*(\mathbf{x}) > K$ holds is open in Ω and the boundary of Ω_+ consists of point $\mathbf{x}$ at which either $u^*(\mathbf{x}) = K$ or which are contained in $\partial\Omega$. Assuming that Ω_+ is nonempty and letting $\mathbf{x}^* \in \Omega_+$, we denote with Ω_+^* the maximal connected component of Ω_+ containing $\mathbf{x}^*$. Then $u^* \in \Omega_+^*$ is solution of the problem

$$\begin{cases} -\nabla \cdot (a(\mathbf{x}, t)\nabla u^*) & = & f(\mathbf{x}, t, K), & \text{in} & \Omega_+^* \times [0, T]; \\ u^* & = & u_D, & \text{on} & \partial\Omega_+^* \cap \Gamma_D \times [0, T], \\ \dfrac{\partial u^*}{\partial \nu} & = & 0, & \text{on} & \partial\Omega_+^* \cap \Gamma_N \times [0, T], \\ u^* & = & K, & \text{on} & \partial\Omega_+^* \setminus \partial\Omega \times [0, T]. \end{cases} \tag{4.24}$$

Since $f(\mathbf{x}, t, K) \geq 0$ in Ω and $\max_{\Gamma_D} u_D \leq K$, we can conclude that $\overline{u}^* = K$ is an upper solution of this problem, which is a contraddiction. Therefore Ω_+ is empty and $u^*(\mathbf{x}) \leq K$ in $\overline{\Omega}$, similarly we obtain $u^*(\mathbf{x}) \geq -K$ in $\overline{\Omega}$. It follows $|u_D^*(\mathbf{x})| \leq K$. Thus any fixed point of $M(\cdot, 1)$ is a weak solution of (4.14).
The operator $u' \rightarrow u'_K$, $L^2(\Omega) \rightarrow L^2(\Omega)$ is continuous, then it is possible to show that the right hand side of the first equation in (4.23) $\sigma f(\mathbf{x}, t, u'_K)$ depends continuously in $L^2(\Omega)$ on $(u', \sigma) \in L^2(\Omega) \times [0, 1]$. Thus, by the continuous dependence of solutions of elliptic equations in $H^1(\Omega)$ on $L^2(\Omega)$-right hand side and $H^1(\Omega)$-boundary data, it follows the continuity of operator M. The range of M is bounded in $H^1(\Omega)$

$$\|u''\|_{1,2,\Omega} \leq c\|f(\mathbf{x}, t, u'_K)\|_{2,\Omega} \leq c\mu(\Omega)^{1/2}\,\overline{f}(t, K),$$

where c is a generic constant and $\mu(\Omega)$ is the measure of Ω. Since $H^1(\Omega)$ is compactly imbedded in $L^2(\Omega)$ we can conclude that M is completely continuous. Moreover $M(u', 0) = 0$ holds for all $u' \in L^2(\Omega)$. The maximum principle implies that $u'' = M(u', \sigma)$ satisfies $\|u''\|_{\infty,\Omega} \leq$ const. indipendently of $u' \in L^2(\Omega)$ and $\sigma \in [0, 1]$ since $\|f(\mathbf{x}, t, u_K)\|_{\infty,\Omega} \leq \overline{f}(t, K)$. Thus the Leray-Schauder Theorem proves the existence of a fixed point u^* of $M(\cdot, 1)$. ∎

Next, we consider the problem

$$
\begin{cases}
-\nabla \cdot (a_1(\mathbf{x}, t)\nabla u_1) &= f(\mathbf{x}, t, u_1 - u_2), & \text{in } \Omega \times [0, T], \\
-\nabla \cdot (a_2(\mathbf{x}, t)\nabla u_2) &= -f(\mathbf{x}, t, u_1 - u_2), & \text{in } \Omega \times [0, T], \\
u_1 &= u_2 = u_D, & \text{on } \Gamma_D \times [0, T], \\
\dfrac{\partial u_1}{\partial \nu} &= \dfrac{\partial u_2}{\partial \nu} = 0, & \text{on } \Gamma_N \times [0, T].
\end{cases}
\tag{4.25}
$$

For this problem we can proove the following Lemma.

Lemma 4.2.2 *Let $a_1(\mathbf{x}, t)$, $a_2(\mathbf{x}, t)$ are bounded functions, continuous in t and such that:*

$$
a_1(\mathbf{x}, t) \geq \underline{a}_1 > 0, \qquad a_2(\mathbf{x}, t) \geq \underline{a}_2 > 0,
\tag{4.26}
$$

for positive constants $\underline{a}_1$, $\underline{a}_2$. Under the assumptions (4.11)-(4.12) and

$$
\underline{f}(t, 0) = \overline{f}(t, 0) = 0, \text{ for all } t \in [0, T],
\tag{4.27}
$$

problem (4.25) has a unique solution $(u_1, u_2) \in C([0, T], (H^1(\Omega))^2)$. This solution satisfies the estimates

$$
\underline{u}_D(t) \leq u_1(\mathbf{x}, t) \leq \overline{u}_D(t), \quad \underline{u}_D(t) \leq u_2(\mathbf{x}, t) \leq \overline{u}_D(t), \quad \text{in } \Omega \times [0, T].
\tag{4.28}
$$

Proof. The proof of the Lemma is based on a fixed point argument. To define a fixed point map, we consider two functions $u_1', u_2' \in C([0, T], L^2(\Omega))$, satisfying the estimates in (4.28). Then, let us consider the two decoupled problems:

$$
\begin{cases}
-\nabla \cdot (a_1(\mathbf{x}, t)\nabla u_1) &= f_1(\mathbf{x}, t, u_1), & \text{in } \Omega \times [0, T], \\
u_1 &= u_D, & \text{on } \Gamma_D \times [0, T], \\
\dfrac{\partial u_1}{\partial \nu} &= 0, & \text{on } \Gamma_N \times [0, T].
\end{cases}
\tag{4.29}
$$

$$
\begin{cases}
-\nabla \cdot (a_2(\mathbf{x}, t)\nabla u_2) &= f_2(\mathbf{x}, t, u_2), & \text{in } \Omega \times [0, T], \\
u_2 &= u_D, & \text{on } \Gamma_D \times [0, T], \\
\dfrac{\partial u_2}{\partial \nu} &= 0, & \text{on } \Gamma_N \times [0, T],
\end{cases}
\tag{4.30}
$$

where we have introduced the functions

$$f_1(\mathbf{x}, t, u_1) := f(\mathbf{x}, t, u_1 - u_2'(\mathbf{x}, t)), \tag{4.31}$$
$$f_2(\mathbf{x}, t, u_2) := -f(\mathbf{x}, t, u_1'(\mathbf{x}, t) - u_2). \tag{4.32}$$

Both problems (4.29) and (4.30) satisfy the hypotesis of Lemma 4.2.1, with a, f, u replaced with a_1, f_1, u_1, and a_2, f_2, u_2, respectively. Specifically, let us consider problem (4.29), first. Recalling the assumptions (4.11), (4.12), and using the estimate (4.28) for u_2', we find

$$\underline{f}(t, u_1 - \underline{u}_D) \leq f_1(\mathbf{x}, t, u_1) \leq \overline{f}(t, u_1 - \overline{u}_D).$$

Then we can introduce the functions

$$\underline{f}_1(t, u_1) := \underline{f}(t, u_1 - \underline{u}_D), \quad \overline{f}_1(t, u_1) := \overline{f}(t, u_1 - \overline{u}_D),$$

and assumption (4.12) holds with $\underline{f} = \underline{f}_1$, $\overline{f} = \overline{f}_1$. Moreover, recalling (4.27), we get

$$\underline{f}_1(t, \underline{u}_D) = \underline{f}(t, 0) = 0, \quad \overline{f}_1(t, \overline{u}_D) = \overline{f}(t, 0) = 0,$$

thus assumption (4.13) holds with $\underline{u} = \underline{u}_D$, $\overline{u} = \overline{u}_D$.

Similarly, for problem (4.30) we find

$$-\overline{f}(t, \underline{u}_D - u_2) \leq f_2(\mathbf{x}, t, u_2) \leq -\underline{f}(t, \overline{u}_D - u_2).$$

Then we can introduce the functions

$$\underline{f}_2(t, u_2) := -\overline{f}(t, \underline{u}_D - u_2), \quad \overline{f}_2(t, u_2) := -\underline{f}(t, \overline{u}_D - u_2),$$

and assumption (4.12) holds with $\underline{f} = \underline{f}_2$, $\overline{f} = \overline{f}_2$. Then, recalling (4.27), also in this case assumption (4.13) holds with $\underline{u} = \underline{u}_D$, $\overline{u} = \overline{u}_D$.

In conclusion, applying Lemma 4.2.1, there exists a unique solution $u_1(\cdot, t) = u_1''(\cdot, t) \in H^1(\Omega)$ of problem (4.29), and a unique solution $u_2(\cdot, t) = u_2''(\cdot, t) \in H^1(\Omega)$ of problem (4.30). These solutions satisfy the estimates in (4.28).

In this way we have defined a map

$$(u_1', u_2') \mapsto M(u_1', u_2') := (u_1'', u_2''),$$

which acts from

$$\mathcal{X} := \{(v_1, v_2) \in C([0, T], (L^2(\Omega))^2) \mid \underline{u}_D \leq v_1 \leq \overline{u}_D, \ \underline{u}_D \leq u_2 \leq \overline{u}_D\}$$

in to itself. It is possible to see that $\mathcal{X}$ is a nonempty, closed, bounded subset of the Banach space $C([0, T], (L^2(\Omega))^2)$, and that the map M is compact. Then, using Schauder's fixed point theorem, we obtain the existence of a couple of functions $(v_1, v_2) \in (H^1(\Omega))^2$ that is solution of problem (4.25), and satisfies the estimate (4.28).

The uniqueness of this solution can be obtained by using the same arguments used for the uniqueness proof in Lemma 4.2.1. ∎

4.3 Proof of the existence result

In this section prove the existence result for the system (4.3). We use this strategy: we decouple by iteration the system into two systems, one containing the Poisson equation and other containing the continuity equations. In the following subsection we introduce an iteration map that will be used also in next chapter.

4.3.1 Iteration map for the device equations

We consider $\boldsymbol{e}_D$, $\boldsymbol{e}_D^* \in \mathbb{R}^{n_D+1}$, with components

$$
\boldsymbol{e}_D = \begin{bmatrix} e_{D,0} \\ e_{D,1} \\ \vdots \\ e_{D,n_D} \end{bmatrix}, \qquad \boldsymbol{e}_D^* = \begin{bmatrix} e_{D,0}^* \\ e_{D,1}^* \\ \vdots \\ e_{D,n_D}^* \end{bmatrix},
$$

and define the following elliptic system

$$
\begin{cases}
-\nabla \cdot (\epsilon_s \nabla \phi^*) = q(N + p^* - n^*), \\
\nabla \cdot \boldsymbol{J}_n = qF^*(n_i^{-2}np - 1), \qquad \boldsymbol{J}_n = -a_n^* \nabla \phi_n, \qquad \text{in } \Omega \\
\nabla \cdot \boldsymbol{J}_p = -qF^*(n_i^{-2}np - 1), \qquad \boldsymbol{J}_p = -a_p^* \nabla \phi_p,
\end{cases} \tag{4.33}
$$

in which we have posed $a_n^* = q\mu_n n^*$, $a_p^* = q\mu_p p^*$, and boundary conditions

$$
\begin{cases}
\phi^* - \phi_{\text{bi}} = e_{D,i}^*, \ \phi_n = \phi_p = e_{D,i}, \quad \text{on } \Gamma_{D,i}, \ i = 0, 1, \ldots, n_D, \\
\dfrac{\partial \phi}{\partial \nu} = \dfrac{\partial \phi_n}{\partial \nu} = \dfrac{\partial \phi_p}{\partial \nu} = 0, \qquad \qquad \text{on } \Gamma_N,
\end{cases} \tag{4.34}
$$

where: $n^* = n(\phi^*, \phi_n^*)$, $p^* = p(\phi^*, \phi_p^*)$, with

$$
n(\phi, \phi_n) = n_i \exp\left(\frac{\phi - \phi_n}{\phi_{\text{th}}}\right), \qquad p(\phi, \phi_n) = n_i \exp\left(\frac{\phi_p - \phi}{\phi_{\text{th}}}\right). \tag{4.35}
$$

The * on F denotes evaluation on n^*, p^*, that is, $F^* = F(n^*, p^*)$.

We divide the system (4.33) in two systems.
First step. The first system is one that includes the nonlinear Poisson equation

$$
\begin{cases}
-\nabla \cdot (\epsilon_s \nabla \phi^*) = q(N + p(\phi^*, \phi_p^*) - n(\phi^*, \phi_n^*)), & \text{in } \Omega, \\
\phi^* - \phi_{\text{bi}} = e_{D,i}^*, & \text{on } \Gamma_{D,i}, \\
\dfrac{\partial \phi}{\partial \nu} = 0, & \text{on } \Gamma_N,
\end{cases} \tag{4.36}
$$

where the built-in potential ϕ_{bi} depends on $N(\mathbf{x})$, as defined in chapter 3. On $\epsilon_s(\mathbf{x})$ and $N(\mathbf{x})$ we make assumptions (**T.3**)-(**T.4**).

Observing that the problem (4.36) has the same structure of problem (4.14), then, using the Lemma (4.2.1), we have that this problem admits a unique solution $\phi^* \in H^1(\Omega)$. Moreover, the solution satisfies the estimate:

$$\inf_{\Gamma_D} \phi_{\text{bi}} + \min_i e^*_{D,i} \leq \phi^* \leq \sup_{\Gamma_D} \phi_{\text{bi}} + \min_i e^*_{D,i}, \quad \text{a.e. in } \Omega. \tag{4.37}$$

Second step. We consider the problem:

$$\begin{cases} -\nabla \cdot (\, a_n^* \nabla \phi_n) = qF^*(n_i^{-2}np - 1), & \\ -\nabla \cdot (\, a_p^* \nabla \phi_p) = -qF^*(n_i^{-2}np - 1), & \text{in } \Omega \\ \phi_n = \phi_p = e_{D,i}, & \text{on } \Gamma_{D,i}, \\ \dfrac{\partial \phi_n}{\partial \nu} = \dfrac{\partial \phi_p}{\partial \nu} = 0, & \text{on } \Gamma_N, \end{cases} \tag{4.38}$$

The functions a_n^*, a_p^*, F^* are evaluated for $\phi = \phi^*$, $\phi_n = \phi_n^*$, $\phi_p = \phi_p^*$. Thanks to (4.35), the term $n_i^{-2}np$ depends only on $\phi_n - \phi_p$, since we have

$$n_i^{-2}np = \exp\left(\frac{\phi_p - \phi_n}{\phi_{\text{th}}}\right).$$

The above problem has the same structure of problem (4.25), then using Lemma (4.2.2) , we find that the problem (4.38) has a unique solution $(\phi_n, \phi_p) \in (H^1(\Omega) \cap L^\infty(\Omega))^2$. This solution satisfies the estimates

$$\min_i e_{D,i} \leq \phi_n \leq \max_i e_{D,i}, \quad \min_i e_{D,i} \leq \phi_p \leq \max_i e_{D,i} \quad \text{a.e. in } \Omega. \tag{4.39}$$

Using the system (4.33) with boundary conditions (4.34), it is possible to define an iteration map for the device current in the following way. For any given $\boldsymbol{e}_D$, $\boldsymbol{e}_D^* \in \mathbb{R}^{n_D+1}$, with components $\boldsymbol{e}_D = (e_{D,0}, \ldots, e_{D,n_D})^\top$, $\boldsymbol{e}_D^* = (e_{D,0}^*, \ldots, e_{D,n_D}^*)^\top$, we introduce the function $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*)$, which maps the function $\boldsymbol{\Phi}^* \equiv (\phi_n^*, \phi_p^*)$, taken in a set $\mathcal{M}$ to be specified later, to the function $\boldsymbol{\Phi} = (\phi_n, \phi_p)$ defined by the elliptic system (4.33) with boundary conditions (4.34). We use the notation

$$\boldsymbol{\Phi} = \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*), \tag{4.40}$$

that is,

$$(\phi_n, \phi_p) = (\phi_n^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*), \phi_p^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)).$$

Thus, for any given $\boldsymbol{e}_D, \boldsymbol{e}_D^* \in \mathbb{R}^{n_D+1}$, we have defined the map

$$\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*) \; : \; \boldsymbol{\Phi}^* \mapsto \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*).$$

We can also view the above map in the following way: for any given $\boldsymbol{e}_D \in \mathbb{R}^{n_D+1}$, we consider the map

$$\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D) \; : \; (\boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \mapsto \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*).$$

This view will be adopted in the next chapter. In this chapter we will always take $\boldsymbol{e}_D = \boldsymbol{e}_D^*$. Nevertheless, for later use, we will considered the map with the most general variation of arguments.

Lemma 4.3.1 (Well-posedness of $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*)$) *For any $\boldsymbol{e}_D, \boldsymbol{e}_D^* \in \mathbb{R}^{n_D+1}$, the problem (4.33)–(4.34) defines uniquely a map*

$$\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*) \,:\, \mathscr{M}(\boldsymbol{e}_D^*) \to \mathscr{M}^\sharp(\boldsymbol{e}_D) := \mathscr{M}(\boldsymbol{e}_D) \cap H^1(\Omega),$$

$$\mathscr{M}(\boldsymbol{e}_D^*) \ni \boldsymbol{\Phi}^* \mapsto \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \in \mathscr{M}^\sharp(\boldsymbol{e}_D).$$

where

$$\mathscr{M}(\boldsymbol{e}_D) = \{\psi \in L^2(\Omega) \mid \min_i e_{D,i} \leq \psi \leq \max_i e_{D,i} \text{ a.e. in } \Omega\}^2.$$

The first equation in (4.33) is decoupled from the other two equations, and defines the electric potential $\phi^* = \phi^*(\boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, which is then used in the next two equations. So the definition of $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D)$ actually takes place in two steps. Thus, the proof of Lemma 4.3.1 will result from the uniqueness of the solutions of the systems (4.36),(4.38).

Using the same considerations we have also that

Lemma 4.3.2 *If $\boldsymbol{\Phi}^* \in \mathscr{M}(\boldsymbol{e}_D^*)$, that is, $\boldsymbol{\Phi}^* \in L_2(\Omega)$ and*

$$\min_i e_{D,i}^* \leq \phi_n^* \leq \max_i e_{D,i}^*, \quad a.e. \ in \ \Omega, \tag{4.41}$$

$$\min_i e_{D,i}^* \leq \phi_p^* \leq \max_i e_{D,i}^*, \quad a.e. \ in \ \Omega, \tag{4.42}$$

then problem (4.36) has a unique solution $\phi^* \in H^1(\Omega)$, which we denote also by $\phi^*(\boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$. Moreover, the solution satisfies the following estimate:

$$\inf_{\Gamma_D} \phi_{\mathrm{bi}} + \min_i e_{D,i}^* \leq \phi^* \leq \sup_{\Gamma_D} \phi_{\mathrm{bi}} + \min_i e_{D,i}^*, \quad a.e. \ in \ \Omega. \tag{4.43}$$

4.3.2 Existence of fixed points

In this section we conclude the proof of the existence theorem 4.1.1, the main result of this chapter.

In the previous subsection we have introduced the iteration map $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*)$, and we have shown that it is well defined from $\mathscr{M}(\boldsymbol{e}_D^*)$ to $\mathscr{M}(\boldsymbol{e}_D) \cap H^1(\Omega)$. In particular, if we take $\boldsymbol{e}_D^* = \boldsymbol{e}_D$, we find that the map $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D)$ is well defined from $\mathscr{M}(\boldsymbol{e}_D)$ to $\mathscr{M}(\boldsymbol{e}_D) \cap H^1(\Omega)$.

We observe that any fixed point of $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D)$ is a solution of the drift-diffusion equations (4.3), as can be seen by inspecting the defining problem (4.33)-(4.34). Moreover, since for any fixed point $\boldsymbol{\Phi}^*$ we have

$$\boldsymbol{\Phi}^* = \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D, \boldsymbol{\Phi}^*) \in \mathscr{M}(\boldsymbol{e}_D),$$

it follows that its components ϕ_n^*, ϕ_p^* satisfy the estimates (4.9), (4.10). Then, by using lemma 4.3.2, the electric potential $\phi^* = \phi^*(\boldsymbol{e}_D, \boldsymbol{\Phi}^*)$ satisfies the estimate (4.8). Thus, theorem 4.1.1 is proved if can show the existence of a fixed point of the map $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D)$.

We have that $\mathscr{M}(\boldsymbol{e}_D)$ is nonempty, bounded, closed, convex subset of $L^2(\Omega)$. Also, $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D)$ is an compact automorphism of $\mathscr{M}(\boldsymbol{e}_D)$, since H^1 is compacly embedded in $L^2(\Omega)$. Then, Schauder's Theorem implies the existence of a fixed point, and the proof of theorem 4.1.1 is completed.

4.4 Device current and passivity

In this section we define in a proper way the electric currents flowing through the Ohmic contacts, and establish some properties which will be used for the coupling to the circuit.

