HYDRODYNAMICAL MODELING OF CHARGE CARRIER TRANSPORT IN SEMICONDUCTORS

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Preface

Enhanced functional integration in modern electron devices requires an accurate modeling of energy transport in semiconductors in order to describe high-field phenomena such as hot electron propagation, impact ionization and heat generation in the bulk material. The standard drift-diffusion models cannot cope with high-field phenomena because they do not comprise energy as a dynamical variable.

Furthermore for many applications in optoelectronics one needs to describe the transient interaction of electromagnetic radiation with carriers in complex semiconductor materials and since the characteristic times are of order of the electron momentum or energy flux relaxation times, some higher moments of the distribution function are necessarily involved. Therefore these phenomena cannot be described within the framework of the drift-diffusion equations (which are valid only in the quasi-stationary limit) Therefore generalizations of the drift-diffusion equations have been sought which would incorporate energy as a dynamical variable and also would not be restricted to quasi-stationary situations. These models are loosely speaking called hydrodynamical models. Hydrodynamical models are obtained from the infinite hierarchy of the moment equations of the Boltzmann transport equation by a suitable truncation procedure. This requires making suitable assumptions on: i) closing the hierarchy by finding appropriate expressions for the $N + 1$ order moment in terms of the previous ones; ii)modeling the production terms on the right hand side of the moment equations which arise from the moments of the collision terms in the Boltzmann transport equation.

One of the earliest hydrodynamical models currently used in applications was originally put forward by Blotekjaer [23] and subsequently investigated by Baccarani and Wordeman [19] and by other authors (see references in [73]). This model is implemented in simulation codes currently used in the microelectronics industry. It consists of a set of balance equations for carrier density, momentum and energy obtained from the Boltzmann transport equation in the parabolic band approximation, closed by a postulated Fourier law as constitutive equation for the heat flux. The production terms for momentum and energy are assumed to be of the relaxation type and the relaxation times are obtained by phenomenological arguments. Other models have also been investigated, some including also non parabolic effects [43, 79, 75, 25, 50, 78, 84, 11, 8, 3, 14, 15, 12, 13].

Most implemented hydrodynamical models suffer from serious theoretical drawbacks due to the ad hoc treatment of the closure problem (lacking a physically convincing motivation) and the modeling of the production terms (usually assumed to be of the relaxation type and this, as we shall see, leads to serious inconsistencies with the Onsager reciprocity relations). Also most numerical methods which have been used to solve the equations are simply an adaptation of methods used for the drift-diffusion equations, e.g. methods appropriate for parabolic systems. However, unless some special (and usually unwarranted) approximations are made, the evolution equations of hydrodynamical models form a hyperbolic system. Therefore their numerical solution requires using schemes which can cope well with the special features of hyperbolic systems. In these lectures we present a general overview of the theory underlying hydrodynamical models. In particular we investigate in depth both the closure problem and the modeling of the production terms and present a recently introduced approach based on the maximum entropy principle (physically set in the framework of extended thermodynamics [63, 49]).

The plan of these lecture notes is the following. In chapter 2 we briefly recall the main concepts of semiconductor physics (energy band structure in semiconductors and Bloch's theorem), introduce the semiclassical Liouville equation, discuss the most relevant scattering processes and introduce phenomenologically the semiclassical Boltzmann equation. Moreover we present some important mathematical questions related to the semiclassical Boltzmann equation, in particular the H theorem, the null space of the collision operator and the existence and uniqueness for the initial value problem.

In chapter 3 we review the general framework in which the macroscopical models of charge transport in semiconductors are set. The diffusion limit and the hydrodynamical limit of the Boltzmann transport equation will be investigated, recovering the celebrated drift-diffusion model and the Blotekjaer-Baccarani-Wordeman model. Some important properties of these models are highlighted and their deficiencies are discussed.

In chapter 4 the extended hydrodynamical models based on moment equations closed with the maximum entropy principle of extended thermodynamics are treated. First the general theory (without restriction on the form of the energy band) will be discussed, then some recent results in the case of parabolic band and in the case of the Kane dispersion relation will be considered.

In chapter 5 some recently introduced numerical methods for solving hyperbolic systems of conservation laws are discussed. These methods are then employed for solving numerically the extended hydrodynamical models previously introduced in the 1D case, for simple benchmark problems. The results are then compared with those obtained by a direct numerical solution of the Boltzmann transport equation via Monte Carlo methods.

Chapter 1

Carriers transport in semiconductors

In this chapter a general review of fundamental features of semiconductor physics which are essential for describing carrier transport is presented. Charge carriers in semiconductors move under the effect of a periodic crystal potential, due to the periodically spaced atomic nuclei, and to the self-consistent potential due to the charged carriers themselves. First we introduce briefly the concept of Bravais lattices and of the Brillouin zone. Then we recall the Bloch theorem for the dynamics of an electron inside a perfect crystal lattice, the band structure, and a heuristic derivation of the Boltzmann-Poisson system for the one-electron distribution function. Finally some important results concerning the H-theorem and null space problem of the collision operator are critically reviewed.

1.1 Energy Band structure in semiconductors

Crystals can be described in terms of Bravais lattices [17], which are the set of vectors of the form

$$L = \{ia_1 + ja_2 + la_3, i, j, l \in \mathcal{Z}\}$$

where a_1, a_2, a_3 are primitive lattice vectors, $\mathcal{Z}$ being the set of relative integers. The reciprocal lattice $\hat{L}$ of the Bravais lattice L is defined by

$$\hat{L} = \{ia^1 + ja^2 + la^3, i, j, l \in \mathcal{Z}\}$$

with the reciprocal lattice vectors a^1, a^2, a^3 defined by

$$a_i \cdot a^j = 2\pi\delta_i^j$$

A connected subset $\mathcal{B} \subseteq \mathcal{R}^3$ is called a *primitive cell* of the lattice if:

1. The volume of $\mathcal{B}$ equals $|a_1 \cdot (a_2 \times a_3)|$

2. The whole space $\mathcal{R}^3$ is covered by the union of translates of $\mathcal{B}$ by the lattice vectors.

The first Brillouin zone $\mathcal{B}$ is the primitive cell of the reciprocal lattice $\hat{L}$ consisting of those points which are closer to the origin than to any other point of $\hat{L}$.

The quantum mechanical dynamics of an electron in the periodic potential of the crystal lattice is governed by *Bloch's Theorem.*

Theorem. *Consider an electron whose motion is governed by the potential V_L generated by the ions located at the points of the crystal lattice L. The Schrödinger equation is*

$$H\psi = \mathcal{E}\psi$$

with the Hamiltonian H given by

$$H = -\frac{\hbar^2}{2m} \triangle - qV_L$$

The bounded eigenstates have the form:

$$\psi(\mathbf{x}) = \exp{(i\mathbf{k}\cdot\mathbf{x})}u_k(x) \quad \text{with } \mathbf{x} \in \mathcal{R}^3$$

and

$$u_{\mathbf{k}}(\mathbf{x}+\mathbf{X}) = u_{\mathbf{k}}(\mathbf{x}) \quad \text{with } \mathbf{x} \in L.$$

Therefore one obtains a second order self-adjoint elliptic problem posed on a primitive cell of the crystal lattice L. It is possible to prove [17] the existence of an infinite sequence of eigenpairs of solutions

$$\mathcal{E}_l(\mathbf{k}),\ u_{k,l}(\mathbf{x}),\ l \in \mathcal{N},$$

$\mathcal{N}$ being the set of non negative integers. From the periodicity condition

$$\psi(\mathbf{x}+\mathbf{X}) = \exp{(i\mathbf{k}\cdot\mathbf{X})}\psi(\mathbf{x})$$

with $\mathbf{x} \in \mathcal{R}^3, \mathbf{X} \in L$, it follows that the set of eigenfunctions ψ and the energies $\mathcal{E}(\mathbf{k})$ are identical for any two wavevectors which differ by a reciprocal lattice vector. Therefore one can constrain the wavevector $\mathbf{k}$ to the Brillouin zone $\mathcal{B}$.