As we will see, the electric currents at the terminals are defined once we have a solution of the drift-diffusion equations. We have seen in chapter 2 that, in principle, these currents depend on the applied potentials. Moreover, we can show that they are invariant under translation of the applied potentials, so they actually depend on the voltage drops with respect to a terminal, chosen as ground terminal for the device.

In fact, theorem 4.1.1 establishes the existence of at least a solution, but says nothing on its uniqueness. In general we do not expect to have uniqueness of solutions without additional assuptions, and there could be more than one solution corresponding to the same applied potentials. Then the previous considerations on the dependence of the currents on the applied potentials are valid only locally, and we cannot define a map that to any applied potentials associate the resulting terminal currents. In this respect, the device-circuit coupled problem does not appear to be well-posed in a simple way.

Nevertheless, we will see in the next chapter a way to give a meaning to this coupled problem. The key idea is that the iteration map defined in the previous section gives rise to a well-defined current, which is Lipschitz-continuous with respect to the applied potentials.

In the next two subsection we define the currents through the terminals of the device, and prove the passivity of the device. Then, we will discuss in more details the current defined by the iteration map $\mathbf{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D)$, and prove some relevant properties.

4.4.1 Device current

To define the electric current flowing through the Ohmic contacts of the device, we introduce the auxiliary functions w_i, $i = 0, 1, \ldots, n_D$, defined by the following elliptic boundary value problem:

$$
\begin{cases}
-\nabla \cdot (\epsilon_D \nabla w_i) &= 0, \quad \text{in } \Omega, \\
w_i &= \delta_{ij}, \quad \text{on } \Gamma_{D,j}, \quad j = 0, 1, \ldots, n_D, \\
\dfrac{\partial w_i}{\partial \nu} &= 0, \quad \text{on } \Gamma_N,
\end{cases}
\tag{4.44}
$$

where δ_{ij} is Kronecker's delta ($\delta_{ij} = 1$ if $i = j$, $\delta_{ij} = 0$ if $i \neq j$).

Then, the electric current $j_{D,i}$ flowing through the ith Ohmic contact $\Gamma_{D,i}$ is defined by the surface integral

$$
j_{D,i}(t) = -\int_\Omega \nabla w_i \cdot (\boldsymbol{J}_n(\mathbf{x}, t) + \boldsymbol{J}_p(\mathbf{x}, t)) \; \mathrm{d}\mathbf{x}.
\tag{4.45}
$$

Remark 4.4.1 *It is possible to see that the definition* (4.45) *leads to the usual definition of current. In fact, summing up the two equations* $\nabla \cdot \boldsymbol{J}_n = -qH$ *and* $\nabla \cdot \boldsymbol{J}_p = qH$ *of the drift-diffusion system* (4.3) *we find that*

$$\nabla \cdot (\boldsymbol{J}_n + \boldsymbol{J}_p) = 0. \tag{4.46}$$

From Gauss divergence theorem, recalling the boundary values of w_i*, we obtain*

$$j_{D,i}(t) = -\int_{\Gamma_{D,i}} \nu \cdot (\boldsymbol{J}_n(\mathbf{x}, t) + \boldsymbol{J}_p(\mathbf{x}, t)) \ \mathrm{d}\sigma(\mathbf{x}), \tag{4.47}$$

that is, the natural definition for the electric current through the i-th Ohmic contact $\Gamma_{D,i}$*, (given in chapter 2,* (2.21)*). The expression in* (4.47) *is equivalent to the one in* (4.45)*, if the right-hand side is well defined.*

By definition, the currents $j_{D,i}$ depend on $e_{D,k}$, $i, k = 0, 1, \ldots, n_D$. Actually the currents are not independent quantities. Furthermore, they depend only on the voltage drops $e_{D,k} - e_{D,0}$, $k = 1, \ldots, n_D$, where $e_{D,0}$ is the potential corresponding to the ground contact, arbitrarily chosen. These concepts are formally expressed in the following propositions.

Proposition 4.4.1 *The currents* $j_{D,i}$*,* $i = 0, 1, \ldots, n_D$*, defined in* (4.45)*, satisfy the relation*

$$\sum_{i=0}^{n_D} j_{D,i}(t) = 0, \tag{4.48}$$

in according with the conservation of charge.

Proof. The function $w_0 + w_1 + \cdots + w_{n_D}$ satisfies the elliptic equation in (4.44) with Dirichlet data identically 1 on Γ_D and uniform Neumann conditions on Γ_N. It is simple to verify that the function 1 satisfies the same problem. Then, from uniqueness, it follows

$$\sum_{i=0}^{n_D} w_i = 1. \tag{4.49}$$

Thus, using (4.49), we have also

$$\nabla \left(\sum_{i=0}^{n_D} w_i \right) = 0,$$

which yields (4.48). ∎

Proposition 4.4.2 *The currents* $j_{D,i}$*,* $i = 0, 1, \ldots, n_D$*, are invariant under the translation of the applied potential*

$$e_{D,k} \rightarrow e_{D,k} + \bar{e}_D, \qquad k = 0, 1, \ldots, n_D. \tag{4.50}$$

Proof. The translation (4.50) produces a translation

$$(\phi, \phi_n, \phi_p) \rightarrow (\phi + \bar{e}_D, \phi_n + \bar{e}_D, \phi_p + \bar{e}_D).$$

The relation (4.45) which defines $j_{D,i}$ depends on n, p, $\nabla \phi$, $\nabla \phi_n$, $\nabla \phi_p$. Recalling (4.5), it follows that $j_{D,i}$ is independent of $\bar{e}_D$. ∎

4.4.2 Passivity condition

Now we introduce a property of the device current, said passivity condition, as we will see, this property is fundamental for the description of the coupling with circuit equations. We remember the definition of applied potential vector $\boldsymbol{e}_D$ and voltage drops vector $\boldsymbol{v}_D$ introduced in chapter 2,

$$
\boldsymbol{e}_D = \begin{bmatrix} e_{D,0} \\ \vdots \\ e_{D,n_D} \end{bmatrix}, \qquad \boldsymbol{v}_D = \begin{bmatrix} e_{D,1} - e_{D,0} \\ \vdots \\ e_{D,n_D} - e_{D,0} \end{bmatrix}, \tag{4.51}
$$

and we define the vectors which components given by (4.45)

$$
\boldsymbol{j}_D = \begin{bmatrix} j_{D,0} \\ \vdots \\ j_{D,n_D} \end{bmatrix}, \qquad \boldsymbol{i}_D = \begin{bmatrix} j_{D,1} \\ \vdots \\ j_{D,n_D} \end{bmatrix}, \tag{4.52}
$$

We notice that

$$
\boldsymbol{e}_D^\top \boldsymbol{j}_D = \boldsymbol{v}_D^\top \boldsymbol{i}_D. \tag{4.53}
$$

Lemma 4.4.1 *For a fixed $t > 0$, let $(\phi, \phi_n, \phi_p)(\mathbf{x}, t)$ be a solution of the drift-diffusion equation (4.3) with boundary condition (4.6). Then, we have the passivity condition*

$$
\boldsymbol{v}_D^\top \boldsymbol{i}_D \geq 0, \tag{4.54}
$$

where $\boldsymbol{v}_D$, $\boldsymbol{i}_D$ are defined in (4.51), (4.52) respectively.

Proof. To prove the passivity condition we consider the equations for ϕ_n, ϕ_p in the system (4.3)

$$
\begin{aligned}
\nabla \cdot (-a_n \nabla \phi_n) &= -qH, \\
\nabla \cdot (-a_p \nabla \phi_p) &= qH,
\end{aligned}
$$

multiplying them for ϕ_n, ϕ_p respectively, integrating over Ω and summing them, we have

$$
-\int_\Omega [\phi_n \nabla \cdot (a_n \nabla \phi_n) + \phi_p \nabla \cdot (a_p \nabla \phi_p)]\, \mathrm{d}\mathbf{x} = \int_\Omega (\phi_n - \phi_p) qH \, \mathrm{d}\mathbf{x} \leq 0,
$$

the inequality come from the expression of H in (4.7). From conservation of charge, we have the identity

$$
\nabla \cdot (a_n \nabla \phi_n) + \nabla \cdot (a_p \nabla \phi_p) = 0,
$$

then we get

$$
-\int_\Omega \left[\left(\phi_n - \sum_{k=0}^{n_D} w_k e_{D,k} \right) \nabla \cdot (a_n \nabla \phi_n) + \left(\phi_p - \sum_{k=0}^{n_D} w_k e_{D,k} \right) \nabla \cdot (a_p \nabla \phi_p) \right] \mathrm{d}\mathbf{x} \leq 0,
$$

where w_k is the auxiliary function defined in (4.44). It is possible to verify that

$$\phi_n - \sum_{k=0}^{n_D} w_k e_{D,k} = 0 \quad \text{and} \quad \phi_p - \sum_{k=0}^{n_D} w_k e_{D,k} = 0, \quad \text{on } \Gamma_D.$$

Then, integrating by parts the previous inequality, and using the definition of $\boldsymbol{j}_D$, we obtain

$$\int_\Omega \left[a_n |\nabla \phi_n|^2 + a_p |\nabla \phi_p|^2 \right] \, \mathrm{d}\mathbf{x} - \boldsymbol{e}_D^\top \boldsymbol{j}_D \leq 0.$$

Using (4.53), the previous inequality gives immediately the passivity condition (4.54). ∎

4.4.3 The current map

The map $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*)$ defines also the modified electron and hole currents, $\boldsymbol{j}_n = \boldsymbol{j}_n^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, $\boldsymbol{j}_p = \boldsymbol{j}_p^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, by the expressions in (4.33), that is,

$$\boldsymbol{j}_n = -a_n^* \nabla \phi_n, \quad \boldsymbol{j}_p = -a_p^* \nabla \phi_p, \tag{4.55}$$

with $\phi_n = \phi_n^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, $\phi_p = \phi_p^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$. We use the notation

$$\boldsymbol{j}_D^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \;=\; \begin{bmatrix} j_{D,0}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \\ \vdots \\ j_{D,n_D}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \end{bmatrix}, \tag{4.56}$$

$$\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \;=\; \begin{bmatrix} j_{D,1}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \\ \vdots \\ j_{D,n_D}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \end{bmatrix}, \tag{4.57}$$

where we have introduced the voltage drops

$$\boldsymbol{v}_D = \widehat{\boldsymbol{A}}^\top \boldsymbol{e}_D. \tag{4.58}$$

Propositions 4.4.1 and 4.4.2 can be extended also to the modified equations (4.33)–(4.34). This explains why we consider $\boldsymbol{i}_D^\sharp$ as a function of $\boldsymbol{v}_D$ instead of $\boldsymbol{i}_D$. We have also the relation

$$\boldsymbol{j}_D^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) = \widehat{\boldsymbol{A}} \boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*). \tag{4.59}$$

Using the result in [5] we have the following Lemma.

Lemma 4.4.2 (Lipschitz-continuity and passivity) *Let us consider* $\boldsymbol{e}_D^* \in \mathbb{R}^{n_D+1}$, *and* $\boldsymbol{\Phi}^* \in \mathcal{M}(\boldsymbol{e}_D^*)$. *Then, the map*

$$\mathbb{R}^{n_D} \ni \boldsymbol{v}_D \mapsto \boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \in \mathbb{R}^{n_D}$$

is Lipschitz-continuous with respect to $\boldsymbol{v}_D$, that is,

$$\|\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D'; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) - \boldsymbol{i}_D^\sharp(\boldsymbol{v}_D''; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)\| \leq c(\boldsymbol{e}_D^*)\|\boldsymbol{v}_D' - \boldsymbol{v}_D''\|, \qquad (4.60)$$

for all $\boldsymbol{v}_D'$, $\boldsymbol{v}_D'' \in \mathbb{R}^{n_D}$, for some positive constant $c(\boldsymbol{e}_D^*)$ depending on $\boldsymbol{e}_D^*$ and on the data of the problem. Moreover, $\boldsymbol{i}_D^\sharp$ satisfies the passivity condition

$$\boldsymbol{v}_D^\top \boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \geq 0. \qquad (4.61)$$

Proof. Let us consider any vectors $\boldsymbol{e}_D', \boldsymbol{e}_D'' \in \mathbb{R}$ such that

$$\boldsymbol{v}' = \widehat{\boldsymbol{A}}^\top \boldsymbol{e}_D', \quad \boldsymbol{v}'' = \widehat{\boldsymbol{A}}^\top \boldsymbol{e}_D''.$$

Let us introduce the two functions $\boldsymbol{\Phi}' = \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D'; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, $\boldsymbol{\Phi}'' = \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D''; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, which for simplicity we denote just by $\boldsymbol{\Phi}' = (\phi_n', \phi_p')$, $\boldsymbol{\Phi}'' = (\phi_n'', \phi_p'')$. We will use the notation $\delta g(\boldsymbol{e}_D, \boldsymbol{\Phi}) = g(\boldsymbol{e}_D', \boldsymbol{\Phi}') - g(\boldsymbol{e}_D'', \boldsymbol{\Phi}'')$ for any suitable g, e.g., $\delta\phi_n = \phi_n' - \phi_n''$ and

$$\begin{aligned}
\delta j_{D,i}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) &= j_{D,i}^\sharp(\boldsymbol{e}_D'; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) - j_{D,i}^\sharp(\boldsymbol{e}_D''; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \\
&= \int_\Omega \nabla w_i \cdot \left(a_n^* \nabla\delta\phi_n + a_p^* \nabla\delta\phi_p\right) \, \mathrm{d}\mathbf{x}.
\end{aligned}$$

Subtracting the equations for $\boldsymbol{\Phi}'$ and $\boldsymbol{\Phi}''$, and omitting to write explicitly the dependence on $\mathbf{x}$, we get

$$-\nabla \cdot (a_n^* \nabla\delta\phi_n) = \delta f(\phi_n - \phi_p), \qquad (4.62)$$
$$-\nabla \cdot (a_p^* \nabla\delta\phi_p) = -\delta f(\phi_n - \phi_p), \qquad (4.63)$$

where we use the notation $f(\psi) = qF^*(\exp(-\psi/\phi_{\mathrm{th}})-1)$. Now we multiply (4.62) and (4.63) by $\delta\phi_n$ and $\delta\phi_p$, respectively. Summing the resulting equations, we obtain

$$-\sum_{\alpha=n,p} \delta\phi_\alpha \nabla \cdot (a_\alpha^* \nabla\delta\phi_\alpha) = \delta(\phi_n - \phi_p)\delta f(\phi_n - \phi_p) \leq 0. \qquad (4.64)$$

The right-hand side is a non-positive quantity since f is a non increasing function. Next, summing up (4.62) and (4.63) , we find

$$-\sum_{\alpha=n,p} \nabla \cdot (a_\alpha^* \nabla\delta\phi_\alpha) = 0.$$

Then the following identity holds:

$$-\int_\Omega \sum_{\alpha=n,p} \left(\delta\phi_\alpha - \sum_{k=0}^{n_D} w_k \delta e_{D,k}\right) \nabla \cdot (a_\alpha^* \nabla\delta\phi_\alpha) \, \mathrm{d}\mathbf{x}$$
$$= -\int_\Omega \sum_{\alpha=n,p} \delta\phi_\alpha \nabla \cdot (a_\alpha^* \nabla\delta\phi_\alpha) \, \mathrm{d}\mathbf{x}. \qquad (4.65)$$

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We note that

$$\left[\delta\phi_\alpha - \sum_{k=0}^{n_D} w_k \delta e_{D,k}\right]_{\Gamma_{D,i}} = \delta e_{D,i} - \sum_{k=0}^{n_D} \delta_{ik}\delta e_{D,k} = 0, \quad \alpha = n, p,$$

that is,

$$\delta\phi_n - \sum_{k=0}^{n_D} w_k \delta e_{D,k} = \delta\phi_p - \sum_{k=0}^{n_D} w_k \delta e_{D,k} = 0, \quad \text{on } \Gamma_D.$$

Integrating by part the left-hand side of (4.65), and recalling (4.64), using the definition of $j_{D,i}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, we obtain

$$\int_\Omega \sum_{\alpha=n,p} a_\alpha^* |\nabla\delta\phi_\alpha|^2 \, \mathrm{d}\mathbf{x} - \sum_{k=0}^{n_D} \delta e_{D,k} \delta j_{D,k}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \, \mathrm{d}\mathbf{x}$$

$$= -\sum_{\alpha=n,p} \int_\Omega \delta\phi_\alpha \nabla \cdot (a_\alpha^* \nabla\delta\phi_\alpha) \, \mathrm{d}\mathbf{x} \le 0, \tag{4.66}$$

which gives

$$\int_\Omega \sum_{\alpha=n,p} a_\alpha^* |\nabla\delta\phi_\alpha|^2 \, \mathrm{d}\mathbf{x} \le \delta\boldsymbol{e}_D^\top \delta\boldsymbol{j}_D^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$$

$$= \delta\boldsymbol{v}_D^\top \delta\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*). \tag{4.67}$$

On the other hand, we have

$$|\delta\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)|^2 \le \sum_{i=1}^{n_D} \|\nabla w_i\|_{L^2}^2 \int_\Omega \left(\sum_{\alpha=n,p} a_\alpha^* \nabla\delta\phi_\alpha\right)^2 \mathrm{d}\mathbf{x}$$

$$\le c \int_\Omega \sum_{\alpha=n,p} a_\alpha^* |\nabla\delta\phi_\alpha|^2 \, \mathrm{d}\mathbf{x}, \tag{4.68}$$

with $c = \sum_{i=1}^{n_D} \|\nabla w_i\|_{L^2}^2 \max\{\|a_n^*\|_{L^\infty}, \|a_p^*\|_{L^\infty}\}$. This constant depends only on the bounds on $\boldsymbol{\Phi}^*$, that is, on $\boldsymbol{e}_D^*$, and on the data of the problem, that is, on the mobility functions and the doping profile. Using (4.67) in (4.68) we obtain

$$|\delta\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)|^2 \le c\delta\boldsymbol{v}_D^\top \delta\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$$

$$\le c |\delta\boldsymbol{v}_D| \left|\delta\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)\right|,$$

dividing by $\left|\delta\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)\right|$ we have

$$|\delta\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)| \le c |\delta\boldsymbol{v}_D|. \tag{4.69}$$

This proves the Lipschitz continuity of $\boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$ with respect to $\boldsymbol{v}_D$.

We can prove the passivity condition as in Lemma 4.4.1. ∎

Proposition 4.4.3 *Under the same assumptions of Lemma 4.2.1, the function*

$$\mathbb{R}^{n+n_L+n_V} \ni \mathbf{x} \mapsto \boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \in \mathbb{R}^{n+n_L+n_V},$$

with

$$\boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) := -\boldsymbol{S}\boldsymbol{i}_D^\sharp(\boldsymbol{S}^\top \boldsymbol{x}; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*),$$

is Lipschitz-continuous with respect to $\boldsymbol{v}_D$, that is,

$$\|\boldsymbol{\sigma}^\sharp(\boldsymbol{x}'; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) - \boldsymbol{\sigma}^\sharp(\boldsymbol{x}''; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)\| \le c(\boldsymbol{e}_D^*)\|\boldsymbol{x}' - \boldsymbol{x}''\|, \tag{4.70}$$

for all $\boldsymbol{x}', \boldsymbol{x}'' \in \mathbb{R}^{n+n_L+n_V}$, for some positive constant $c(\boldsymbol{e}_D^*)$ depending on $\boldsymbol{e}_D^*$ and on the data of the problem. Moreover, $\boldsymbol{\sigma}^\sharp$ satisfies the passivity condition

$$\boldsymbol{x}^\top \boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \le 0. \tag{4.71}$$

Chapter 5

Analysis of the circuit-device coupled model

In the previous chapter we have discussed the steady-state drift-diffusion model for semiconductor devices introduced in chapter 3 and in chapter 2 we have described the circuits using the MNA formalism. In this chapter we discuss the coupling between the steady-state drift-diffusion model and the circuit of index-1 and index-2, and we prove the existence results in both cases.

5.1 The circuit-device coupled problem

In this section we summarize the equations that will be considered. We have used two similar symbols for two different concepts: we have used the notation $\boldsymbol{x}(t)$ to denote the circuit variables, and the notation $\mathbf{x}$ to denote the semiconductor space variable.

We consider a circuit containing only one device. The case of circuits with many devices can be dealt using the same arguments, but the notation would be much heavier.