The function $\mathcal{E}_l = \mathcal{E}_l(\mathbf{k})$ on the Brillouin zone describes the l-th energy band of the crystal.

Semiconductors are characterized by a sizable energy gap between the valence and the conduction bands, which are almost fully filled at thermal equilibrium. Upon thermal excitation electrons from the valence band can jump to the conduction band leaving behind holes (in the language of quasi-particles). Therefore the transport of charge is achieved through both negatively charged (electrons) and positively charged (holes) carriers.

The energy band structure of crystals can be obtained at the cost of intensive numerical calculations (and also semiphenomenologically) by the quantum theory of solids [17]. However, in order to describe electron transport, for most applications, a simplified description is adopted which is based on a simple analytical model. This is the so called parabolic band and effective mass approximation, where the energy curve corresponding to a given energy band is approximated by a parabola near its minimum. In the sequel for the sake of simplicity only one conduction band will be considered.

In the parabolic approximation, if we denote by $\mathcal{E}$ the energy of the considered conduction band measured from the band minimum, we have that the first Brillouin zone, $\mathcal{B}$, coincides with $\mathcal{R}^3$ and

$$\mathcal{E} = \frac{\hbar^2 |\mathbf{k}|^2}{2m^*}, \tag{1.1}$$

with m^* the effective electron mass (for silicon m^*=0.32 m_e, with m_e the electron mass in vacuum), $\hbar\mathbf{k}$ the *crystal momentum* and $\hbar$ the Planck constant h divided by 2π.

In the approximation of the Kane dispersion relation, which takes into account the non-parabolicity at high energy, $\mathcal{E}$ still depends only on k, the modulus of $\mathbf{k}$, $\mathcal{B} = \mathcal{R}^3$, but

$$\mathcal{E}(k)\,[1 + \alpha\mathcal{E}(k)] = \frac{\hbar^2 k^2}{2m^*}, \quad \mathbf{k} \in \mathcal{B}, \tag{1.2}$$

where α is the non parabolicity parameter (for Silicon α=0.5 eV^{-1}).

In the Monte Carlo simulations the anisotropic version of (1.1) and (1.2) are used

$$\mathcal{E} = \frac{\hbar^2}{2}\left[\frac{k_l^2}{m_l^*} + \frac{k_t^2}{m_t^*}\right],$$

$$\mathcal{E}(k)\,[1 + \alpha\mathcal{E}(k)] = \frac{\hbar^2}{2}\left[\frac{k_l^2}{m_l^*} + \frac{k_t^2}{m_t^*}\right],$$

where m_l^* and m_t^* are the longitudinal and the transverse effective electron masses.

However it is always possible to recover the isotropic cases from the anisotropic ones by means of the Herring-Vogt [45] transformation, with $m^* = \left((m_t^*)^2 m_l^*\right)^{1/3}$.

The electron velocity $v(\mathbf{k})$ in a generic band depends on the energy $\mathcal{E}$ measured from the conduction band minimum by the relation

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

Explicitly we get for parabolic band

$$v^i = \frac{\hbar k^i}{m^*}, \tag{1.3}$$

while in the approximation of the Kane dispersion relation

$$v^i = \frac{\hbar k^i}{m^*\,[1 + 2\alpha\mathcal{E}(k)]}. \tag{1.4}$$

1.2 The semiclassical Liouville equation

Under the assumption that external forces (electric field $\mathbf{E}^{ext}$) are almost constant over a length comparable to the physical dimensions of the wave packet describing the motion of an electron for an ensemble of M electrons belonging to the same energy band with wavevectors $\mathbf{k}_i, i = 1, ...M$, one obtains the following equation for the joint probability density $f(\mathbf{x}_i, \mathbf{k}_i, t)$, with e the absolute value of the electron charge,

$$\frac{\partial f}{\partial t} + \sum \mathbf{v}(\mathbf{k}_i) \cdot \nabla_{x_i} f - \frac{1}{\hbar} e\,\mathbf{E}^{ext} \cdot \nabla_{k_i} f = 0.$$