Network equations. We consider the compact form for the network equations

$$\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x}), \quad \text{in } [t_0, t_1], \tag{5.1}$$

with consistent initial data. The unknown is

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{e} \\ \boldsymbol{i}_L \\ \boldsymbol{i}_V \end{bmatrix}.$$

Device equations. For the semiconductor device we consider the steady-state drift-diffusion model discussed in details in previous chapters.

$$\begin{cases} -\nabla \cdot (\epsilon_s \nabla \phi) = q(N + p - n), \\ \nabla \cdot \boldsymbol{J}_n = -qH, \qquad \boldsymbol{J}_n = -a_n \nabla \phi_n, \qquad \text{in } \Omega \\ \nabla \cdot \boldsymbol{J}_p = qH, \qquad \boldsymbol{J}_p = -a_p \nabla \phi_p, \end{cases} \tag{5.2}$$

As unknowns we choose the electric potential $\phi(\mathbf{x}, t)$, and the carriers potentials $(\phi_n(\mathbf{x}, t), \phi_p(\mathbf{x}, t)) =: \mathbf{\Phi}(\mathbf{x}, t)$. For the system (5.2), we assign the following mixed boundary conditions

$$\begin{cases} \phi - \phi_{\text{bi}} = \phi_n = \phi_p = e_{D,i}(t), & \text{on } \Gamma_{D,i}, \ i = 0, 1, \ldots, n_D, \\ \dfrac{\partial \phi}{\partial \nu} = \dfrac{\partial \phi_n}{\partial \nu} = \dfrac{\partial \phi_p}{\partial \nu} = 0, & \text{on } \Gamma_N. \end{cases} \tag{5.3}$$

The unknowns of the problem (5.2)-(5.3) depend parametrically on $t \in [t_0, t_1]$ through the boundary data $e_{D,i} = e_{D,i}(t)$.

The densities n, p, are related to the quasi-Fermi potentials ϕ_n, ϕ_p by the Maxwell-Boltzmann relations by equations (4.5).

For the generation-recombination term $H = H(n, p)$ and for the mobilities we assume hypothesis (**T.5**) (**T.6**) given in chapter 4.

Coupling conditions.

In chapter 2 we have defined the potentials $e_{D,k}$ as the external electric potentials applied to the device. They are determined by the equations for the electric network. Recalling equation (2.32) in chapter 2, the network-to-device coupling condition are:

$$\boldsymbol{e}_D = \boldsymbol{S}_D^\top \boldsymbol{e}, \tag{5.4}$$

where

$$\boldsymbol{e}_D = \begin{bmatrix} e_{D,0} \\ \vdots \\ e_{D,n_D} \end{bmatrix}$$

and the selection matrix $\boldsymbol{S}_D$ is defined in (2.30).

The relation that expresses the coupling device-to-network is given by equation (2.37), that is

$$\boldsymbol{\sigma}(\boldsymbol{x}) = -\boldsymbol{\mathcal{A}} \boldsymbol{i}_D(\boldsymbol{\mathcal{A}}^\top \boldsymbol{x}), \tag{5.5}$$

with

$$\boldsymbol{\mathcal{A}} = \begin{bmatrix} \boldsymbol{A}_D \\ \boldsymbol{O} \\ \boldsymbol{O} \end{bmatrix},$$

where $\boldsymbol{A}_D$ is the incidence semiconductor matrix, and $\boldsymbol{i}_D$ is the current vector defined in (4.52).

We note that $\boldsymbol{S}_D$ is related to $\boldsymbol{A}_D$ by the identity $\boldsymbol{A}_D = \boldsymbol{S}_D \widehat{\boldsymbol{A}}$. Then recalling (2.33), we find

$$\boldsymbol{\mathcal{A}}^\top \boldsymbol{x} = \boldsymbol{A}_D^\top \boldsymbol{e} = \boldsymbol{v}_D,$$

thus

$$\boldsymbol{\sigma}(\boldsymbol{x}) = -\boldsymbol{\mathcal{A}} \boldsymbol{i}_D(\boldsymbol{v}_D). \tag{5.6}$$

For this coupled problem we can prove an existence theorem if the DAE circuit equations are of index-1 and also if they are of index-2. The difference between these systems will be described in the following sections.

5.2   Existence theorem for index-1 model

We consider the coupled problem (5.1)-(5.2), with boundary conditions for the device system given by (5.3). First of all we have to introduce the initial conditions for the network system. In the index-1 case, as discussed in chapter 2, it is possible to show that the network system (5.1) is equivalent to the two projected equations

$$\dot{\boldsymbol{y}} = \boldsymbol{P}\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x})\right], \qquad (5.7)$$
$$\boldsymbol{z} = \boldsymbol{Q}\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x})\right], \qquad (5.8)$$

for the differential part $\boldsymbol{y} = \boldsymbol{P}\boldsymbol{x}$, and the algebraic part $\boldsymbol{z} = \boldsymbol{Q}\boldsymbol{x}$, where the matrix $\boldsymbol{Q}$ is a projector onto $\ker \boldsymbol{E}$, $\boldsymbol{P}$ is its complementary projector. In (5.7), (5.8) we have used the matrices $\boldsymbol{E}_1 = \boldsymbol{E} - \boldsymbol{A}\boldsymbol{Q}$, $\boldsymbol{A}_1 = \boldsymbol{A}\boldsymbol{P}$. We assume the index-1 condition

$$\boldsymbol{E} \text{ is singular}, \quad \boldsymbol{E}_1 \text{ is nonsingular}, \qquad (5.9)$$

and the following additional topological condition

$$\boldsymbol{\mathcal{A}}^\top \boldsymbol{Q} = \boldsymbol{O}. \qquad (5.10)$$

Recalling proposition 2.6.1 in chapter 2, the topological conditions (5.9), (5.10) imply

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{y}), \quad \boldsymbol{Q}\boldsymbol{E}_1^{-1}\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{0}.$$

Thus equation (5.8) become

$$\boldsymbol{z} = \boldsymbol{Q}\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t)\right]. \qquad (5.11)$$

We need to assign initial conditions only for the differential part of $\boldsymbol{x}$, and subsequently determining consistent initial data for the algebraic part, that is,

$$\boldsymbol{P}\boldsymbol{x}(t_0) = \boldsymbol{y}_0,$$

and thus

$$\boldsymbol{z}_0 = \boldsymbol{Q}\boldsymbol{E}_1^{-1}\left[\boldsymbol{A}_1\boldsymbol{y}_0 + \boldsymbol{B}\boldsymbol{u}(t)\right].$$

Now we are ready to introduce the existence result of the coupled index-1 problem.

Theorem 5.2.1 *The problem* (5.1)–(5.2), *with the topological conditions* (5.9)–(5.10), *admits a solution,* $(\boldsymbol{x}, \boldsymbol{\Phi}) \in C^0([t_0, t_1]) \times C^0([t_0, t_1]; H^1(\Omega) \cap L_\infty(\Omega))$, *with* $\boldsymbol{P}\boldsymbol{x} \in C^1([t_0, t_1])$. *Moreover, any solution satisfies the estimates:*

$$|\boldsymbol{P}\boldsymbol{x}(t)|^2 \leq c_y e^{k(t-t_0)} \left(|\boldsymbol{y}_0|^2 + \|\boldsymbol{u}\|_{L^2([t_0,t_1])}^2 \right), \tag{5.12}$$

$$|\boldsymbol{Q}\boldsymbol{x}(t)|^2 \leq c_z \left(|\mathbf{P}x(t)|^2 + |\boldsymbol{u}(t)|^2 \right), \tag{5.13}$$

$$\inf_{\Gamma_D} \phi_{\mathrm{bi}} + \min_i e_{D,i} \leq \phi \leq \sup_{\Gamma_D} \phi_{\mathrm{bi}} + \max_i e_{D,i}, \tag{5.14}$$

$$\min_i e_{D,i} \leq \phi_n \leq \max_i e_{D,i}, \tag{5.15}$$

$$\min_i e_{D,i} \leq \phi_p \leq \max_i e_{D,i}, \tag{5.16}$$

for some positive constants c_y, c_z *and* k *depending only on* $\boldsymbol{E}$, $\boldsymbol{A}$.

The proof of the main result requires several steps. First we prove a priori estimates for the network variables, employing the passivity condition. Next we define an iteration map, extending the map used in the previous chapter to prove the existence result for the steady-state semiconductor device equation. Finally we show that the iteration map is a fixed point map.

For simplicity, we present the above steps separately in the following three subsections.

5.2.1 A priori estimates

For any finite dimensional vector space $\mathbb{R}^m$, let $|\cdot|$ denote the Euclidean vector norm, that is, for $\boldsymbol{w} \in \mathbb{R}^m$ we have $|\boldsymbol{w}|^2 = \boldsymbol{w}^\top \boldsymbol{w} \equiv \boldsymbol{w} \cdot \boldsymbol{w}$.

In the following Lemma we prove the a priori estimates for the network unknowns.

Lemma 5.2.2 *Let* $\boldsymbol{E}$ *be symmetric, positive semidefinite, and let the index-1 topological condition* (5.9), *and the additional topological condition* (5.10) *be satisfied. Furthermore, let* $\boldsymbol{x} \in C^0([t_0, t_1])$ *be a solution of the network equation* (5.1), *with consistent initial value* $\boldsymbol{x}_0$. *We assume that* $\boldsymbol{\sigma}$ *satisfies the passivity condition*

$$\boldsymbol{x}^\top \boldsymbol{\sigma}(\boldsymbol{x}) \leq 0. \tag{5.17}$$

Then, for all $t \in [t_0, t_1]$, *the differential part* $\boldsymbol{y} = \boldsymbol{P}\boldsymbol{x}$, *and the algebraic part* $\boldsymbol{z} = \boldsymbol{Q}\boldsymbol{x}$ *of the solution, satisfy the estimates*

$$|\boldsymbol{y}(t)|^2 \leq c_y e^{k(t-t_0)} \left(|\boldsymbol{y}_0|^2 + \|\boldsymbol{u}\|_{L^2([t_0,t_1])}^2 \right), \tag{5.18}$$

$$|\boldsymbol{z}(t)|^2 \leq c_z \left(|\boldsymbol{y}(t)|^2 + |\boldsymbol{u}(t)|^2 \right), \tag{5.19}$$

for some positive constants c_y, c_z *and* k *depending only on* $\boldsymbol{E}$, $\boldsymbol{A}$.

Proof. Equation (5.11) implies immediately (5.19).

Next we prove (5.18). Multiplying (5.1) by $\boldsymbol{y}^\top = \boldsymbol{x}^\top \boldsymbol{P}^\top$, we get

$$\boldsymbol{y}^\top \boldsymbol{E} \dot{\boldsymbol{y}} = \boldsymbol{y}^\top \boldsymbol{A} \boldsymbol{y} + \boldsymbol{y}^\top \boldsymbol{A} \boldsymbol{z} + \boldsymbol{y}^\top \boldsymbol{B} \boldsymbol{u} + \boldsymbol{y}^\top \boldsymbol{\sigma}. \tag{5.20}$$

Noting that it is possible write the differential part of $\boldsymbol{x}$ in the following way

$$\boldsymbol{y} = \boldsymbol{x} - \boldsymbol{Q}\boldsymbol{x},$$

recalling (5.10) and the passivity condition (5.17), we find

$$\boldsymbol{y}^\top \boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{\sigma}(\boldsymbol{x}) - \boldsymbol{x}^\top \boldsymbol{Q}^\top \boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{\sigma}(\boldsymbol{x}) \leq 0.$$

Then, we use the previous inequality and (5.19) in (5.20), we integrate over $[t_0, t]$, and apply Cauchy-Schwarz and Young inequalities, obtaining

$$\boldsymbol{y}^\top \boldsymbol{E} \boldsymbol{y} \leq \boldsymbol{y}_0^\top \boldsymbol{E} \boldsymbol{y}_0 + c \int_{t_0}^t \left(|\boldsymbol{y}(\tau)|^2 + |\boldsymbol{u}(\tau)|^2 \right) \, \mathrm{d}\tau. \tag{5.21}$$

Since $\boldsymbol{E}$ is positive semidefinite, it is positive definite when restricted to $\boldsymbol{P}\mathbb{R}^m$, with $m = n + n_L + n_V$, that is,

$$c_1 |\boldsymbol{y}|^2 \leq \boldsymbol{y}^\top \boldsymbol{E} \boldsymbol{y} \leq c_2 |\boldsymbol{y}|^2,$$

for two positive constants c_1, c_2. Then, from (5.21) we find

$$|\boldsymbol{y}|^2 \leq c_y \left(|\boldsymbol{y}_0|^2 + \|\boldsymbol{u}\|_{L^2([t_0, t_1])}^2 \right) + k \int_{t_0}^t |\boldsymbol{y}(\tau)|^2 \, \mathrm{d}\tau,$$

with c_y, k positive constants. Estimate (5.18) follows from Gronwall's lemma. ∎

We can prove that the passivity condition (5.17), assumed in previous Lemma, is satisfied for our problem. In fact from Lemma 4.4.1, we have

$$\boldsymbol{v}_D^\top \boldsymbol{i}_D \geq 0,$$

and, using (5.6) we have

$$\boldsymbol{x}^\top \boldsymbol{\sigma} = -\boldsymbol{x}^\top \boldsymbol{\mathcal{A}} \boldsymbol{i}_D = -\boldsymbol{v}_D^\top \boldsymbol{i}_D,$$

that implies the passivity condition for $\boldsymbol{\sigma}$.

5.2.2 Iteration map for the coupled problem

In this subsection, we introduce an iteration map for both the device variables and network variables by estending the map $\mathbf{\Phi}^\sharp$ defined in (4.40), in the previous chapter. The map $\mathbf{\Phi}^\sharp$ is defined by $\mathbf{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \mathbf{\Phi}^*) = (\phi_n, \phi_p)$, solution of the following problem:

$$
\begin{cases}
-\nabla \cdot (\epsilon_s \nabla \phi^*) = q(N + p^* - n^*), & \\
\nabla \cdot \boldsymbol{J}_n = qF^*(n_i^{-2}np - 1), & \boldsymbol{J}_n = -q\mu_n^* n^* \nabla \phi_n, \quad \text{in } \Omega \qquad (5.22) \\
\nabla \cdot \boldsymbol{J}_p = -qF^*(n_i^{-2}np - 1), & \boldsymbol{J}_p = -q\mu_p^* p^* \nabla \phi_p,
\end{cases}
$$

with boundary conditions

$$
\begin{cases}
\phi^* - \phi_{\text{bi}} = e_{D,i}^*, \ \phi_n = \phi_p = e_{D,i}, & \text{on } \Gamma_{D,i}, \ i = 0, 1, \ldots, n_D, \\
\dfrac{\partial \phi}{\partial \nu} = \dfrac{\partial \phi_n}{\partial \nu} = \dfrac{\partial \phi_p}{\partial \nu} = 0, & \text{on } \Gamma_N.
\end{cases}
\qquad (5.23)
$$

The definition of the iteration map for the device equation given above, depends on the Lemmas 4.2.1, 4.2.2, in chapter 4, which apply to equations with a parametric dependence on time. Thus, all the discussion in the previous chapter can be extended to functions $\boldsymbol{e}_D^*(t)$, $\mathbf{\Phi}^*(t)$ in the spaces $C^0([t_0, t_1], \mathbb{R}^{n_D+1})$, $C^0([t_0, t_1], L^2(\Omega))$, respectively, defining the set $\mathcal{M}(\boldsymbol{e}_D) \subset C^0([t_0, t_1], L^2(\Omega))$ by

$$
\begin{aligned}
\mathcal{M}(\boldsymbol{e}_D) \ = \ & \{\psi \in C^0([t_0, t_1], L^2(\Omega)) \mid \\
& \min_i e_{D,i} \leq \psi \leq \max_i e_{D,i} \text{ a.e. in } \Omega, \text{for all } t \in [t_0, t_1]\}^2.
\end{aligned}
$$

In particular, as we have shown in Lemma 4.4.2, in the previous chapter, for any $\boldsymbol{e}_D^*(t) \in C^0([t_0, t_1], \mathbb{R}^{n_D+1})$, $\mathbf{\Phi}^* \in \mathcal{M}(\boldsymbol{e}_D^*)$, the map

$$
\begin{aligned}
C^0([t_0, t_1], \mathbb{R}^{n_D}) \ni \boldsymbol{v}_D \ \mapsto \ & \boldsymbol{i}_D^\sharp(\boldsymbol{v}_D; \boldsymbol{e}_D^*, \mathbf{\Phi}^*) \in C^0([t_0, t_1], \mathbb{R}^{n_D}), \\
& \boldsymbol{v}_D = \widehat{\boldsymbol{A}}^\top \boldsymbol{e}_D,
\end{aligned}
$$

is Lipschitz continuous and satisfies the passivity condition (4.61).

We fix $(\boldsymbol{e}_D^*, \mathbf{\Phi}^*)$ in an appropriate set M, which will be rendered explicit later, and we solve the coupled system

$$
\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D^*, \mathbf{\Phi}^*), \quad \text{in } [t_0, t_1], \qquad (5.24)
$$

$$
\boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D^*, \mathbf{\Phi}^*) = -\boldsymbol{\mathcal{A}}\boldsymbol{i}_D^\sharp(\boldsymbol{\mathcal{A}}^\top \boldsymbol{x}; \boldsymbol{e}_D^*, \mathbf{\Phi}^*), \qquad (5.25)
$$

$$
\boldsymbol{P}\boldsymbol{x}(t_0) = \boldsymbol{y}_0, \qquad (5.26)
$$

which is just a modified version of the original coupled system (5.1)–(5.2). The network equation (5.1) is replaced by (5.24), with a modified coupling term $\boldsymbol{\sigma}^\sharp$. The device-to-network coupling condition (5.5) is replaced by (5.25), with a modified current vector $\boldsymbol{i}_D^\sharp$. Denoting by $\boldsymbol{\mathcal{S}}$ the matrix

$$
\boldsymbol{\mathcal{S}} = \begin{bmatrix} \boldsymbol{S}_D \\ \boldsymbol{O} \\ \boldsymbol{O} \end{bmatrix}, \qquad (5.27)
$$

we can see that the device equations (5.2) are implicit in the notation for the modified current $i_D^\sharp(\mathcal{A}^\top x; e_D^*, \Phi^*)$, defined by $\Phi = \Phi^\sharp(\mathcal{S}^\top x; e_D^*, \Phi^*)$, which satisfies the system (5.22)-(5.23).

Since the modified nonlinear coupling term $\sigma^\sharp$ is Lipschitz-continuous, we can regard (5.24), (5.26) as an index-1 differential-algebraic system, which admits a unique solution x, depending on the pair (e_D^*, Φ^*). Then, x determines uniquely the device variable $\Phi = \Phi^\sharp(e_D; e_D^*, \Phi^*)$. In this way, the coupled system (5.24)–(5.26) defines a map

$$T \ : \ (e_D^*, \Phi^*) \mapsto (e_D, \Phi) = (\mathcal{S}x, \Phi^\sharp(e_D; e_D^*, \Phi^*)).$$

To make this statement more precise, we need to specify the set M where the map T acts.

5.2.3   Existence of fixed point

In this section we define the set M where the map T is defind. We use the a priori estimates found in chapter 4.

We can apply Lemma 5.2.2, because of the passivity condition, and the solution x uniquely defined by (5.24)-(5.26) satisfies the estimates (5.18)–(5.19):

$$|Px(t)|^2 \le c_y e^{k(t-t_0)} \left(|y_0|^2 + \|u\|_{L^2([t_0,t_1])}^2 \right), \tag{5.28}$$

$$|Qx(t)|^2 \le c_z \left(|Px(t)|^2 + |Q^\top u(t)|^2 \right). \tag{5.29}$$

In particular, the applied potentials $e_D = \mathcal{S}^\top x$ are bounded by a constant which depends only on the data of the network problem and on the time interval $[t_0, t_1]$,

$$\|e_D\|_{C^0} \le C_D(t_0, t_1). \tag{5.30}$$

This estimate defines a bounded subset B of $C^0([t_0, t_1], \mathbb{R}^{n_D+1})$,

$$\mathsf{B} = \left\{ e_D \ : \ \|e_D\|_{C^0} \le C_D(t_0, t_1) \right\}. \tag{5.31}$$

Let us consider the subset M of $C^0([t_0, t_1], \mathbb{R}^{n_D+1}) \times C^0([t_0, t_1], L^2(\Omega))$, defined by

$$\mathsf{M} = \left\{ (e_D, \Phi) \ : \ e_D \in \mathsf{B}, \ \Phi \in \mathcal{M}(e_D) \right\}.$$

Lemma 5.2.3 (Fixed-point map) *The set M is a nonempty, bounded, closed, convex subset of $C^0([t_0, t_1], \mathbb{R}^{n_D+1}) \times C^0([t_0, t_1], L^2(\Omega))$. The map T is a compact automorphism of M.*

Proof. The first part of the Lemma is immediate.