By proceeding as in the classical theory one obtains the *hierarchy BBGKY of equations*. Then under the usual assumptions [62] (low correlations, separation between long range and short range forces, etc.) one obtains formally the *semiclassical Vlasov equation*

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla f - \frac{1}{\hbar} e \, \mathbf{E} \cdot \nabla_k f = 0$$

for the *one particle distribution function* $f(\mathbf{x}, \mathbf{k}, t)$. Here the electric field $\mathbf{E}(x, t)$ is the sum of the external electric field and the self-consistent one due to the long range electrostatic interactions.

1.3 Scattering processes

The above description of electron motion is valid for an ideal perfectly periodic crystal. Real semiconductors cannot be considered as ideal periodic crystals for several reasons. In fact strict periodicity is destroyed by:

- doping with impurities (which is done in order to control the electrical conductivity);
- thermal vibrations of the ions off their equilibrium positions in the lattice.

These effects can be taken into account in a perturbative way, by describing the interaction of the electrons with the lattice of ions as being only approximately periodic. The weak deviations from periodicity are treated as small perturbations of the background periodic ion potential. In particular the effect of the thermal vibrations of the ions on the electron dynamics can be described quantum mechanically as *scattering with quasi-particles (phonons) representing the thermal lattice vibrations.*

The perturbations from the strict periodicity (which can be interpreted as scattering effects) will obviously affect the semiclassical Liouville equation. Formally these effects are taken into account *by introducing a non zero right hand side in the semiclassical Vlasov equation*, i.e. it is assumed that the influence of the scattering can be described by a non vanishing RHS of the transport equation. In this way one obtains the *semiclassical Boltzmann equation for electrons in the conduction band in semiconductors*

$$\frac{\partial f}{\partial t} + v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} - \frac{eE^i}{\hbar} \frac{\partial f}{\partial k^i} = \mathcal{C}[f], \tag{1.5}$$

where $\mathcal{C}[f]$ represents the effects due to scattering with phonons, impurities and with other electrons.

The electric field which is calculated by solving the Poisson equation for the electric potential ϕ

$$E_i = -\frac{\partial \phi}{\partial x_i}, \tag{1.6}$$

$$\epsilon \Delta \phi = -e(N_D - N_A - n), \tag{1.7}$$

N_D and N_A being the donor and acceptor density respectively (which are fixed ions implanted in the semiconductors and depending only on the position) and n the electron number density

$$n = \int_B f d^3\mathbf{k}.$$

The expression of the collision term has been investigated in the quantum theory of scattering.

The main scattering mechanisms in a semiconductor are the electron-phonon interaction, the interaction with impurities, electron-electron scatterings and interaction with stationary imperfections of the crystal as vacancies, external and internal crystal boundaries. In many situations the electron-electron collision term can be neglected since the electron density is not too high. However in the case of high doping electron-electron collisions must be taken into account because they might produce sizable effects. Retaining the electron-electron collision term greatly increases the complexity of the collision operator on the RHS of the semiclassical Boltzmann equation. In fact the collision operator for the electron-electron scattering is a highly nonlinear one, being quartic in the distribution function.

For each type of interaction mechanism, the collision operator can be schematically written as

$$\mathcal{C}[f] = \int_{\mathcal{B}} \left[P(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') - P(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) \right] \, d^3\mathbf{k} \tag{1.8}$$

with $P(\mathbf{k}, \mathbf{k}')$ the scattering probability per unit time from a state $\mathbf{k}$ to a state $\mathbf{k}'$. The first term in (1.8) represents the gain and the second one the loss.