To prove the second part, we need to show that $T(\mathsf{M}) \subset \mathsf{M}$, and that $T(\mathsf{M})$ is precompact in M. The inclusion $T(\mathsf{M}) \subset \mathsf{M}$ follows by construction. To prove that $T(\mathsf{M})$ is precompact in M, we note that

$$T(\mathsf{M}) \subset \mathsf{B} \times \mathcal{T}(\mathsf{B}),$$

with

$$\begin{aligned}
\mathcal{T}(\mathsf{B}) \;=\; & \{\boldsymbol{\Phi} \in C^0([t_0, t_1], H^1(\Omega)) \mid \\
& \boldsymbol{\Phi} = \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}_D^*), \;\; \boldsymbol{e}_D \in \mathsf{B}, \;\; (\boldsymbol{e}_D^*, \boldsymbol{\Phi}_D^*) \in \mathsf{M}\}.
\end{aligned}$$

The set $\mathcal{T}(\mathsf{B})$ is a compact subset of $C^0([t_0, t_1], L^2(\Omega))$. Then also $\mathsf{B} \times \mathcal{T}(\mathsf{B})$ is a compact subset of $C^0([t_0, t_1], \mathbb{R}^{n_D+1}) \times C^0([t_0, t_1], L^2(\Omega))$, and thus $T(\mathsf{M})$ is a compact subset of the same functional space. It follows that $T(\mathsf{M})$ is precompact in M. ∎

The previous Lemma implies that the map T fulfills the hypothesis of Schauder's fixed point theorem. Than, T admit a fixed point, which satisfies

$$\begin{aligned}
\boldsymbol{E}\dot{\boldsymbol{x}} &= \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D, \boldsymbol{\Phi}), \quad \text{in } [t_0, t_1], & (5.32) \\
\boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D, \boldsymbol{\Phi}) &= -\boldsymbol{A}\boldsymbol{i}_D^\sharp(\boldsymbol{\mathcal{A}}^\top \boldsymbol{x}; \boldsymbol{e}_D, \boldsymbol{\Phi}), & (5.33) \\
\boldsymbol{e}_D &= \boldsymbol{\mathcal{S}}^\top \boldsymbol{x}, & (5.34) \\
\boldsymbol{P}\boldsymbol{x}(t_0) &= \boldsymbol{y}_0. & (5.35)
\end{aligned}$$

By definition,
$$\boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{\mathcal{S}}^\top \boldsymbol{x}, \boldsymbol{\Phi}) = \boldsymbol{\sigma}(\boldsymbol{x}; \boldsymbol{\mathcal{S}}^\top \boldsymbol{x}, \boldsymbol{\Phi}), \tag{5.36}$$

and the fixed point $(\boldsymbol{e}_D, \boldsymbol{\Phi})$ leads to a solution $(\mathbf{x}, \boldsymbol{\Phi}, \phi)$ of the original problem (5.1)–(5.2), with $\boldsymbol{x}$ solution of (5.33), and $\phi = \phi(\boldsymbol{e}_D, \boldsymbol{\Phi})$. Thus the main result, Theorem 5.2.1, is proved.

5.3   Existence theorem for index-2 model

In this section we consider index-2 conditions for the coupled model (5.1)-(5.3). As we have discussed in chapter 2, these conditions are given by

$$\begin{aligned}
\boldsymbol{E}_0 \equiv \boldsymbol{E}, \qquad \boldsymbol{E}_1 &= \boldsymbol{E}_0 - \boldsymbol{A}_0 \boldsymbol{Q}_0 \quad \text{are singular}, & (5.37) \\
\boldsymbol{E}_2 &= \boldsymbol{E}_1 - \boldsymbol{A}_1 \boldsymbol{Q}_1 \quad \text{is nonsingular}, & (5.38)
\end{aligned}$$

together with the additional conditions

$$\boldsymbol{\mathcal{A}}^\top \boldsymbol{Q}_0 = \boldsymbol{O}, \quad \boldsymbol{P}_0 \boldsymbol{Q}_1 \boldsymbol{E}_2^{-1} \boldsymbol{\mathcal{A}} = \boldsymbol{O}, \quad \boldsymbol{Q}_0 \boldsymbol{E}_2^{-1} \boldsymbol{\mathcal{A}} = \boldsymbol{O}. \tag{5.39}$$

In the previous equations, $\boldsymbol{Q}_0$, $\boldsymbol{Q}_1$ are projectors onto $\ker \boldsymbol{E}_0$, $\ker \boldsymbol{E}_1$ respectively, $\boldsymbol{A} \equiv \boldsymbol{A}_0$, $\boldsymbol{A}_1 = \boldsymbol{A}_0 \boldsymbol{P}_0$ and $\boldsymbol{P}_0$ is the complementary projector of $\boldsymbol{Q}_0$. Considering the conditions (5.37), (5.38), we have decomposed the network equation (5.1) in the following projected equations:

$$\begin{aligned}
\dot{\boldsymbol{y}} &= \boldsymbol{P}_0 \boldsymbol{P}_1 \boldsymbol{E}_2^{-1} \left[\boldsymbol{A}_2 \boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x}) \right], & (5.40) \\
\boldsymbol{z} &= \boldsymbol{Q}_0 \boldsymbol{Q}_1 \dot{\boldsymbol{w}} + \boldsymbol{Q}_0 \boldsymbol{P}_1 \boldsymbol{E}_2^{-1} \left[\boldsymbol{A}_2 \boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x}) \right], & (5.41) \\
\boldsymbol{w} &= \boldsymbol{P}_0 \boldsymbol{Q}_1 \boldsymbol{E}_2^{-1} \left[\boldsymbol{A}_2 \boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}(\boldsymbol{x}) \right], & (5.42)
\end{aligned}$$

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with
$$y = P_0 P_1 x, \qquad w = P_0 Q_1 x, \qquad z = Q_0 x, \qquad (5.43)$$

and P_1 complementary projectors of Q_1 and $A_2 = A_1 P_1$. The equations (5.40)–(5.42) are coupled through the coupling term with the device σ. Using the additional conditions (5.39) we obtain

$$
\begin{aligned}
\dot{y} &= P_0 P_1 E_2^{-1} \left[A_2 y + B u(t) + \sigma(y + w) \right], & (5.44) \\
z &= Q_0 Q_1 \dot{w} + Q_0 P_1 E_2^{-1} \left[A_2 y + B u(t) \right], & (5.45) \\
w &= P_0 Q_1 E_2^{-1} \left[A_2 y + B u(t) \right]. & (5.46)
\end{aligned}
$$

Then we can assign the following initial data for the network equation (5.1) in the coupled problem

$$P_0 P_1 x(t_0) = y_0. \qquad (5.47)$$

In the following subsection we prove the existence result for the coupled index-2 model.

Theorem 5.3.1 *The problem (5.1)–(5.2), with the index-2 conditions (5.37)–(5.38), and the additional conditions (5.39), admits a solution, $(x, \Phi) \in C^0([t_0, t_1]) \times C^0([t_0, t_1]; H^1(\Omega) \cap L_\infty(\Omega))$, with $P_0 P_1 x \in C^1([t_0, t_1])$. Moreover, any solution satisfies the estimates:*

$$|P_0 P_1 x(t)|^2 \le c_y e^{k(t-t_0)} \left(|y_0|^2 + |u_0|^2 + \|u\|_{H^1([t_0,t_1])} \right), \qquad (5.48)$$

$$|P_0 Q_1 x(t)|^2 \le c_w e^{k(t-t_0)} \left(|y_0|^2 + |u_0|^2 + \|u\|_{H^1([t_0,t_1])} \right), \qquad (5.49)$$

$$|Q_0 x(t)|^2 \le c_z \left(|y(t)| + |\dot{y}(t)| + |u(t)| + |\dot{u}(t)| \right), \qquad (5.50)$$

$$\inf_{\Gamma_D} \phi_{\mathrm{bi}} + \min_i e_{D,i} \le \phi \le \sup_{\Gamma_D} \phi_{\mathrm{bi}} + \max_i e_{D,i}, \qquad (5.51)$$

$$\min_i e_{D,i} \le \phi_n \le \max_i e_{D,i}, \qquad (5.52)$$

$$\min_i e_{D,i} \le \phi_p \le \max_i e_{D,i}, \qquad (5.53)$$

for some positive constants c_y, c_w, c_z and k depending only on E_0, A_0.

5.3.1 A priori estimates

Lemma 5.3.2 *Let E be symmetric and positive semidefinite, and let the index-2 topological conditions (5.37), (5.38), and the additional topological condition (5.39) be satisfied. Furthermore, let $x \in C^0([t_0, t_1])$ be a solution of the network equation (5.1), with consistent initial value x_0. We assume that A and σ satisfies the passivity conditions*

$$x^\top A x \le 0 \qquad (5.54)$$

$$x^\top \sigma(x) \le 0. \qquad (5.55)$$

Then, for all $t \in [t_0, t_1]$, the differential part $\boldsymbol{y} = \boldsymbol{P}_0\boldsymbol{P}_1 x$, and the algebraic parts $\boldsymbol{w} = \boldsymbol{P}_0\boldsymbol{Q}_1 x$, $\boldsymbol{z} = \boldsymbol{Q}_0 x$ of the solution, satisfy the estimates

$$|\boldsymbol{y}(t)|^2 \le c_y e^{k(t-t_0)}\left(|\boldsymbol{y}_0|^2 + |\boldsymbol{u}_0|^2 + \|\boldsymbol{u}\|_{H^1([t_0,t_1])}\right), \tag{5.56}$$

$$|\boldsymbol{w}(t)|^2 \le c_w e^{k(t-t_0)}\left(|\boldsymbol{y}_0|^2 + |\boldsymbol{u}_0|^2 + \|\boldsymbol{u}\|_{H^1([t_0,t_1])}\right), \tag{5.57}$$

$$|\boldsymbol{z}(t)| \le c_z \left(|\boldsymbol{y}(t)| + |\dot{\boldsymbol{y}}(t)| + |\boldsymbol{u}(t)| + |\dot{\boldsymbol{u}}(t)|\right), \tag{5.58}$$

for some positive constants c_y, c_w, c_z and k depending only on $\boldsymbol{E}$, $\boldsymbol{A}$.

Proof. Multiplying (5.1) by $\boldsymbol{x}^\top$, and using the passivity properties (5.54) and (5.55), we obtain

$$\boldsymbol{x}^\top \boldsymbol{E}\dot{\boldsymbol{x}} \le \boldsymbol{x}^\top \boldsymbol{B}\boldsymbol{u}(t).$$

Here we can replace $\boldsymbol{x}^\top$ with $\boldsymbol{P}_0\boldsymbol{x}^\top$ because of the symmetry of $\boldsymbol{E}$ and definition of $\boldsymbol{P}_0$. Then, we obtain

$$(\boldsymbol{P}_0\boldsymbol{x})^\top \boldsymbol{E}(\boldsymbol{P}_0\dot{\boldsymbol{x}}) \le \boldsymbol{x}^\top \boldsymbol{B}\boldsymbol{u}(t).$$

Using again the symmetry of $\boldsymbol{E}$, we find

$$\frac{1}{2}(\boldsymbol{P}_0\boldsymbol{x})^\top \boldsymbol{E}(\boldsymbol{P}_0\boldsymbol{x}) \le \frac{1}{2}(\boldsymbol{P}_0\boldsymbol{x}_0)^\top \boldsymbol{E}(\boldsymbol{P}_0\boldsymbol{x}_0) + \int_{t_0}^{t_1} \boldsymbol{x}^\top(\tau)\boldsymbol{B}\boldsymbol{u}(\tau)\,\mathrm{d}\tau. \tag{5.59}$$

$$\boldsymbol{P}_0\boldsymbol{Q}_1 + \boldsymbol{Q}_0\boldsymbol{P}_1 = \boldsymbol{P}_0\boldsymbol{Q}_1 - \boldsymbol{Q}_0\boldsymbol{Q}_1 + \boldsymbol{Q}_0$$

Using the decomposition (5.44)-(5.45) and the hypotesis (5.39), we have

$$
\begin{aligned}
\boldsymbol{x}^\top \boldsymbol{B}\boldsymbol{u} &= \boldsymbol{y}^\top \boldsymbol{B}\boldsymbol{u} + \boldsymbol{w}^\top \boldsymbol{B}\boldsymbol{u} + \boldsymbol{z}^\top \boldsymbol{B}\boldsymbol{u} \\
&= \boldsymbol{y}^\top \boldsymbol{B}\boldsymbol{u} + [\boldsymbol{P}_0\boldsymbol{Q}_1\boldsymbol{E}_2^{-1}(\boldsymbol{A}_2\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u})]^\top \boldsymbol{B}\boldsymbol{u} \\
&\quad + [\boldsymbol{Q}_0\boldsymbol{Q}_1(\dot{\boldsymbol{w}} - \boldsymbol{w}) + \boldsymbol{Q}_0\boldsymbol{E}_2^{-1}(\boldsymbol{A}_2\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u})]^\top \boldsymbol{B}\boldsymbol{u} \\
&= \boldsymbol{y}^\top[\boldsymbol{I} + \boldsymbol{A}_2^\top \boldsymbol{M}^\top]\boldsymbol{B}\boldsymbol{u} + \boldsymbol{u}^\top \boldsymbol{B}^\top \boldsymbol{M}^\top \boldsymbol{B}\boldsymbol{u} \\
&\quad - \boldsymbol{w}^\top(\boldsymbol{Q}_0\boldsymbol{Q}_1)^\top B(\boldsymbol{u} + \dot{\boldsymbol{u}}) + \frac{\mathrm{d}}{\mathrm{d}t}[\boldsymbol{w}^\top(\boldsymbol{Q}_0\boldsymbol{Q}_1)^\top \boldsymbol{B}\boldsymbol{u}]
\end{aligned}
$$

with $\boldsymbol{M} = (\boldsymbol{I} - \boldsymbol{P}_0\boldsymbol{P}_1)\boldsymbol{E}_2^{-1}$. In the last equality there appear no terms quadratic in the components of $\boldsymbol{x}$. Then, using the Schwarz inequality, we find

$$
\begin{aligned}
\int_{t_0}^{t_1} \boldsymbol{x}^\top(\tau)\boldsymbol{B}\boldsymbol{u}(\tau)\,\mathrm{d}\tau \le\ & c\int_{t_0}^{t_1}\left(\|\boldsymbol{y}(\tau)\|^2 + \|\boldsymbol{u}(\tau)\|^2\right)\mathrm{d}\tau \\
& + c\int_{t_0}^{t_1}\left(\|\boldsymbol{w}(\tau)\|^2 + \|\boldsymbol{u}(\tau)\|^2 + \|\dot{\boldsymbol{u}}(\tau)\|^2\right)\mathrm{d}\tau \\
& + \boldsymbol{w}^\top(\boldsymbol{Q}_0\boldsymbol{Q}_1)^\top \boldsymbol{B}\boldsymbol{u} - \boldsymbol{w}_0^\top(\boldsymbol{Q}_0\boldsymbol{Q}_1)^\top \boldsymbol{B}\boldsymbol{u}_0 \\
\le\ & c\int_{t_0}^{t_1}\left(\|\boldsymbol{y}(\tau)\|^2 + \|\boldsymbol{w}(\tau)\|^2\right)\mathrm{d}\tau + c\|\boldsymbol{u}\|_{H^1([t_0,t_1])} \\
& + \delta\|\boldsymbol{w}(t)\|^2 + c(\delta)\|\boldsymbol{u}(t)\|^2 - \boldsymbol{w}_0^\top(\boldsymbol{Q}_0\boldsymbol{Q}_1)^\top \boldsymbol{B}\boldsymbol{u}_0,
\end{aligned}
$$

where δ is a small positive real number which will be chosen later.

On the other hand, we have

$$
\begin{aligned}
\frac{1}{2}(\boldsymbol{P}_0\boldsymbol{x})^\top \boldsymbol{E}(\boldsymbol{P}_0\boldsymbol{x}) &\geq c\|\boldsymbol{P}_0\boldsymbol{x}\|^2 \\
&\geq c_E(\|\boldsymbol{y}\|^2 + \|\boldsymbol{w}\|^2).
\end{aligned}
$$

Using the previous two inequalities in (5.59) and choosing $\delta = \frac{c_E}{2}$, we get

$$
\begin{aligned}
\frac{1}{2}c_E(\|\boldsymbol{y}\|^2 + \|\boldsymbol{w}\|^2) &\leq \frac{1}{2}(\boldsymbol{P}_0\boldsymbol{x}_0)^\top \boldsymbol{E}(\boldsymbol{P}_0\boldsymbol{x}_0) - \boldsymbol{w}_0^\top(\boldsymbol{Q}_0\boldsymbol{Q}_1)^\top \boldsymbol{B}\boldsymbol{u}_0 \\
&\quad + c\|\boldsymbol{u}\|_{H^1([t_0,t_1])} + c\int_{t_0}^{t_1}(\|\boldsymbol{y}(\tau)\|^2 + \|\boldsymbol{w}(\tau)\|^2)\,\mathrm{d}\tau.
\end{aligned}
$$

Here we have used the Sobolev embedding $H^1([t_0, t_1]) \subset C^0([t_0, t_1])$. From Gronwall Lemma, we find the inequality

$$
\|\boldsymbol{y}\|^2 + \|\boldsymbol{w}\|^2 \leq C_0 e^{c(t-t_0)}, \tag{5.60}
$$

with $C_0 = c_0(|\boldsymbol{y}_0|^2 + |\boldsymbol{u}_0|^2 + \|\boldsymbol{u}\|_{H^1([t_0,t_1])})$.

Finally we obtain (5.58) considering that

$$
\begin{aligned}
\boldsymbol{z} &= \boldsymbol{Q}_0\boldsymbol{Q}_1\dot{\boldsymbol{w}} + \boldsymbol{Q}_0\boldsymbol{P}_1\boldsymbol{E}_2^{-1}[\boldsymbol{A}_2\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}] \\
&= \boldsymbol{Q}_0\boldsymbol{Q}_1\boldsymbol{E}_2^{-1}[\boldsymbol{A}_2\dot{\boldsymbol{y}} + \boldsymbol{B}\dot{\boldsymbol{u}}] + \boldsymbol{Q}_0\boldsymbol{P}_1\boldsymbol{E}_2^{-1}[\boldsymbol{A}_2\boldsymbol{y} + \boldsymbol{B}\boldsymbol{u}].
\end{aligned}
$$

$\blacksquare$

Now, as for the index-1 case, we can apply Lemma 4.4.1 to prove that the passivity condition (5.55) is satisfied also in this case.

5.3.2 Iteration map for the coupled problem and existence of fixed points

As in the previous section, also in this subsection we introduce an iteration map for both the device variables and network variables by estending the map $\boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$, defined in the previous chapter, to functions $\boldsymbol{e}_D^*(t)$, $\boldsymbol{\Phi}^*(t)$ in the spaces $C^0([t_0, t_1], \mathbb{R}^{n_D+1})$, $C^0([t_0, t_1], L^2(\Omega))$, respectively, defining the set $\mathcal{M}(\boldsymbol{e}_D^*) \subset C^0([t_0, t_1], L^2(\Omega))$.

We fix $(\boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$ in an appropriate set M', which will be rendered explicit later, and we solve the coupled system

$$
\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*), \quad \text{in } [t_0, t_1], \tag{5.61}
$$

$$
\boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) = -\boldsymbol{\mathcal{A}}\boldsymbol{i}_D^\sharp(\boldsymbol{\mathcal{A}}^\top\boldsymbol{x}; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*), \tag{5.62}
$$

$$
\boldsymbol{P}_0\boldsymbol{P}_1\boldsymbol{x}(t_0) = \boldsymbol{y}_0, \tag{5.63}
$$

which is just a modified version of the original coupled system (5.1)–(5.2).

Since the modified nonlinear coupling term $\boldsymbol{\sigma}^\sharp$ is Lipschitz-continuous, we can regard (5.61), (5.63) as an index-2 ordinary differential-algebraic system, which

admits a unique solution $\boldsymbol{x}$, depending on the pair $(\boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$. Then, $\boldsymbol{x}$ determines uniquely the device variable $\boldsymbol{\Phi} = \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)$. In this way, the coupled system (5.24)–(5.26) defines a map

$$T' \; : \; (\boldsymbol{e}_D^*, \boldsymbol{\Phi}^*) \mapsto (\boldsymbol{e}_D, \boldsymbol{\Phi}) = (\boldsymbol{\mathcal{S}}\boldsymbol{x}, \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}^*)).$$

To specify the set M' where the map T' acts, we use the a priori estimates found in chapter 4.

We can apply Lemma 5.3.2, because of the passivity condition, and the solution $\boldsymbol{x}$ uniquely defined by (5.61)-(5.63) satisfies the estimates (5.56)–(5.58):

$$|\boldsymbol{y}(t)|^2 \le c_y e^{k(t-t_0)} \left(|\boldsymbol{y}_0|^2 + |\boldsymbol{u}_0|^2 + \|\boldsymbol{u}\|_{H^1([t_0,t_1])} \right), \tag{5.64}$$

$$|\boldsymbol{w}(t)|^2 \le c_w e^{k(t-t_0)} \left(|\boldsymbol{y}_0|^2 + |\boldsymbol{u}_0|^2 + \|\boldsymbol{u}\|_{H^1([t_0,t_1])} \right), \tag{5.65}$$

$$|\boldsymbol{z}(t)| \le c_z \left(|\boldsymbol{y}(t)| + |\dot{\boldsymbol{y}}(t)| + |\boldsymbol{u}(t)| + |\dot{\boldsymbol{u}}(t)| \right), \tag{5.66}$$

In particular, the applied potentials $\boldsymbol{e}_D = \boldsymbol{\mathcal{S}}^\top \boldsymbol{x}$ are bounded by a constant which depends only on the data of the network problem, on their time derivatives, and on the time interval $[t_0, t_1]$,

$$\|\boldsymbol{e}_D\|_{C^0} \le C_D'(t_0, t_1). \tag{5.67}$$

This estimate defines a bounded subset B' of $C^0([t_0, t_1], \mathbb{R}^{n_D+1})$,

$$\mathsf{B}' = \left\{ \boldsymbol{e}_D \; : \; \|\boldsymbol{e}_D\|_{C^0} \le C_D'(t_0, t_1) \right\}. \tag{5.68}$$

Let us consider the subset M of $C^0([t_0, t_1], \mathbb{R}^{n_D+1}) \times C^0([t_0, t_1], L^2(\Omega))$, defined by

$$\mathsf{M} = \left\{ (\boldsymbol{e}_D, \boldsymbol{\Phi}) \; : \; \boldsymbol{e}_D \in \mathsf{B}, \; \boldsymbol{\Phi} \in \mathcal{M}(\boldsymbol{e}_D) \right\}.$$

Lemma 5.3.3 (Fixed-point map) *The set M is a nonempty, bounded, closed, convex subset of $C^0([t_0, t_1], \mathbb{R}^{n_D+1}) \times C^0([t_0, t_1], L^2(\Omega))$. The map T is a compact automorphism of M.*

Proof. The first part of the Lemma is immediate.

To prove the second part, we need to show that $T(\mathsf{M}) \subset \mathsf{M}$, and that $T(\mathsf{M})$ is precompact in M. The inclusion $T(\mathsf{M}) \subset \mathsf{M}$ follows by construction. To prove that $T(\mathsf{M})$ is precompact in M, we note that

$$T(\mathsf{M}) \subset \mathsf{B} \times \mathcal{T}(\mathsf{B}),$$

with

$$\begin{aligned} \mathcal{T}(\mathsf{B}) \;\; = \;\; & \{ \boldsymbol{\Phi} \in C^0([t_0, t_1], H^1(\Omega)) \; | \\ & \boldsymbol{\Phi} = \boldsymbol{\Phi}^\sharp(\boldsymbol{e}_D; \boldsymbol{e}_D^*, \boldsymbol{\Phi}_D^*), \; \boldsymbol{e}_D \in \mathsf{B}, \; (\boldsymbol{e}_D^*, \boldsymbol{\Phi}_D^*) \in \mathsf{M} \}. \end{aligned}$$

The set $\mathcal{T}(\mathsf{B})$ is a compact subset of $C^0([t_0, t_1], L^2(\Omega))$. Then also $\mathsf{B} \times \mathcal{T}(\mathsf{B})$ is a compact subset of $C^0([t_0, t_1], \mathbb{R}^{n_D+1}) \times C^0([t_0, t_1], L^2(\Omega))$, and thus $T(\mathsf{M})$ is a compact subset of the same functional space. It follows that $T(\mathsf{M})$ is precompact in M. ∎

The previous Lemma implies that the map T fulfills the hypothesis of Schauder's fixed point theorem. Than, T admit a fixed point, which satisfies

$$\boldsymbol{E}\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}(t) + \boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D, \boldsymbol{\Phi}), \quad \text{in } [t_0, t_1], \tag{5.69}$$

$$\boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{e}_D, \boldsymbol{\Phi}) = -\boldsymbol{A}\boldsymbol{i}_D^\sharp(\boldsymbol{\mathcal{A}}^\top \boldsymbol{x}; \boldsymbol{e}_D, \boldsymbol{\Phi}), \tag{5.70}$$

$$\boldsymbol{e}_D = \boldsymbol{\mathcal{S}}^\top \boldsymbol{x}, \tag{5.71}$$

$$\boldsymbol{P}_0 \boldsymbol{P}_1 \boldsymbol{x}(t_0) = \boldsymbol{y}_0. \tag{5.72}$$

By definition,

$$\boldsymbol{\sigma}^\sharp(\boldsymbol{x}; \boldsymbol{\mathcal{S}}^\top \boldsymbol{x}, \boldsymbol{\Phi}) = \boldsymbol{\sigma}(\boldsymbol{x}; \boldsymbol{\mathcal{S}}^\top \boldsymbol{x}, \boldsymbol{\Phi}), \tag{5.73}$$

and the fixed point $(\boldsymbol{e}_D, \boldsymbol{\Phi})$ leads to a solution $(\mathbf{x}, \boldsymbol{\Phi}, \phi)$ of the original problem (5.1)–(5.2), with $\boldsymbol{x}$ solution of (5.70), and $\phi = \phi(\boldsymbol{e}_D, \boldsymbol{\Phi})$. Thus the main result, Theorem 5.2.1, is proved.

Chapter 6

Mathematical modeling of thermal effects in devices

In this chapter we present a systematic way to derive models for the thermal effects in a semiconductor device. The methodology we present is consistent with the linear irreversible thermodynamics.

6.1 Thermodynamic approach and energy transport model

In this section we describe a semiconductor in a state near equilibrium using the approach of the Linear Irreversible Thermodynamics.

We assume that it is possible to define an *entropy* S for a thermodynamic system around equilibrium. The entropy of the system will depend on some extensive thermodynamic quantities, which we denote by E_i, with i varying in an index set I. Than we can write the Gibbs relations

$$\mathrm{d}S = \sum_{i \in I} I_i \, \mathrm{d}E_i, \qquad I_i = \frac{\partial S}{\partial E_i}. \tag{6.1}$$

We assume that each thermodynamic quantity E_i, $i \in I$, satisfies a balance equation of the form

$$\frac{\partial E_i}{\partial t} + \nabla \cdot \boldsymbol{j}_i = H_i, \qquad i \in I, \tag{6.2}$$

where $\boldsymbol{j}_i$ is the flux density and H_i is the production term of the quantity E_i. We assume also that the Gibbs relations (6.1) are valid also in non equilibrium states. Using these relation and (6.2) we can obtain an entropy balance equation

in the following way:

$$\frac{\partial S}{\partial t} = \sum_{i \in I} I_i \frac{\partial E_i}{\partial t}$$

$$= \sum_{i \in I} I_i(-\nabla \cdot \boldsymbol{j}_i + H_i)$$

$$= -\nabla \cdot \left(\sum_{i \in I} I_i \boldsymbol{j}_i\right) + \sum_{i \in I} \nabla I_i \cdot \boldsymbol{j}_i + \sum_{i \in I} I_i H_i.$$

If we identify the entropy flux

$$\boldsymbol{j}^S = \sum_{i \in I} I_i \boldsymbol{j}_i, \tag{6.3}$$

and the entropy production term

$$H^S = \sum_{i \in I} \nabla I_i \cdot \boldsymbol{j}_i + \sum_{i \in I} I_i H_i, \tag{6.4}$$

we obtain the entropy balance equation

$$\frac{\partial S}{\partial t} + \nabla \cdot \boldsymbol{j}^S = H^S \geq 0. \tag{6.5}$$

The inequality expresses the second principle of thermodynamics. The entropy production term, defined in (6.4), is the sum of the flux densities, called *thermodynamic fluxes*, multiplied by the gradients of the conjugate quantities I_i, that is $\boldsymbol{X} := \nabla I_i$, called *thermodynamic forces*, plus a combination of the production terms. According to the Linear Irreversible Thermodynamics, the thermodynamic fluxes depend linearly on the thermodynamic forces, that is, there exist matrices L_{ij} such that

$$\boldsymbol{j}_i = \sum_{j \in I} L_{ij} \boldsymbol{X}_j, \qquad i \in I. \tag{6.6}$$

The second principle of thermodynamics, expressed in (6.5), is satisfied if the following inequalities hold:

$$\sum_{i \in I} \nabla I_i \cdot \boldsymbol{j}_i \geq 0, \tag{6.7}$$

$$\sum_{i \in I} I_i H_i \geq 0. \tag{6.8}$$

Using (6.6), the inequality related to the thermodynamic fluxes (6.7), becomes

$$\sum_{i,j \in I} \boldsymbol{X} \cdot (L_{ij} \boldsymbol{X}_j) \geq 0, \tag{6.9}$$

which implies that the matrix $(L_{ij})_{i,j \in I}$ positive definite. In addition, we know that the Onsager reciprocity principle is valid, that requires the symmetry conditions

$$L_{ij} = L_{ji}, \qquad i, j \in I.$$

The inequality (6.8) provides a constraint on the production terms, which must hold for a thermodynamically compatible model.

Now we apply this theory to a semiconductor, in which we want to consider thermal effect. If we take into account the thermal effects, besides the thermodynamic effects of electrons and holes, we have to analyze in terms of the thermodynamic behavior the whole lattice. To this aim we describe the first two thermodynamic systems as immersed in a thermal bath of phonons, which represents the thermodynamic contents of the lattice. This means that we assume that the concentration of phonons in the lattice depends only on the temperature of the lattice, or rather on its internal energy. Phonons are quasi-particles which correspond to the oscillations of the nuclei of the semiconductor around the equilibrium configuration which determine the lattice. They are bosons, that is, many phonons may occupy the same quantum state.

Summing up, we consider three thermodynamic subsystems:

1. Electron in conduction band, whose thermodynamic state is identified by the chemical potential μ_c and the temperature T_c.

2. Holes in valence band, whose thermodynamic state is identified by the chemical potential μ_v and the temperature T_v.

3. Phonons in the lattice, whose thermodynamic state is identified the temperature T_L.

For the chemical potentials μ_c and μ_v we have

$$\mu_c = \mathcal{E}_{F,c}, \quad \mu_v = -\mathcal{E}_{F,v},$$

where $\mathcal{E}_{F,c}$, and $\mathcal{E}_{F,v}$ are defined in chapter 3. The minus sign in μ_v depends on the fact that a hole is lack of an electron so $-\mu_v$ is the chemical potential for electrons in valence band, in accordance with the definition of $\mathcal{E}_{F,v}$. If we introduce the entropy functions S_c, S_v and S_L for the electrons in conduction band, the holes in valence band and the phonons in the lattice, respectively, we can write the Gibbs relations

$$dS_c = -\frac{\mu_c}{T_c}\, dn_c + \frac{1}{T_c}\, du_c, \tag{6.10}$$

$$dS_v = -\frac{\mu_v}{T_v}\, dn_v + \frac{1}{T_c}\, du_v, \tag{6.11}$$

$$dS_L = \frac{1}{T_L}\, du_L, \tag{6.12}$$

where u_c, u_v, u_L are the internal energy corresponding to the three subsystems above described. The quantities n_c, u_c, p_v, u_v, u_L satisfy the balance laws

$$\frac{\partial n_c}{\partial t} + \nabla \cdot \boldsymbol{j}_c = H_c, \tag{6.13}$$

$$\frac{\partial u_c}{\partial t} + \nabla \cdot \boldsymbol{j}_c^u = H_c^u + q\boldsymbol{j}_c \cdot \nabla \phi, \tag{6.14}$$

$$\frac{\partial p_v}{\partial t} + \nabla \cdot \boldsymbol{j}_v = H_v, \tag{6.15}$$

$$\frac{\partial u_v}{\partial t} + \nabla \cdot \boldsymbol{j}_v^u = H_v^u - q\boldsymbol{j}_v \cdot \nabla \phi, \tag{6.16}$$

$$\frac{\partial u_L}{\partial t} + \nabla \cdot \boldsymbol{j}_L^u = H_L^u. \tag{6.17}$$

The terms $q\boldsymbol{j}_c \cdot \nabla \phi$, and $-q\boldsymbol{j}_v \cdot \nabla \phi$, that appear in equations (6.14) and (6.16) represent the dissipation due to Joule effect.

The entropy is an additive quantity, then the total entropy of the system is $S = S_c + S_v + S_L$, which satisfies the Gibbs relation

$$\mathrm{d}S = -\frac{\mu_c}{T_c}\,\mathrm{d}n_c + \frac{1}{T_c}\,\mathrm{d}u_c - \frac{\mu_v}{T_v}\,\mathrm{d}n_v + \frac{1}{T_c}\,\mathrm{d}u_v + \frac{1}{T_L}\,\mathrm{d}u_L. \tag{6.18}$$

Using the approach described at the beginning of this section, we obtain the following balance equation for the entropy of the system

$$
\begin{aligned}
\frac{\partial S}{\partial t} = \; & - \; \frac{\mu_c}{T_c}[-\nabla \cdot \boldsymbol{j}_c + H_c] \\
& + \; \frac{1}{T_c}[-\nabla \cdot \boldsymbol{j}_c^u + H_c^u + q\boldsymbol{j}_c \cdot \nabla \phi] \\
& - \; \frac{\mu_v}{T_v}[-\nabla \cdot \boldsymbol{j}_v + H_v] \\
& + \; \frac{1}{T_v}[-\nabla \cdot \boldsymbol{j}_v^u + H_v^u - q\boldsymbol{j}_v \cdot \nabla \phi] \\
& + \; \frac{1}{T_L}[-\nabla \cdot \boldsymbol{j}_L^u + H_L^u],
\end{aligned}
$$

that is equivalent to

$$
\begin{aligned}
\frac{\partial S}{\partial t} = \; & - \; \nabla\frac{\mu_c}{T_c} \cdot \boldsymbol{j}_c + \nabla\frac{1}{T_c} \cdot \boldsymbol{j}_c - \nabla\frac{\mu_v}{T_v} \cdot \boldsymbol{j}_v + \nabla\frac{1}{T_v} \cdot \boldsymbol{j}_v \nabla\frac{1}{T_L} \cdot \boldsymbol{j}_L^u \\
& - \; \nabla \cdot \left(\frac{\mu_c}{T_c}\boldsymbol{j}_c + \frac{1}{T_c}\boldsymbol{j}_c^u + \frac{\mu_v}{T_v}\boldsymbol{j}_v + \frac{1}{T_v}\boldsymbol{j}_v^u + \frac{1}{T_L}\boldsymbol{j}_L^u \right) \\
& - \; \frac{\mu_c}{T_c}H_c + \frac{1}{T_c}H_c^u - \frac{\mu_v}{T_v}H_v + \frac{1}{T_v}H_v^u + \frac{1}{T_L}H_L^u \\
& + \; \frac{1}{T_c}q\boldsymbol{j}_c \cdot \nabla \phi + \frac{1}{T_v}q\boldsymbol{j}_v \cdot \nabla \phi.
\end{aligned}
$$

Then we can write

$$\frac{\partial S}{\partial t} + \nabla \cdot \boldsymbol{j}^S = \sum_{i=1}^{5} \boldsymbol{X}_i \cdot \boldsymbol{j}_i + \sum_{i=1}^{5} I_i H_i,$$

with thermodynamic forces

$$\boldsymbol{X}_1 = \nabla I_1 + q I_2 \nabla \phi \equiv \nabla\left(-\frac{\mu_c}{T_c}\right) + \frac{q}{T_c}\nabla\phi,$$

$$\boldsymbol{X}_2 = \nabla I_2 \equiv \nabla\left(\frac{1}{T_c}\right),$$

$$\boldsymbol{X}_3 = \nabla I_3 - q I_4 \nabla \phi \equiv \nabla\left(-\frac{\mu_v}{T_v}\right) - \frac{q}{T_v}\nabla\phi,$$

$$\boldsymbol{X}_4 = \nabla I_4 \equiv \nabla\left(\frac{1}{T_v}\right),$$

$$\boldsymbol{X}_5 = \nabla I_5 \equiv \nabla\left(\frac{1}{T_L}\right),$$

and production terms

$$H_1 = H_c, \quad H_2 = H_c^u, \quad H_3 = H_v, \quad H_4 = H_v^u, \quad H_5 = H_L^u.$$

The presence of the electric charge affects the definition of the thermodynamic forces, but it is possible assume that the fluxes depend linearly on the forces

$$\boldsymbol{j}_i = \sum_{j=1}^{5} L_{ij} \boldsymbol{X}, \qquad i = 1, \dots 5. \tag{6.19}$$

Finally we must consider, for the electric potential ϕ, the Poisson equation because of the presence of the charge

$$-\nabla \cdot (\epsilon_D \nabla \phi) = \rho \equiv q(N_d^+ - N_a^-) - q n_c + q p_v. \tag{6.20}$$

The system (6.13)-(6.17) with costitutive relations (6.19), coupled with Poisson equation (6.20), is the most general energy transport model for semiconductor.

This thermodynamic approach does not give a way to determine the explicit form of the matrices L_{ij}, nor the expression for the production term. It just give a general form of the equations and the "measure" for the matrices. Then we have to consider other approaches or fitting the data given by the measurement. The Linear Irreversible Thermodynamics provides only the general constraints on L_{ij} and H_i by the second principle of thermodynamics, that are:

$$(L_{ij})_{i,j \in I}, \quad \text{symmetric and positive definite,} \tag{6.21}$$

$$\sum_{i \in I} I_i H_i \geq 0. \tag{6.22}$$

The last thing that we want to note in this section concerns the choice of unknowns in energy transport system above introduced. We can choose for the equations (6.13)-(6.17), (6.20) the variables n_c, u_c, p_v, u_v, u_L and ϕ. Another choice, provided by the constitutive relations (6.19), could be

$$\frac{\mu_c}{T_c} - \frac{q\phi}{T_c}, \quad -\frac{1}{T_c}, \quad \frac{\mu_v}{T_v} - \frac{q\phi}{T_v}, \quad -\frac{1}{T_v}, \quad -\frac{1}{T_L}, \quad \phi,$$

that are related to the opposite of variables I_i.

It is possible to determine the relations between the first type of variables and the second from the following relations introduced in chapter (3). For the electrons on conduction band, we have

$$n_c(\mu_c, T_c) = y \int_{\mathcal{B}} F_{\mathrm{FD}}(\mathcal{E}_c(\mathbf{k}); \mu_c, T_c) \, \mathrm{d}\mathbf{k}, \tag{6.23}$$

where $y = 2/(2\pi)^3$. For the holes in valence band, recalling that $\mu_v = -\mathcal{E}_{F,v}$ and noting that

$$
\begin{aligned}
1 - F_{\mathrm{FD}}(-\mathcal{E}; \mu_v, T_v) &= 1 - \frac{1}{\exp\frac{\mathcal{E}+\mu_v}{k_B T_v} + 1} \\
&= \frac{1}{1 + \exp\frac{-\mathcal{E}-\mu_v}{k_B T_v}} \\
&= F_{\mathrm{FD}}(-\mathcal{E}; \mu_v, T_v),
\end{aligned}
$$

we have also

$$p_v(\mu_v, T_v) = y \int_{\mathcal{B}} F_{\mathrm{FD}}(-\mathcal{E}_v(\mathbf{k}); \mu_v, T_v) \, \mathrm{d}\mathbf{k}. \tag{6.24}$$

Similarly we obtain expressions for internal energies

$$
\begin{aligned}
u_c(\mu_c, T_c) &= y \int_{\mathcal{B}} \mathcal{E}_c(\mathbf{k}) F_{\mathrm{FD}}(\mathcal{E}_c(\mathbf{k}); \mu_c, T_c) \, \mathrm{d}\mathbf{k}, \\
u_v(\mu_v, T_v) &= y \int_{\mathcal{B}} (-\mathcal{E}_v(\mathbf{k})) F_{\mathrm{FD}}(-\mathcal{E}_v(\mathbf{k}); \mu_v, T_v) \, \mathrm{d}\mathbf{k}.
\end{aligned}
$$

For the phonons internal energy u_L, using the Bose-Einstein distribution N_{B}, introduced in chapter 3, equation (3.49), we have the following expression

$$u_L(T_L) = z \int_{\mathcal{B}} \hbar\omega(\mathbf{q}) N_{\mathrm{B}}(\hbar\omega; T_L) \, \mathrm{d}\mathbf{q},$$

where $z = 3/(2\pi)^3$.

6.2 Electron-phonon kinetic model

We consider an ensemble of electrons, with charge $-q_e$, in a semiconductor with n_{ph} relevant families of phonons. We denote by $f(\mathbf{x}, \mathbf{k}, t)$ the electron distribution

function, and by $g_i(\mathbf{x}, \mathbf{q}, t)$, $i = 1, \ldots, n_{\text{ph}}$, the phonon distribution functions, with $\mathbf{x} \in \Omega \subset \mathbb{R}^3$, $\mathbf{k}, \mathbf{q} \in \mathcal{B} \subset \mathbb{R}^3$, $t \in \mathbb{R}^+$, where Ω is the domain of the semiconductor, and $\mathcal{B}$ is the first Brillouin zone of the inverse lattice.

For simplicity we use the scaling:

$$\frac{f}{y} \to f, \quad \frac{g_i}{z} \to g_i,$$

keeping the same name. Thus the distribution functions f, g_i must now be interpreted as occupation probabilities.

These distribution functions satisfy the Bloch-Boltzmann-Peierls (BBP) equations:

$$\begin{cases} \dfrac{\partial f}{\partial t} + \boldsymbol{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \dfrac{q_e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f = \mathcal{C}_0^{\text{el}}(f) + \sum_{i=1}^{n_{\text{ph}}} \mathcal{C}_i^{\text{el}}(f, g_i), \\ \dfrac{\partial g_i}{\partial t} + \boldsymbol{c}_i(\mathbf{q}) \cdot \nabla_{\mathbf{x}} g_i = \mathcal{C}_i^{\text{ph}}(f, g_i), \quad i = 1, \ldots, n_{\text{ph}}. \end{cases} \tag{6.25}$$

Below we explain the meaning of the terms appearing in (6.25). The term $\mathcal{E}(\mathbf{k})$ is the electron dispersion relation (conduction energy band), and $\boldsymbol{v}(\mathbf{k})$ is the carrier electron velocity related to the energy by the relation

$$\boldsymbol{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k}), \tag{6.26}$$

where the $\hbar$ is the reduced Planck constant. The group velocities of the phonons are indicated with

$$\boldsymbol{c}_i(\mathbf{q}) = \nabla_{\mathbf{q}} \omega_i(\mathbf{q}), \quad i = 1, \ldots, n_{\text{ph}},$$

where $\omega_i(\mathbf{q})$ are the phonons dispersion relations, $i = 1, \ldots, n_{\text{ph}}$.