From the principle of detailed balance [62] it follows that

$$P(\mathbf{k}', \mathbf{k}) = P(\mathbf{k}, \mathbf{k}') \exp\left(-\frac{\mathcal{E} - \mathcal{E}'}{k_B T_L} \right), \tag{1.9}$$

where $\mathcal{E} = \mathcal{E}(\mathbf{k})$ and $\mathcal{E}' = \mathcal{E}(\mathbf{k}')$, k_B being the Boltzmannn constant and T_L being the lattice temperature which will be taken as constant.

In the case of acoustic phonon scattering in the elastic approximation we have

$$P(\mathbf{k}, \mathbf{k}') = \frac{k_B T_L \Xi_d^2}{4\pi^2 \hbar \rho v_s^2} \delta(\mathcal{E} - \mathcal{E}') \mathcal{G}(\mathbf{k}, \mathbf{k}') \tag{1.10}$$

where δ is the Dirac delta function, Ξ_d is the deformation potential of acoustic phonons, ρ the mass density of the material and v_s the sound velocity of the longitudinal acoustic mode.

G(**k**, **k**') represents the overlap factor which depends on the band structure. For parabolic bands it is nearly equal to unity. If the Kane dispersion relation is considered one has [32]

$$\mathcal{G}(\mathbf{k}, \mathbf{k}') = (aa' + cc' \, \mathbf{l} \cdot \mathbf{l}')^2 \tag{1.11}$$

where $\mathbf{l}$ and $\mathbf{l}'$ are the unit vectors of direction $\mathbf{k}$ and $\mathbf{k}'$ respectively and

$$a = \sqrt{\frac{1 + \alpha\mathcal{E}}{1 + 2\alpha\mathcal{E}}}, \quad a' = \sqrt{\frac{1 + \alpha\mathcal{E}'}{1 + 2\alpha\mathcal{E}'}}, \quad c = \sqrt{\frac{\alpha\mathcal{E}}{1 + 2\alpha\mathcal{E}}}, \quad c' = \sqrt{\frac{\alpha\mathcal{E}'}{1 + 2\alpha\mathcal{E}'}}.$$

In the case of non-polar optical phonon interaction the scattering rate reads

$$P(\mathbf{k}, \mathbf{k}') = \frac{(D_t K)^2}{8\pi^2 \rho \omega} \left(n_B + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\mathcal{E}' - \mathcal{E} \mp \hbar\omega) \mathcal{G}(\mathbf{k}, \mathbf{k}'), \tag{1.12}$$

where $D_t K$ is the deformation potential for non polar optical phonons, $\hbar\omega$ is the longitudinal optical phonon energy and n_B is the phonon equilibrium distribution according to the Bose-Einstein statistics

$$n_B = \frac{1}{\exp(\hbar\omega/k_B T_L) - 1}.$$

The double choice of sign means that we must consider the sum of the two cases with the upper and lower sign.

At last for the scattering with impurities we shall adopt the Grinberg-Luryi approximation [41], which is well suited for a quasi isotropic distribution function

$$\mathcal{C}_{imp}[f] = -\frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau_{imp}} \tag{1.13}$$

where f_0 is the isotropic part of the distribution function and $1/\tau_{imp}$ is the scattering rate due to the interaction with impurities of charge Ze,

$$\frac{1}{\tau_{imp}} = \frac{\pi\hbar k e^4 Z^2 N_{imp}}{2m^* \mathcal{E}_0^2 \mathcal{E}^2}\left[\ln\left(\frac{1+\gamma}{\gamma}\right) + \frac{1}{1+\gamma}\right],$$

with N_{imp} concentration of impurities and γ screening parameter

$$\gamma = \frac{\hbar^2 b^2}{8m^* \mathcal{E}},$$

b being the inverse screening length. We observe that the nonparabolicity will enter only in the calculation of the moments of the impurity scattering through the elementary volume in the integrals.