The operator $\mathcal{C}_0^{\text{el}}(f)$, represents the collision electron-impurities and is given by

$$\mathcal{C}_0^{\text{el}}(f) = \int_{\mathcal{B}} [P_0(\mathbf{k}', \mathbf{k}) f'(1 - f) - P_0(\mathbf{k}, \mathbf{k}') f(1 - f')] \, d\mathbf{k}', \tag{6.27}$$

where $P_0(\mathbf{k}', \mathbf{k})$ is the transition probability per unit time from a state $\mathbf{k}'$ to a state $\mathbf{k}$, we assume that these collisions are elastic and anisotropic, and we assume that P_0 does not depend on temperature. In equation (6.27) and in the following, we use the short notation $\mathcal{E} = \mathcal{E}(\mathbf{k})$, $\mathcal{E}' = \mathcal{E}(\mathbf{k}')$, $f = f(\mathbf{x}, \mathbf{k}, t)$ and $f' = f(\mathbf{x}, \mathbf{k}', t)$.

The other two collision terms in equations (6.25), $\mathcal{C}_i^{\text{el}}(f, g_i)$, $\mathcal{C}_i^{\text{ph}}(f, g_i)$, are the collision operator between electrons and phonons. To obtain the form of this collision operator we have to sum the probabilities of the phenomena of collision that we have chosen.

1. Probability that an electron goes from a state $\mathbf{k}'$ to a state $\mathbf{k}$ releasing the i-th phonon

$$s(\mathbf{q}) \delta(\mathcal{E} - \mathcal{E}' + \hbar \omega_i) \delta(\mathbf{k} - \mathbf{k}' + \mathbf{q})(g_i + 1) f'(1 - f).$$

2. Probability that an electron goes from a state $\mathbf{k}$ to a state $\mathbf{k}'$ assimilating the i-th phonon

$$s(\mathbf{q})\delta(\mathcal{E} - \mathcal{E}' + \hbar\omega_i)\delta(\mathbf{k} - \mathbf{k}' + \mathbf{q})g_i f(1 - f').$$

3. Probability that an electron goes from a state $\mathbf{k}'$ to a state $\mathbf{k}$ assimilating the i-th phonon

$$s(\mathbf{q})\delta(\mathcal{E} - \mathcal{E}' - \hbar\omega_i)\delta(\mathbf{k} - \mathbf{k}' - \mathbf{q})g_i f'(1 - f).$$

4. Probability that an electron goes from a state $\mathbf{k}$ to a state $\mathbf{k}'$ releasing the i-th phonon

$$s(\mathbf{q})\delta(\mathcal{E} - \mathcal{E}' - \hbar\omega_i)\delta(\mathbf{k} - \mathbf{k}' - \mathbf{q})(g_i + 1)f(1 - f').$$

Here, $s(\mathbf{q})$ is the Fourier transform of the scattering potential, and δ is the delta function definted in chapter 3.

Using these considerations we can write

$$
\begin{aligned}
\mathcal{C}_i^{\mathrm{el}}(f, g_i) &= \int_{\mathcal{B}} w_i^+(\mathbf{k}, \mathbf{k}', \mathbf{q}^+)[(g_i^+ + 1)f'(1 - f) - g_i^+ f(1 - f')]\,\mathrm{d}\mathbf{k}' \\
&+ \int_{\mathcal{B}} w_i^-(\mathbf{k}, \mathbf{k}', \mathbf{q}^-)[g_i^- f'(1 - f) - (g_i^- + 1)f(1 - f')]\,\mathrm{d}\mathbf{k}' \\
&= \int_{\mathcal{B}} [P_i(\mathbf{k}', \mathbf{k}; g_i)f'(1 - f) - P_i(\mathbf{k}, \mathbf{k}'; g_i)f(1 - f')]\,\mathrm{d}\mathbf{k}'.
\end{aligned}
$$

with $\mathbf{q}^\pm = \pm(\mathbf{k}' - \mathbf{k})$.

Noting that

$$\omega_i^\pm(\mathbf{k}, \mathbf{k}', \mathbf{q}) = \omega^\mp(\mathbf{k}', \mathbf{k}, \mathbf{q})$$

and

$$\delta(\mathbf{k} - \mathbf{k}' \pm \mathbf{q}) = \delta(\mathbf{k} - \mathbf{k}' \mp \mathbf{q}),$$

the phonon collision operator has the form

$$
\begin{aligned}
\mathcal{C}_i^{\mathrm{ph}}(f, g_i) &= 2\int_{\mathcal{B}}\int_{\mathcal{B}} s_i(\mathbf{q})\{\delta(\mathcal{E} - \mathcal{E}' + \hbar\omega_i)\delta(\mathbf{k} - \mathbf{k}' + \mathbf{q})(g_i + 1)f'(1 - f) \\
&\qquad -\delta(\mathcal{E} - \mathcal{E}' + \hbar\omega_i)\delta(\mathbf{k} - \mathbf{k}' + \mathbf{q})g_i f(1 - f')\}\,\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}'. \\
&= 2\int_{\mathcal{B}}\int_{\mathcal{B}} s_i(\mathbf{q})\delta(\mathcal{E} - \mathcal{E}' + \hbar\omega_i)\delta(\mathbf{k} - \mathbf{k}' + \mathbf{q}) \times \\
&\qquad \{(g_i + 1)f'(1 - f) - g_i f(1 - f')\}\,\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}'. \\
&= 2\int_{\mathcal{B}} s_i(\mathbf{q})\delta(\mathcal{E}^* - \mathcal{E}' + \hbar\omega_i)\{(g_i + 1)f'(1 - f^*) - g_i f^*(1 - f')\}\,\mathrm{d}\mathbf{k}'.
\end{aligned}
$$

in the last integral $f^* = f(\mathbf{x}, \mathbf{k}^*, t)$, where $\mathbf{k}^* = \mathbf{k}' - \mathbf{q}$.

6.3 Maximum Entropy Principle

Macroscopic models for semiconductors can be obtained from a suitable finite subset of the infinite moment equations hierarchy of the Bloch-Boltzmann-Pierls equations. To this aim we consider the sets of weight functions for electrons and for phonons:

$$\mathscr{W}^{\mathrm{el}} = \{\psi^\alpha(\mathbf{k}) \,:\, \alpha \in I\}, \quad \mathscr{W}_i^{\mathrm{ph}} = \{\psi_i^\alpha(\mathbf{q}) \,:\, \alpha \in I_i\}, \quad i = 1, \dots, n_{\mathrm{ph}},$$

with I, I_i index sets, and introduce the electron and phonon moments:

$$M^\alpha(\mathbf{x}, t) = \int_{\mathscr{B}} \psi^\alpha(\mathbf{k}) f(\mathbf{x}, \mathbf{k}, t) \, d\mathbf{k}, \quad \alpha \in I,$$

$$M_i^\alpha(\mathbf{x}, t) = \int_{\mathscr{B}} \psi_i^\alpha(\mathbf{q}) g_i(\mathbf{x}, \mathbf{q}, t) \, d\mathbf{q}, \quad \alpha \in I_i, \ i = 1, \dots, n_{\mathrm{ph}}.$$

This moments satisfy the coupled electron-phonon moment equations

$$\begin{cases} \dfrac{\partial M^\alpha}{\partial t} + \nabla \cdot \mathbf{M}^\alpha + q_e \mathbf{E} \cdot \mathbf{N}^\alpha = \mathcal{C}_0^\alpha + \mathcal{C}^\alpha, \quad \alpha \in I, \\ \dfrac{\partial M_i^\alpha}{\partial t} + \nabla \cdot \mathbf{M}_i^{\alpha_i} = \mathcal{C}_i^{\alpha_i}, \quad \alpha \in I_i, \end{cases} \tag{6.28}$$

with

$$\mathbf{M}^\alpha(f) = \int_{\mathscr{B}} \psi^\alpha \boldsymbol{v} f \, d\mathbf{k}, \quad \mathbf{N}^\alpha(f) = \int_{\mathscr{B}} \frac{1}{\hbar} \nabla_{\mathbf{k}} \psi^\alpha f \, d\mathbf{k}, \tag{6.29}$$

$$\mathbf{M}_i^{\alpha_i}(g_i) = \int_{\mathscr{B}} \psi_i^{\alpha_i} \boldsymbol{c}_i g_i \, d\mathbf{q}, \tag{6.30}$$

$$\mathcal{C}_0^\alpha(f) = \int_{\mathscr{B}} \psi^\alpha \mathcal{C}_0^{\mathrm{el}}(f) \, d\mathbf{k}, \quad \mathcal{C}^\alpha(f, g_i) = \sum_{i=1}^{n_{\mathrm{ph}}} \int_{\mathscr{B}} \psi^\alpha \mathcal{C}_i^{\mathrm{el}}(f, g_i) \, d\mathbf{k}, \tag{6.31}$$

$$\mathcal{C}_i^{\alpha_i}(f, g_i) = \int_{\mathscr{B}} \psi_i^{\alpha_i} \mathcal{C}_i^{\mathrm{ph}}(f, g_i) \, d\mathbf{q}. \tag{6.32}$$

System (6.28) is not closed, since the new moments in (6.29),(6.30) depend on ψ^α and $\psi_i^{\alpha_i}$, and the collision term in (6.31),(6.32) are not express in terms of moments of f or g_i.

To solve this closure problem we use the Maximum Entropy Principle. We introduce the entropy functional

$$H(f, g_1, \dots, g_{n_{\mathrm{ph}}}) = H^{\mathrm{el}}(f) + H_1^{\mathrm{ph}}(g_1) + \cdots + H_{n_{\mathrm{ph}}}^{\mathrm{ph}}(g_{n_{\mathrm{ph}}}). \tag{6.33}$$

where

$$H^{\mathrm{el}}(f) = -\int_{\mathscr{B}} [f \log f + (1 - f) \log(1 - f)] \, d\mathbf{k},$$

$$H_i^{\mathrm{ph}}(g_i) = H^{\mathrm{ph}}(g_i) = -\int_{\mathscr{B}} [g_i \log g_i - (1 + g_i) \log(1 + g_i)] \, d\mathbf{q},$$

equivalent to

$$H^{\mathrm{el}}(f) = \int_{\mathscr{B}} h^+(f)\,\mathrm{d}\mathbf{k},$$

$$H^{\mathrm{ph}}(g) = \int_{\mathscr{B}} h^-(g)\,\mathrm{d}\mathbf{q},$$

with $h^{\pm}(f) = -\left[f \log f \pm (1 \mp f) \log(1 \mp f)\right]$.

The maximum entropy principle (hereafter MEP) leads to a systematic way for obtaining constitutive relations on the basis of information theory. According to the MEP if a given number of moments are known, the distribution function f_{ME}, or respectively g_{ME}, which can be used to evaluate the unknown moments of f and g, corresponds to the extremal of the entropy functional under the constraints that it yields exactly the known moments.

In other words the maximum entropy principle says that if we know the moment M^α and $M_i^{\alpha_i}$, $\alpha \in I$, $\alpha_i \in I_i$, we need to find $(f, \boldsymbol{g}) = (f, g_1, \ldots, g_{n_{\mathrm{ph}}})$ that maximizes the entropy functional H in (6.33) with the constraints

$$\int_{\mathscr{B}} \psi^\alpha f\,\mathrm{d}\mathbf{k} = M^\alpha,\ \alpha \in I, \qquad \int_{\mathscr{B}} \psi_i^{\alpha_i} g_i\,\mathrm{d}\mathbf{q} = M_i^{\alpha_i},\ \alpha_i \in I_i. \tag{6.34}$$

This is equivalent to find $(f, \boldsymbol{g}, \lambda^\alpha, \lambda_i^{\alpha_i})$ that minimizes

$$
\begin{aligned}
\mathscr{H} &= -H(f, \boldsymbol{g}) + \sum_{\alpha \in I} \lambda^\alpha (M^\alpha(f) - M^\alpha) + \sum_{i=1}^{n_{\mathrm{ph}}} \sum_{\alpha_i \in I_i} \lambda_i^{\alpha_i}(M_i^{\alpha_i}(g_i) - M_i^{\alpha_i}) \\
&= \int_{\mathscr{B}} \{-h^+(f) + \sum_{\alpha \in I} \lambda^\alpha \psi^\alpha f\}\,\mathrm{d}\mathbf{k} + \sum_{i=1}^{n_{\mathrm{ph}}} \int_{\mathscr{B}} \{-h^-(g_i) + \sum_{\alpha_i \in I_i} \lambda_i^{\alpha_i} \psi_i^{\alpha_i} g_i\}\,\mathrm{d}\mathbf{q} \\
&\quad - \sum_{\alpha \in I} \lambda^\alpha M^\alpha - \sum_{i=1}^{n_{\mathrm{ph}}} \sum_{\alpha_i \in I_i} \lambda_i^{\alpha_i} M_i^{\alpha_i}.
\end{aligned}
$$

To this aim, we compute the Fréchet derivatives of the functional $\mathcal{H}$ with respect to f and g_i, and we equal them to zero

$$
\begin{aligned}
\frac{\delta \mathscr{H}}{\delta f}(f, \boldsymbol{g})[\eta] &= \int_{\mathscr{B}} \left\{-\frac{\mathrm{d}h^+}{\mathrm{d}f}(f) + \chi\right\} \eta\,\mathrm{d}\mathbf{k} = 0, \\
\frac{\delta \mathscr{H}}{\delta g_i}(f, \boldsymbol{g})[\eta_i] &= \int_{\mathscr{B}} \left\{-\frac{\mathrm{d}h^-}{\mathrm{d}g_i}(g_i) + \chi_i\right\} \eta_i\,\mathrm{d}\mathbf{q} = 0,
\end{aligned}
$$

with

$$\chi := \sum_{\alpha \in I} \lambda^\alpha \psi^\alpha, \qquad \chi_i := \sum_{\alpha_i \in I_i} \lambda_i^{\alpha_i} \psi_i^{\alpha_i}.$$

Because of

$$\frac{\mathrm{d}h^+}{\mathrm{d}f} = -\log \frac{f}{1-f}, \qquad \frac{\mathrm{d}h^-}{\mathrm{d}g_i} = -\log \frac{g_i}{1+g_i},$$

we have

$$\log \frac{f^{\mathrm{ME}}}{1 - f^{\mathrm{ME}}} = -\chi, \qquad \log \frac{g_i^{\mathrm{ME}}}{1 + g_i^{\mathrm{ME}}} = -\chi_i$$

and, inverting the above equations, we obtain the maximum entropy distribution fuctions indicate with f^{ME} and g_i^{ME},

$$f^{\mathrm{ME}} = \frac{1}{\exp \chi + 1}, \qquad g_i^{\mathrm{ME}} = \frac{1}{\exp \chi_i - 1} \tag{6.35}$$

The Lagrangian multipliers are implicitly defined as functions of the moments $\{M^\alpha, \alpha \in I\}$, $\{M_i^\alpha, \alpha \in I_i\}$ by the constraints

$$\int_{\mathscr{B}} \psi^\alpha f^{\mathrm{ME}} \, \mathrm{d}\mathbf{k} = M^\alpha, \ \alpha \in I, \qquad \int_{\mathscr{B}} \psi_i^{\alpha_i} g_i^{\mathrm{ME}} \, \mathrm{d}\mathbf{q} = M_i^{\alpha_i}, \ \alpha_i \in I_i. \tag{6.36}$$

We choose the following sets of weight functions

$$\mathscr{W}^{\mathrm{el}} = \{1, \boldsymbol{v}, \mathcal{E}, \mathcal{E}\boldsymbol{v}\}, \quad \mathscr{W}_i^{\mathrm{ph}} = \{\hbar\omega_i, \hbar\omega_i \boldsymbol{c}_i\},$$

thus we consider electron and phonon moments $M^\alpha(f)$ and $M_i^{\alpha_i}(g_i)$:

$$\text{electron number density} \quad n = n(f) \ := \ y \int_{\mathscr{B}} f(\mathbf{x}, \mathbf{k}, t) \, \mathrm{d}\mathbf{k},$$

$$\text{electron current density} \quad \boldsymbol{j} = \boldsymbol{j}(f) \ := \ y \int_{\mathscr{B}} \boldsymbol{v} f(\mathbf{x}, \mathbf{k}, t) \, \mathrm{d}\mathbf{k},$$

$$\text{energy electron density} \quad W = W(f) \ := \ y \int_{\mathscr{B}} \mathcal{E} f(\mathbf{x}, \mathbf{k}, t) \, \mathrm{d}\mathbf{k},$$

$$\text{energy electron flux} \quad \boldsymbol{j}^W = \boldsymbol{j}^W(f) \ := \ y \int_{\mathscr{B}} \mathcal{E}\boldsymbol{v} f(\mathbf{x}, \mathbf{k}, t) \, \mathrm{d}\mathbf{k},$$

$$\text{energy phonon density} \quad W_i = W_i(g_i) \ := \ z \int_{\mathscr{B}} \hbar\omega_i(\mathbf{q}) g_i(\mathbf{x}, \mathbf{q}, t) \, \mathrm{d}\mathbf{q},$$

$$\text{energy phonon flux} \quad \boldsymbol{j}_i^W = \boldsymbol{j}_i^W(g_i) \ := \ z \int_{\mathscr{B}} \hbar\omega_i(\mathbf{q}) \boldsymbol{c}(\mathbf{q}) g_i(\mathbf{x}, \mathbf{q}, t) \, \mathrm{d}\mathbf{q}.$$

This moments satisfy the coupled electron-phonon moment equations

$$\begin{cases} \dfrac{\partial n}{\partial t} & + \ \nabla \cdot \boldsymbol{j} & = \ 0, \\[2mm] \dfrac{\partial \boldsymbol{j}}{\partial t} & + \ \nabla \cdot \mathscr{J} + q_e \mathbf{E} \cdot \mathscr{R} & = \ \boldsymbol{\mathcal{C}}_0 + \boldsymbol{\mathcal{C}}, \\[2mm] \dfrac{\partial W}{\partial t} & + \ \nabla \cdot \boldsymbol{j}^W + q_e \mathbf{E} \cdot \boldsymbol{j} & = \ \mathcal{C}_0^W + \mathcal{C}^W, \\[2mm] \dfrac{\partial \boldsymbol{j}^W}{\partial t} & + \ \nabla \cdot \mathscr{J}^W + q_e \mathbf{E} \cdot \mathscr{R}^W & = \ \boldsymbol{\mathcal{C}}_0^W + \boldsymbol{\mathcal{C}}^W, \\[2mm] \dfrac{\partial W_i}{\partial t} & + \ \nabla \cdot \boldsymbol{j}_i^W & = \ \mathcal{C}_i^W, \\[2mm] \dfrac{\partial \boldsymbol{j}_i^W}{\partial t} & + \ \nabla \cdot \mathscr{J}_i^W & = \ \boldsymbol{\mathcal{C}}_i^W, \quad i = 1, \ldots, n_{\mathrm{ph}}, \end{cases} \tag{6.37}$$

with

$$\mathscr{J}(f) \;=\; y \int_{\mathscr{B}} \boldsymbol{v} \otimes \boldsymbol{v} f \, \mathrm{d}\mathbf{k},$$

$$\mathscr{J}^{W}(f) \;=\; y \int_{\mathscr{B}} \mathcal{E}\boldsymbol{v} \otimes \boldsymbol{v} f \, \mathrm{d}\mathbf{k},$$

$$\mathscr{J}^{W}_{i}(g_i) \;=\; z \int_{\mathscr{B}} \hbar\omega_i \boldsymbol{c}_i \otimes \boldsymbol{c}_i g_i \, \mathrm{d}\mathbf{q},$$

and

$$\mathscr{R}(f) \;=\; y \int_{\mathscr{B}} \frac{1}{\hbar^2}\nabla_{\mathbf{k}} \otimes \nabla_{\mathbf{k}}\mathcal{E} f \, \mathrm{d}\mathbf{k},$$

$$\mathscr{R}^{W}(f) \;=\; y \int_{\mathscr{B}} \left[\boldsymbol{v} \otimes \boldsymbol{v} + \mathcal{E}\frac{1}{\hbar^2}\nabla_{\mathbf{k}} \otimes \nabla_{\mathbf{k}}\mathcal{E} \right] f \, \mathrm{d}\mathbf{k}.$$

For the collision terms we have

$$
\begin{aligned}
\boldsymbol{\mathcal{C}}_0 &= y \int_{\mathscr{B}} \boldsymbol{v}(\mathbf{k})\mathcal{C}_0^{\mathrm{el}}(f) \, \mathrm{d}\mathbf{k}, & \boldsymbol{\mathcal{C}} &= \sum_{i=1}^{n_{\mathrm{ph}}} y \int_{\mathscr{B}} \boldsymbol{v}(\mathbf{k})\mathcal{C}_i^{\mathrm{el}}(f,g_i) \, \mathrm{d}\mathbf{k} \\[4pt]
\mathcal{C}_0^{W} &= y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k})\mathcal{C}_0^{\mathrm{el}}(f) \, \mathrm{d}\mathbf{k}, & \mathcal{C}^{W} &= \sum_{i=1}^{n_{\mathrm{ph}}} y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k})\mathcal{C}_i^{\mathrm{el}}(f,g_i) \, \mathrm{d}\mathbf{k} \\[4pt]
\boldsymbol{\mathcal{C}}_0^{W} &= y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k})\boldsymbol{v}(\mathbf{k})\mathcal{C}_0^{\mathrm{el}}(f) \, \mathrm{d}\mathbf{k}, & \boldsymbol{\mathcal{C}}^{W} &= \sum_{i=1}^{n_{\mathrm{ph}}} y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k})\boldsymbol{v}(\mathbf{k})\mathcal{C}_i^{\mathrm{el}}(f,g_i) \, \mathrm{d}\mathbf{k} \\[4pt]
\mathcal{C}_i^{W} &= z \int_{\mathscr{B}} \hbar\omega_i \mathcal{C}_i^{\mathrm{ph}}(f,g_i) \, \mathrm{d}\mathbf{q}, & \boldsymbol{\mathcal{C}}_i^{W} &= z \int_{\mathscr{B}} \hbar\omega_i \boldsymbol{c}_i \mathcal{C}_i^{\mathrm{ph}}(f,g_i) \, \mathrm{d}\mathbf{q}
\end{aligned}
\tag{6.38}
$$

Now we apply the Maximum Entropy Principle and we obtain the maximum entropy distribution functions f^{ME}, g_i^{ME}, definited in (6.35), depending on the Lagrange multipliers, more precisely depending on

$$
\begin{aligned}
\chi &= \lambda + \boldsymbol{v} \cdot \boldsymbol{\lambda} + \mathcal{E}\lambda^{W} + \mathcal{E}\boldsymbol{v} \cdot \boldsymbol{\lambda}^{W}, & (6.39) \\
\chi_i &= \hbar\omega_i \lambda_i^{W} + \hbar\omega_i \boldsymbol{c}_i \cdot \boldsymbol{\lambda}_i^{W}. & (6.40)
\end{aligned}
$$

The Lagrange multipliers are implicitly defined as functions of the known moments, that is,

$$
\begin{aligned}
n(f^{\mathrm{ME}}) &= n, & \boldsymbol{j}(f^{\mathrm{ME}}) &= \boldsymbol{j}, \\
W(f^{\mathrm{ME}}) &= W, & \boldsymbol{j}^{W}(f^{\mathrm{ME}}) &= \boldsymbol{j}^{W}, \\
W_i(f^{\mathrm{ME}}) &= W_i, & \boldsymbol{j}_i^{W}(f^{\mathrm{ME}}) &= \boldsymbol{j}_i^{W}.
\end{aligned}
\tag{6.41}
$$

6.4 Diffusive limit

In this section we consider the diffusive limit of the MEP-based models (6.37). First we have to identify the smallness parameter from the collision term.

First scaling. We introduce the first scaling for the transition probability $P_0(\mathbf{k}, \mathbf{k}')$ in the collision term for electron-impurities $\mathcal{C}_0^{\text{el}}$ in (6.27)

$$P_0(\mathbf{k}, \mathbf{k}') = \frac{1}{\epsilon}\hat{P}_0(\mathbf{k}, \mathbf{k}').\tag{6.42}$$

The scaling for the other transition probabilities is in the terms $s_i(\mathbf{q})$ and $\hbar\omega_i$ in $\mathcal{C}_i^{\text{el}}$ and $\mathcal{C}_i^{\text{ph}}$

$$s_i(\mathbf{q}) = \frac{\sigma}{\epsilon}\hat{s}_i(\mathbf{q}), \qquad \hbar\omega_i = \sigma\hbar\hat{\omega}_i.\tag{6.43}$$

This second part of the first scaling, uses other small parameters σ that will be later related to the small parameter ϵ in (6.42).

Second scaling. The second scaling, that we propose for the Lagrange multipliers, corresponding to the fluxes, is the following

$$\boldsymbol{\lambda} = \epsilon\hat{\boldsymbol{\lambda}}, \quad \boldsymbol{\lambda}^W = \epsilon\hat{\boldsymbol{\lambda}}^W, \quad \boldsymbol{\lambda}_i^W = \epsilon\hat{\boldsymbol{\lambda}}_i^W.\tag{6.44}$$

Using both previous scaling, we can write χ and χ_i, defined in (6.39), (6.40), as follows

$$\chi = \chi^{(0)} + \epsilon\chi^{(1)},\tag{6.45}$$

$$\chi_i = \sigma\left(\chi_i^{(0)} + \epsilon\chi_i^{(1)}\right)\tag{6.46}$$

in which we have posed

$$
\begin{aligned}
\chi^{(0)} &= \lambda + \mathcal{E}\lambda^W, & \chi^{(1)} &= \boldsymbol{v}\cdot\hat{\boldsymbol{\lambda}} + \mathcal{E}\boldsymbol{v}\cdot\hat{\boldsymbol{\lambda}}^W, \\
\chi_i^{(0)} &= \hbar\hat{\omega}_i, & \chi_i^{(1)} &= \hbar\hat{\omega}_i\boldsymbol{c}_i\cdot\hat{\boldsymbol{\lambda}}^W.
\end{aligned}\tag{6.47}
$$

Now we introduce a lemma that that will allow us to write the distribution functions, in (6.35), in series form.

We use a parameter ν which can take values $-1, 0, 1$, in order to characterize in an unified way the expansion of the Fermi-Dirac, Maxwell and Bose-Einstein distributions, respectively.

Lemma 6.4.1 *Let*

$$f_\nu(x) = \frac{1}{e^{a+bx} + \nu},\tag{6.48}$$

with $a, b \in \mathbb{R}$. Then

$$f_\nu(x) = f_\nu^{(0)}\sum_{n=0}^{\infty}(-1)^n b^n x^n p_{\nu,n}(f_\nu^{(0)})\tag{6.49}$$

with $\nu = -1, 0, 1$, and

$$f_\nu^{(0)} = \frac{1}{e^a + \nu},$$

and the function $p_{\nu,n}$ is defined iteratively by

$$p_{\nu,0}(s) = 1, \quad p_{\nu,n}(s) = \frac{1}{n}(1 - \nu s)\frac{\mathrm{d}}{\mathrm{d}s}[sp_{\nu,(n-1)}(s)], \quad n \geq 1.$$

Proof. The first observation, easly to show, is the following relation between the function f, definited in (6.48), and its first defivative

$$f'_\nu(x) = -bf_\nu(1 - \nu f_\nu). \tag{6.50}$$

Now we prove, by induction, that

$$f_\nu^{(n)}(x) = n!(-1)^n b^n f_\nu(x) p_{\nu,n}(f_\nu(x)), \quad n \geq 1. \tag{6.51}$$

The first step of induction, for $n = 0$, is trivial. Let us now assume that (6.51) is true for some $n = \ell$ and prove that it follows for $n = \ell + 1$. To this aim we compute

$$
\begin{aligned}
f_\nu^{(\ell+1)}(x) &= \frac{d}{dx}\left[f_\nu^{(\ell)}(x)\right] \\
&= \frac{d}{dx}\left[\ell!(-1)^\ell b^\ell f_\nu(x) p_{\nu,\ell}(f_\nu(x))\right] \\
&= (-1)^\ell b^\ell \ell! \frac{d}{dx}\left[f_\nu(x) p_{\nu,\ell}(f_\nu(x))\right] \\
&= (-1)^\ell b^\ell \ell! \left[\frac{d}{df_\nu}(f_\nu(x) p_{\nu,\ell}(f_\nu(x)))\right] f'_\nu(x) \\
&= (-1)^\ell b^\ell \ell! [-bf_\nu(x)(1 - \nu f_\nu(x))]\left[\frac{d}{df_\nu}(f_\nu(x) p_{\nu,\ell}(f_\nu(x)))\right] \\
&= (-1)^{\ell+1} b^{\ell+1} (\ell+1)! f_\nu(x) p_{\nu,(\ell+1)}(f_\nu(x)),
\end{aligned}
$$

where the last equality follows from (6.50). Evaluating the derivatives at $x = 0$ we obtain the series in the right hand side of (6.49). ∎

Using the previous Lemma, we can write both maximum entropy distribution functions

$$f^{ME} = \frac{1}{\exp\left(\chi^{(0)} + \epsilon\chi^{(1)}\right) + 1}, \quad g_{i,\sigma}^{ME} = \frac{1}{\exp\left(\sigma(\chi_i^{(0)} + \epsilon\chi_i^{(1)})\right) - 1}, \tag{6.52}$$

as

$$f^{ME} = \sum_{\ell=0}^{\infty} \epsilon^\ell f^{(\ell)}, \qquad g_{i,\sigma}^{ME} = \sum_{\ell=0}^{\infty} \epsilon^\ell g_{i,\sigma}^{(\ell)}, \tag{6.53}$$

with

$$
\begin{aligned}
f^{(\ell)} &= f^{(0)}(-1)^\ell p_\ell^+(f^{(0)})(\chi^{(1)})^\ell \\
g_{i,\sigma}^{(\ell)} &= g_{i,\sigma}^{(0)}(-1)^\ell \sigma^\ell p_\ell^-(g_{i,\sigma}^{(0)}))(\chi_i^{(1)})^\ell
\end{aligned}
$$

where

$$f^{(0)} = \frac{1}{\exp\chi^{(0)} + 1}, \quad g_{i,\sigma}^{(0)} = \frac{1}{\exp\sigma\chi_i^{(0)} - 1},$$

and the functions $p_\ell^\pm$ are defined iteratively by

$$p_0^\pm(x) = 1, \quad p_\ell^\pm(x) = \frac{1}{\ell}(1 \mp x)\frac{d}{dx}[x p_{\ell-1}(x)], \quad \ell \geq 1,$$

and χ, χ_i defined in (6.45) and (6.46).

It is possible to see that, since

$$\lim_{\sigma \to 0} \sigma g_{i,\sigma}^{(0)} = \frac{1}{\chi_i^{(0)}}, \tag{6.54}$$

and that the leading order coefficient of the polynomial p_ℓ^- is equal to 1, we have

$$\lim_{\sigma \to 0} \sigma g_{i,\sigma}^{(\ell)} = \frac{1}{\chi_i^{(0)}}\left(\frac{\chi_i^{(1)}}{\chi_i^{(0)}}\right)^\ell.$$

In the expansions (6.49), we have that,

$$f^{(\ell)}(-\mathbf{k}) = \begin{cases} f^{(\ell)}(\mathbf{k}), & \text{if } \ell \text{ is even}, \\ -f^{(\ell)}(\mathbf{k}), & \text{if } \ell \text{ is odd}, \end{cases}$$

and similarly

$$g_{i,\sigma}^{(\ell)}(-\mathbf{q}) = \begin{cases} g_{i,\sigma}^{(\ell)}(\mathbf{q}), & \text{if } \ell \text{ is even}, \\ -g_{i,\sigma}^{(\ell)}(\mathbf{q}), & \text{if } \ell \text{ is odd}. \end{cases}$$

Using this property, and the fact that $\mathcal{E}(\mathbf{k})$ is even functions, expansions (6.49) lead to analogous expansions for each term in (6.37). For the electron number density n we have

$$\begin{aligned} n = n(f^{\mathrm{ME}}) &= \sum_{\ell=0}^\infty \epsilon^\ell y \int_{\mathscr{B}} f^{(\ell)}(\mathbf{k})\, d\mathbf{k} = \sum_{\ell=0}^\infty \epsilon^{2\ell} y \int_{\mathscr{B}} f^{(2\ell)}(\mathbf{k})\, d\mathbf{k} \\ &= \sum_{\ell=0}^\infty \epsilon^{2\ell} n^{(2\ell)}(\mathbf{k}). \end{aligned}$$

In a similar way, we obtain

$$\begin{aligned} \mathscr{J} = \mathscr{J}(f^{\mathrm{ME}}) &= \sum_{\ell=0}^\infty \epsilon^\ell y \int_{\mathscr{B}} \mathbf{v}(\mathbf{k}) \otimes \mathbf{v}(\mathbf{k}) f^{(\ell)}(\mathbf{k})\, d\mathbf{k} \\ &= \sum_{\ell=0}^\infty \epsilon^{2\ell} \mathscr{J}^{(2\ell)}(\mathbf{k}), \end{aligned}$$

remembering that $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}(\mathbf{k})$, then it is an odd function. Using the same argument, we have for the other term

$$\begin{aligned} \mathscr{R} = \mathscr{R}(f^{\mathrm{ME}}) &= \sum_{\ell=0}^\infty \epsilon^\ell y \int_{\mathscr{B}} \frac{1}{\hbar^2}\nabla_{\mathbf{k}} \otimes \nabla_{\mathbf{k}}\mathcal{E}(\mathbf{k}) f^{(\ell)}(\mathbf{k})\, d\mathbf{k} \\ &= \sum_{\ell=0}^\infty \epsilon^{2\ell} \mathscr{R}^{(2\ell)}(\mathbf{k}). \end{aligned}$$

Similarly for the energy electron density, we have

$$
\begin{aligned}
W = W(f^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k}) f^{(\ell)}(\mathbf{k}) \, \mathrm{d}\mathbf{k} = \sum_{\ell=0}^{\infty} \epsilon^{2\ell} y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k}) f^{(2\ell)}(\mathbf{k}) \, \mathrm{d}\mathbf{k} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell} W^{(2\ell)}(\mathbf{k}).
\end{aligned}
$$

and

$$
\begin{aligned}
\mathscr{J}^{W} = \mathscr{J}^{W}(f^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k}) \boldsymbol{v}(\mathbf{k}) \otimes \boldsymbol{v}(\mathbf{k}) f^{(\ell)}(\mathbf{k}) \, \mathrm{d}\mathbf{k} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell} \mathscr{J}^{W,(2\ell)}(\mathbf{k}),
\end{aligned}
$$

$$
\begin{aligned}
\mathscr{R}^{W} = \mathscr{R}^{W}(f^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} y \int_{\mathscr{B}} \left[\boldsymbol{v}(\mathbf{k}) \otimes \boldsymbol{v}(\mathbf{k}) + \mathcal{E}(\mathbf{k}) \frac{1}{\hbar^2} \nabla_{\mathbf{k}} \otimes \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k}) \right] f^{(\ell)}(\mathbf{k}) \, \mathrm{d}\mathbf{k} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell} \mathscr{R}^{W,(2\ell)}(\mathbf{k}).
\end{aligned}
$$

Taking into account that $\omega_i(\mathbf{q})$ is an even function, for the energy phonon density, we have

$$
\begin{aligned}
W_i = W_i(g_{i,\sigma}^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} z \int_{\mathscr{B}} \hbar\omega_i(\mathbf{q}) g_{i,\sigma}^{(\ell)}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell} W_i^{(2\ell)}(\mathbf{q}),
\end{aligned}
$$

and

$$
\begin{aligned}
\mathscr{J}_i^{W} = \mathscr{J}_i^{W}(g_{i,\sigma}^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} z \int_{\mathscr{B}} \hbar\omega_i(\mathbf{q}) \boldsymbol{c}_i(\mathbf{q}) \otimes \boldsymbol{c}_i(\mathbf{q}) g_{i,\sigma}^{(\ell)}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell} \mathscr{J}_i^{W,(2\ell)}(\mathbf{q}),
\end{aligned}
$$

Instead for the electron current density $\boldsymbol{j}$ and for the energy fluxes for electron

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and phonon $\boldsymbol{j}^W$ and $\boldsymbol{j}_i^W$ respectively, we have

$$
\begin{aligned}
\boldsymbol{j} = \boldsymbol{j}(f^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} y \int_{\mathscr{B}} \boldsymbol{v}(\mathbf{k}) f^{(\ell)}(\mathbf{k}) \, \mathrm{d}\mathbf{k} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell+1} \boldsymbol{j}^{(2\ell+1)}(\mathbf{k}). \quad (6.55)
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{j}^W = \boldsymbol{j}^W(f^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} y \int_{\mathscr{B}} \mathcal{E}(\mathbf{k}) \boldsymbol{v}(\mathbf{k}) f^{(\ell)}(\mathbf{k}) \, \mathrm{d}\mathbf{k} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell+1} \boldsymbol{j}^{W,(2\ell+1)}(\mathbf{k}). \quad (6.56)
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{j}_i^W = \boldsymbol{j}_i^W(g_{i,\sigma}^{\mathrm{ME}}) &= \sum_{\ell=0}^{\infty} \epsilon^{\ell} z \int_{\mathscr{B}} \hbar \omega_i(\mathbf{q}) \boldsymbol{c}_i(\mathbf{q}) g_{i,\sigma}^{(\ell)}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \\
&= \sum_{\ell=0}^{\infty} \epsilon^{2\ell+1} \boldsymbol{j}_i^{W,(2\ell+1)}(\mathbf{q}). \quad (6.57)
\end{aligned}
$$

Third scaling. These expressions lead to the third and last following scaling

$$
t = \frac{\hat{t}}{\epsilon}, \quad \boldsymbol{j} = \epsilon \hat{\boldsymbol{j}}, \quad \boldsymbol{j}^W = \epsilon \hat{\boldsymbol{j}}^W, \quad \boldsymbol{j}_i^W = \epsilon \hat{\boldsymbol{j}}_i^W. \quad (6.58)
$$

Applying the three scalings introduced in (6.42), (6.43), (6.44) and (6.58) to system (6.37), the system of the moment equations becomes

$$
\begin{cases}
\dfrac{\partial n}{\partial \hat{t}} + \nabla \cdot \hat{\boldsymbol{j}} = 0, \\[2mm]
\epsilon^2 \dfrac{\partial \hat{\boldsymbol{j}}}{\partial \hat{t}} + \nabla \cdot \mathscr{J} + q_e \mathbf{E} \cdot \mathscr{R} = \frac{1}{\epsilon} \hat{\mathcal{C}}_0 + \frac{\sigma}{\epsilon} \hat{\mathcal{C}}, \\[2mm]
\dfrac{\partial W}{\partial \hat{t}} + \nabla \cdot \hat{\boldsymbol{j}}^W + q_e \mathbf{E} \cdot \hat{\boldsymbol{j}} = \frac{1}{\epsilon^2} \hat{\mathcal{C}}_0^W + \frac{\sigma}{\epsilon^2} \hat{\mathcal{C}}^W, \\[2mm]
\epsilon^2 \dfrac{\partial \hat{\boldsymbol{j}}^W}{\partial \hat{t}} + \nabla \cdot \mathscr{J}^W + q_e \mathbf{E} \cdot \mathscr{R}^W = \frac{1}{\epsilon} \hat{\mathcal{C}}_0^W + \frac{\sigma}{\epsilon} \hat{\mathcal{C}}^W, \\[2mm]
\dfrac{\partial W_i}{\partial \hat{t}} + \nabla \cdot \hat{\boldsymbol{j}}_i^W = \frac{\sigma}{\epsilon^2} \hat{\mathcal{C}}_i^W, \\[2mm]
\epsilon^2 \dfrac{\partial \hat{\boldsymbol{j}}_i^W}{\partial \hat{t}} + \nabla \cdot \mathscr{J}_i^W = \frac{\sigma}{\epsilon} \hat{\mathcal{C}}_i^W, \quad i = 1, \dots, n_{\mathrm{ph}}.
\end{cases} \quad (6.59)
$$

The $\hat{}$ on the collision terms, in the system (6.59), refers to the use of the scaled quantities introduced in (6.42), (6.43).

Next, we need to see the consequences on the collision terms of the three scalings that we have introduced. This is done in the following proposition.

Proposition 6.4.1 *Using the scalings (6.42), (6.43), (6.44) and (6.58) in the collision terms, definited in (6.38), we obtain that*

1. *The terms $\frac{1}{\epsilon}\hat{\mathcal{C}}_0$ and $\frac{1}{\epsilon}\hat{\mathcal{C}}_0^W$ are $\mathcal{O}(1)$ around $\epsilon = 0$.*

2. *The terms $\frac{\sigma}{\epsilon}\hat{\mathcal{C}}$, $\frac{\sigma}{\epsilon}\hat{\mathcal{C}}^W$, $\frac{\sigma}{\epsilon}\hat{\mathcal{C}}_i^W$ are $\mathcal{O}(1)$ around $\epsilon = 0$ and $\sigma = 0$.*

3. *The terms $\frac{1}{\epsilon^2}\hat{\mathcal{C}}_0^W$, $\frac{\sigma}{\epsilon^2}\hat{\mathcal{C}}^W$, $\frac{\sigma}{\epsilon^2}\hat{\mathcal{C}}_i^W$ are of order $\mathcal{O}(1)$ around $\epsilon = 0$, assuming*

$$\sigma = \mathcal{O}(\epsilon^2).$$

Proof. We define

$$\mathscr{F}(\mathbf{k}', \mathbf{k}) = f(\mathbf{k}')(1 - f(\mathbf{k})), \tag{6.60}$$

then, the collision term, describing the scattering electron-impurities, has the form

$$\mathcal{C}_0^{\text{el}} = \int_{\mathscr{B}} [P_0(\mathbf{k}', \mathbf{k})\mathscr{F}(\mathbf{k}', \mathbf{k}) - P_0(\mathbf{k}, \mathbf{k}')\mathscr{F}(\mathbf{k}, \mathbf{k}')] \, \mathrm{d}\mathbf{k}. \tag{6.61}$$

If we introduce the expansion for the distribution function f, given in (6.53), we can write

$$\mathscr{F}(\mathbf{k}', \mathbf{k}) = \sum_{\ell=0}^{\infty} \mathscr{F}^{(\ell)}(\mathbf{k}', \mathbf{k}) \tag{6.62}$$

with $\mathscr{F}^{(0)}(\mathbf{k}', \mathbf{k}) = f^{(0)}(\mathbf{k}')(1 - f^{(0)}(\mathbf{k}))$ and

$$\mathscr{F}^{(\ell)}(\mathbf{k}', \mathbf{k}) = \sum_{m=0}^{\ell} (-1)^\ell \epsilon^\ell p_{\ell-m}^+(f^{(0)'}) \left(\chi^{(1)'}\right)^{\ell-m} p_m^+(f^{(0)}) \left(\chi^{(1)}\right)^m$$

in which

$$f^{(0)} = f^{(0)}(\mathbf{k}), \quad f^{(0)'} = f^{(0)}(\mathbf{k}'),$$

and

$$\chi^{(1)} = \chi^{(1)}(\mathbf{k}), \quad \chi^{(1)'} = \chi^{(1)}(\mathbf{k}').$$

Then we can write

$$\begin{aligned}
\frac{1}{\epsilon}\hat{\mathcal{C}}_0 &= \frac{1}{\epsilon}\int_{\mathscr{B}}\int_{\mathscr{B}} \boldsymbol{v}(\mathbf{k})[\hat{P}_0(\mathbf{k}', \mathbf{k})\mathscr{F}(\mathbf{k}', \mathbf{k}) - \hat{P}_0(\mathbf{k}, \mathbf{k}')\mathscr{F}(\mathbf{k}, \mathbf{k}')] \, \mathrm{d}\mathbf{k}' \, \mathrm{d}\mathbf{k} \\
&= \frac{1}{\epsilon}\sum_{\ell=0}^{\infty}\int_{\mathscr{B}}\int_{\mathscr{B}} \boldsymbol{v}(\mathbf{k}) \left[\hat{P}_0(\mathbf{k}', \mathbf{k})\mathscr{F}^{(\ell)}(\mathbf{k}', \mathbf{k}) - \hat{P}_0(\mathbf{k}, \mathbf{k}')\mathscr{F}^{(\ell)}(\mathbf{k}, \mathbf{k}')\right] \, \mathrm{d}\mathbf{k}' \, \mathrm{d}\mathbf{k} \\
&=: \frac{1}{\epsilon}\sum_{\ell=0}^{\infty} \epsilon^\ell \hat{\mathcal{C}}_0^{(\ell)}.
\end{aligned}$$

Recalling the expressions in (6.47) for $\chi^{(0)}$ and $\chi^{(1)}$, we notice that

$$\chi^{(0)}(-\mathbf{k}) = \chi^{(0)}(\mathbf{k}), \quad \chi^{(1)}(-\mathbf{k}) = -\chi^{(1)}(\mathbf{k}),$$

thus we find $\mathscr{F}^{(0)}(-\mathbf{k}', -\mathbf{k}) = \mathscr{F}^{(0)}(\mathbf{k}', \mathbf{k})$ and

$$
\mathscr{F}^{(\ell)}(-\mathbf{k}', -\mathbf{k}) = \begin{cases} \mathscr{F}^{(\ell)}(\mathbf{k}', \mathbf{k}), & \text{if } \ell \text{ is even,} \\ -\mathscr{F}^{(\ell)}(\mathbf{k}', \mathbf{k}), & \text{if } \ell \text{ is odd.} \end{cases} \tag{6.63}
$$

Moreover, we have $P_0(-\mathbf{k}', -\mathbf{k}) = P_0(\mathbf{k}', \mathbf{k})$. Then, since $\boldsymbol{v}(-\mathbf{k}) = -\boldsymbol{v}(\mathbf{k})$, the previous expansion reduces to

$$
\frac{1}{\epsilon} \hat{\boldsymbol{\mathcal{C}}}_0 = \sum_{\ell=0}^{\infty} \epsilon^{2\ell} \hat{\boldsymbol{\mathcal{C}}}_0^{(2\ell+1)}.
$$

In the same way, since $\mathcal{E}(-\mathbf{k})\boldsymbol{v}(-\mathbf{k}) = -\mathcal{E}(\mathbf{k})\boldsymbol{v}(\mathbf{k})$, we find

$$
\frac{1}{\epsilon} \hat{\boldsymbol{\mathcal{C}}}_0^W = \sum_{\ell=0}^{\infty} \epsilon^{2\ell} \hat{\boldsymbol{\mathcal{C}}}_0^{W,(2\ell+1)}.
$$

In particular we have:

$$
\frac{1}{\epsilon} \hat{\boldsymbol{\mathcal{C}}}_0 = \hat{\boldsymbol{\mathcal{C}}}_0^{(1)} + \mathcal{O}(\epsilon),
$$

$$
\frac{1}{\epsilon} \hat{\boldsymbol{\mathcal{C}}}_0^W = \hat{\boldsymbol{\mathcal{C}}}_0^{W,(1)} + \mathcal{O}(\epsilon),
$$

which proves the first statement.

Recalling the form of the electron-phonon collision term, given in the previous section, and the definition of the function $\mathscr{F}$, we have

$$
\mathcal{C}_i^{\text{el}}(f, g_i) = \int_{\mathscr{B}} [P_i(\mathbf{k}', \mathbf{k}; g_i)\mathscr{F}(\mathbf{k}', \mathbf{k}) - P_i(\mathbf{k}, \mathbf{k}'; g_i)\mathscr{F}(\mathbf{k}, \mathbf{k}')] \, d\mathbf{k}'.
$$

in which the transition rates is given by

$$
P_i(\mathbf{k}, \mathbf{k}'; g_i) = w_i^+(\mathbf{k}, \mathbf{k}', \mathbf{q}^+)g_i^+ + w_i^-(\mathbf{k}, \mathbf{k}', \mathbf{q}^-)g_i^- + w_i^-(\mathbf{k}, \mathbf{k}', \mathbf{q}^-)
$$

where
$$
w_i^{\pm}(\mathbf{k}, \mathbf{k}', \mathbf{q}) = s_i(\mathbf{q})\delta[\mathcal{E}(\mathbf{k}) - \mathcal{E}(\mathbf{k}') \pm \hbar\omega_i(\mathbf{q})].
$$
and $g_i^{\pm} = g_i(\mathbf{q}^{\pm})$, with $\mathbf{q}^{\pm} = \pm(\mathbf{k}' - \mathbf{k}))$.
We notice that $w_i^{\pm}(-\mathbf{k}, -\mathbf{k}', -\mathbf{q}) = w_i^{\pm}(\mathbf{k}, \mathbf{k}', \mathbf{q})$.

We define the function

$$
\mathscr{G}_i(\mathbf{k}', \mathbf{k}, \mathbf{q}) = g_i(\mathbf{q})\mathscr{F}(\mathbf{k}', \mathbf{k}).
$$

Using the scaling (6.43) and the expansion given in (6.53) for the distibution function g_i we can write

$$
\mathscr{G}_i(\mathbf{k}', \mathbf{k}, \mathbf{q}) = \sum_{\ell=0}^{\infty} \mathscr{G}_{i,\sigma}^{(\ell)}(\mathbf{k}', \mathbf{k}, \mathbf{q}),
$$

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with

$$\mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k}',\mathbf{k},\mathbf{q}) = \sum_{m=0}^{\ell} g_{\sigma}^{(0)}(\mathbf{q})(-1)^{m}\sigma^{m}p_{m}^{-}(g_{\sigma}^{(0)}(\mathbf{q}))(\chi^{(1)}(\mathbf{q}))^{m}\mathscr{F}^{(\ell-m)}(\mathbf{k}',\mathbf{k}).$$

Thus we have that

$$
\begin{aligned}
\frac{\sigma}{\epsilon}\hat{\mathcal{C}} &= \frac{\sigma}{\epsilon}\sum_{i=1}^{n_{\mathrm{ph}}}\int_{\mathscr{B}}\int_{\mathscr{B}}\boldsymbol{v}(\mathbf{k})[\hat{s}_{i}(\mathbf{q}^{+})\delta(\mathcal{E}(\mathbf{k}')-\mathcal{E}(\mathbf{k})+\hbar\omega_{i}(\mathbf{q}^{+}))\mathcal{G}_{i,\sigma}(\mathbf{k}',\mathbf{k},\mathbf{q}^{+}) \\
&\quad +\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k}')-\mathcal{E}(\mathbf{k})-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathcal{G}_{i,\sigma}(\mathbf{k}',\mathbf{k},\mathbf{q}^{-}) \\
&\quad +\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathscr{F}(\mathbf{k},\mathbf{k}') \\
&\quad -\hat{s}_{i}(\mathbf{q}^{+})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')+\hbar\hat{\omega}_{i}(\mathbf{q}^{+}))\mathcal{G}_{i,\sigma}(\mathbf{k},\mathbf{k}',\mathbf{q}^{+}) \\
&\quad -\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathcal{G}_{i,\sigma}(\mathbf{k},\mathbf{k}',\mathbf{q}^{-}) \\
&\quad -\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathscr{F}(\mathbf{k},\mathbf{k}')]\quad\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}' \\
&= \frac{\sigma}{\epsilon}\sum_{\ell=0}^{\infty}\sum_{i=1}^{n_{\mathrm{ph}}}\int_{\mathscr{B}}\int_{\mathscr{B}}\boldsymbol{v}(\mathbf{k})[\hat{s}_{i}(\mathbf{q}^{+})\delta(\mathcal{E}(\mathbf{k}')-\mathcal{E}(\mathbf{k})+\hbar\hat{\omega}_{i}(\mathbf{q}^{+}))\mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k}',\mathbf{k},\mathbf{q}^{+}) \\
&\quad +\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k}')-\mathcal{E}(\mathbf{k})-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k}',\mathbf{k},\mathbf{q}^{-}) \\
&\quad +\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathscr{F}^{(\ell)}(\mathbf{k},\mathbf{k}') \\
&\quad -\hat{s}_{i}(\mathbf{q}^{+})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')+\hbar\hat{\omega}_{i}(\mathbf{q}^{+}))\mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k},\mathbf{k}',\mathbf{q}^{+}) \\
&\quad -\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k},\mathbf{k}',\mathbf{q}^{-}) \\
&\quad -\hat{s}_{i}(\mathbf{q}^{-})\delta(\mathcal{E}(\mathbf{k})-\mathcal{E}(\mathbf{k}')-\hbar\hat{\omega}_{i}(\mathbf{q}^{-}))\mathscr{F}^{(\ell)}(\mathbf{k},\mathbf{k}')]\quad\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}' \\
&=: \frac{\sigma}{\epsilon}\sum_{\ell=0}^{\infty}\epsilon^{\ell}\hat{\mathcal{C}}_{\sigma}^{(\ell)}.
\end{aligned}
$$

Using (6.63) and since $g_{i,\sigma}^{(0)}(-\mathbf{q}) = g_{i,\sigma}^{(0)}(\mathbf{q})$, $\chi^{(1)}(-\mathbf{q}) = -\chi^{(1)}(\mathbf{q})$, we have that

$$
\begin{aligned}
&\mathcal{G}_{i,\sigma}^{(\ell)}(-\mathbf{k}',-\mathbf{k},-\mathbf{q}) \\
&= \sum_{m=0}^{\ell} g_{i,\sigma}^{(0)}(\mathbf{q})(-1)^{m}\sigma^{m}p_{m}^{-}(g_{i,\sigma}^{(0)}(\mathbf{q}))(-1)^{m}(\chi^{(1)}(\mathbf{q}))^{m}(-1)^{\ell-m}\mathscr{F}^{(\ell-m)}(\mathbf{k}',\mathbf{k}) \\
&= (-1)^{(\ell)}\mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k}',\mathbf{k},\mathbf{q}),
\end{aligned}
$$

then

$$\mathcal{G}_{i,\sigma}^{(\ell)}(-\mathbf{k}',-\mathbf{k},-\mathbf{q}) = \begin{cases} \mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k}',\mathbf{k},\mathbf{q}), & \text{if } \ell \text{ is even,} \\ -\mathcal{G}_{i,\sigma}^{(\ell)}(\mathbf{k}',\mathbf{k},\mathbf{q}), & \text{if } \ell \text{ is odd.} \end{cases} \tag{6.64}$$

Then, since $\omega_{i}(-\mathbf{q}) = \omega_{i}(\mathbf{q})$, we have

$$\frac{\sigma}{\epsilon}\hat{\mathcal{C}} = \sigma\sum_{\ell=0}^{\infty}\epsilon^{2\ell}\hat{\mathcal{C}}_{\sigma}^{(2\ell+1)}, \tag{6.65}$$

$$\frac{\sigma}{\epsilon}\hat{\mathcal{C}}^{W} = \sigma\sum_{\ell=0}^{\infty}\epsilon^{2\ell}\hat{\mathcal{C}}_{\sigma}^{W,(2\ell+1)}. \tag{6.66}$$

Recalling the expression for the phonon-electron scattering, using the definition of the functions $\mathscr{F}, \mathscr{G}$, we have

$$\mathcal{C}_i^{\mathrm{ph}}(f, g_i) = 2 \int_{\mathcal{B}} \{s_i(\mathbf{q})\delta(\mathcal{E}^* - \mathcal{E}' + \hbar\omega_i)[\mathscr{G}(\mathbf{k}', \mathbf{k}^*\mathbf{q}) - \mathscr{F}(\mathbf{k}', \mathbf{k}^*) - \mathscr{G}(\mathbf{k}^*, \mathbf{k}', \mathbf{q})]\} \, \mathrm{d}\mathbf{k}',$$

with $\mathbf{k}^* = \mathbf{k}' - \mathbf{q}$. Then, doing the same consideration made above, considering that $\boldsymbol{c}_i(-\mathbf{q}) = -\boldsymbol{c}_i(\mathbf{q})$ we can find

$$\frac{\sigma}{\epsilon}\hat{\mathcal{C}}_i^W = \sigma \sum_{\ell=0}^{\infty} \epsilon^{2\ell} \hat{\mathcal{C}}_i^{W,(2\ell+1)}. \tag{6.67}$$

The relations (6.65), (6.66), (6.67), in particular imply

$$\frac{\sigma}{\epsilon}\hat{\mathcal{C}} = \sigma\hat{\mathcal{C}}^{(1)} + \mathcal{O}(\epsilon),$$
$$\frac{\sigma}{\epsilon}\hat{\mathcal{C}}^W = \sigma\hat{\mathcal{C}}^{W,(1)} + \mathcal{O}(\epsilon).$$
$$\frac{\sigma}{\epsilon}\hat{\mathcal{C}}_i^W = \sigma\hat{\mathcal{C}}_i^{W,(1)} + \mathcal{O}(\epsilon).$$

Using (6.54) we can prove the second statement of the proposition.

To prove the third statement, we consider the following expansion for $\mathcal{C}_0^W$:

$$\frac{1}{\epsilon^2}\hat{\mathcal{C}}_0^W = \frac{1}{\epsilon^2} \sum_{\ell=0}^{\infty} \epsilon^{2\ell} \hat{\mathcal{C}}_0^{W,(2\ell)}. \tag{6.68}$$

with

$$\hat{\mathcal{C}}_0^{W,(\ell)} = \int_{\mathcal{B}} \int_{\mathcal{B}} \mathcal{E}(\mathbf{k}) \left[\hat{P}_0(\mathbf{k}', \mathbf{k})\mathscr{F}^{(\ell)}(\mathbf{k}', \mathbf{k}) - \hat{P}_0(\mathbf{k}, \mathbf{k}')\mathscr{F}^{(\ell)}(\mathbf{k}, \mathbf{k}') \right] \, \mathrm{d}\mathbf{k}' \, \mathrm{d}\mathbf{k}.$$

The expansion does not contain the odd terms in ϵ since $\mathcal{E}(\mathbf{k})$ is an even function. From (6.68) we find

$$\frac{1}{\epsilon^2}\hat{\mathcal{C}}_0^W = \frac{1}{\epsilon^2}\hat{\mathcal{C}}_0^{W,(0)} + \hat{\mathcal{C}}_0^{W,(2)} + \mathcal{O}(\epsilon^2).$$

We have

$$\begin{aligned}
\hat{\mathcal{C}}_0^{W,(0)} &= \int_{\mathcal{B}} \int_{\mathcal{B}} \mathcal{E}(\mathbf{k}) \left[\hat{P}_0(\mathbf{k}', \mathbf{k})\mathscr{F}^{(0)}(\mathbf{k}', \mathbf{k}) - \hat{P}_0(\mathbf{k}, \mathbf{k}')\mathscr{F}^{(0)}(\mathbf{k}, \mathbf{k}') \right] \, \mathrm{d}\mathbf{k}' \, \mathrm{d}\mathbf{k} \\
&= \int_{\mathcal{B}} \int_{\mathcal{B}} (\mathcal{E}(\mathbf{k}) - \mathcal{E}(\mathbf{k}'))\hat{P}_0(\mathbf{k}', \mathbf{k})\mathscr{F}^{(0)}(\mathbf{k}', \mathbf{k}) \, \mathrm{d}\mathbf{k}' \, \mathrm{d}\mathbf{k} \\
&= 0
\end{aligned}$$

The remaning terms $\frac{\sigma}{\epsilon^2}\hat{\mathcal{C}}^W$, $\frac{\sigma}{\epsilon^2}\hat{\mathcal{C}}_i^W$ can be treated in a similar way. Thus we obtain

■

Denoting by (0) the leading order terms of the right-hand side of the previous scaled equations, using (6.49), we find

$$\begin{pmatrix} \hat{\mathcal{C}}^{(0)} \\ \hat{\mathcal{C}}^{W(0)} \end{pmatrix} = \mathcal{B} \begin{pmatrix} \hat{\boldsymbol{\lambda}} \\ \hat{\boldsymbol{\lambda}}^W \end{pmatrix} = -\mathcal{B}\mathcal{A}^{-1} \begin{pmatrix} \hat{\boldsymbol{j}} \\ \hat{\boldsymbol{j}}^W \end{pmatrix}, \quad \hat{\mathcal{C}}_i^{W(0)} = b_i \hat{\boldsymbol{\lambda}}_i^W = -b_i a_i^{-1} \hat{\boldsymbol{j}}_i^W.$$

In conclusion, taking the formal limit of (6.37), after the three scaling we obtain the following limit system:

$$\begin{cases} \dfrac{\partial n}{\partial \hat{t}} + \nabla \cdot \hat{\boldsymbol{j}} & = 0, \\[2mm] \nabla \cdot \mathscr{J} + q_e \mathbf{E} \cdot \mathscr{R} & = \hat{\boldsymbol{c}}^{(0)}, \\[2mm] \dfrac{\partial W}{\partial \hat{t}} + \nabla \cdot \hat{\boldsymbol{j}}^W + q_e \mathbf{E} \cdot \hat{\boldsymbol{j}} & = \hat{\mathcal{C}}^{W(0)}, \\[2mm] \nabla \cdot \mathscr{J}^W + q_e \mathbf{E} \cdot \mathscr{R}^W & = \hat{\boldsymbol{c}}^{W(0)}, \\[2mm] \dfrac{\partial W_i}{\partial \hat{t}} + \nabla \cdot \hat{\boldsymbol{j}}_i^W & = \hat{\mathcal{C}}_i^{W(0)}, \\[2mm] \nabla \cdot \mathscr{J}_i^W & = \hat{\boldsymbol{c}}_i^{W,(0)}, \quad i = 1, \ldots, n_{\mathrm{ph}}. \end{cases} \tag{6.69}$$

The equations on the left column constitute the energy transport system, while the equations on the right column are the constitutive relations for the flux, which can be written in the compact form

$$\begin{pmatrix} \hat{\boldsymbol{j}} \\ \hat{\boldsymbol{j}}^W \end{pmatrix} = -\mathcal{A}\mathcal{B}^{-1} \begin{pmatrix} \nabla \cdot \mathscr{J}^{(0)} + q_e \mathbf{E} \cdot \mathscr{R}^{(0)} \\ \nabla \cdot \mathscr{J}^{W(0)} + e\mathbf{E} \cdot (\mathscr{J}^{(0)} + \mathscr{R}^{W(0)}) \end{pmatrix} \tag{6.70}$$
$$\hat{\boldsymbol{j}}_i^W = -a_i b_i^{-1} \nabla \cdot \mathscr{J}_i^{W(0)}, \quad i = 1, \ldots, n_{\mathrm{ph}}.$$

All the coefficients in the above expressions are given in closed form. The limit model (6.69), (6.70) is consistent with linear irreversible thermodynamics.

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