1.4 H-Theorem and the null space of the collision operator

H-theorems were obtained in [69, 70] under the same assumption that the transition probability are bounded functions. In [57, 58, 59] an H-theorem has been derived for the physical electron-phonon operator in the homogeneous case without electric field. The same problem has also been discussed in [53] in the parabolic case.

Here we give a new proof in the case of an arbitrary form of the energy band and in the presence of an electric field, neglecting the electron-electron interaction and assuming the electron gas sufficiently dilute to neglect the degeneracy effects.

As showed in the previous section the typical form of the collision operator $\mathcal{C}[f]$ is

$$\mathcal{C}[f] = \int_{\mathcal{B}} \left[P(\mathbf{k}', \mathbf{k}) f(\mathbf{k}')\left(1 - f(\mathbf{k})\right) - P(\mathbf{k}, \mathbf{k}') f(\mathbf{k})\left(1 - f(\mathbf{k}')\right)\right] d^3\mathbf{k}. \tag{1.14}$$

The terms $1 - f(\mathbf{k})$ account for the Pauli exclusion principle. $P(\mathbf{k}, \mathbf{k}')$ is the transition probability from the state $\mathbf{k}$ to the state $\mathbf{k}'$. It can be written as [45]

$$P(\mathbf{k}, \mathbf{k}') = \mathcal{G}(\mathbf{k}, \mathbf{k}')\left[(n_B + 1)\delta(\mathcal{E}' - \mathcal{E} + \hbar\omega_q) + n_B \delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q)\right] \tag{1.15}$$

where $\delta(x)$ is the Dirac distribution and $\mathcal{G}(\mathbf{k},\mathbf{k}')$ is the so-called overlap factor which depends on the band structure and the particular type of interaction [45] and enjoys the properties

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

$\hbar\omega_q$ stands for the phonon energy. In the case of acoustic phonons it can be neglected.

Under the assumption that the electron gas is dilute the collision operator can be linearized with respect to f and becomes

$$\mathcal{C}[f] = \int_{\mathcal{B}} \left[P(\mathbf{k}',\mathbf{k})f(\mathbf{k}') - P(\mathbf{k},\mathbf{k}')f(\mathbf{k})\right] d^3\mathbf{k}. \tag{1.16}$$

For the moments of the collision term with respect to the weight function $\psi(\mathbf{k})$ the following chain of identities can be proved

$$\begin{aligned}
&\int_{\mathcal{B}} \mathcal{C}[f]\psi(\mathbf{k})d^3\mathbf{k} = \int_{\mathcal{B}} \left[P(\mathbf{k}',\mathbf{k})f(\mathbf{k}') - P(\mathbf{k},\mathbf{k}')f(\mathbf{k})\right] \psi(\mathbf{k})d^3\mathbf{k}d^3\mathbf{k}' = \\
&\int_{\mathcal{B}} P(\mathbf{k},\mathbf{k}')f(\mathbf{k}) \left(\psi(\mathbf{k}') - \psi(\mathbf{k})\right) d^3\mathbf{k}d^3\mathbf{k}' = \\
&\int_{\mathcal{B}} \mathcal{G}(\mathbf{k},\mathbf{k}') \left[(n_q+1)\delta(\mathcal{E}' - \mathcal{E} + \hbar\omega_q) + n_q\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q)\right] \times \\
&f(\mathbf{k}) \left(\psi(\mathbf{k}') - \psi(\mathbf{k})\right) d^3\mathbf{k}d^3\mathbf{k}' = \\
&\int_{\mathcal{B}} \mathcal{G}(\mathbf{k},\mathbf{k}')\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q) \left[(n_q+1)f(\mathbf{k}') - n_q f(\mathbf{k})\right] \left(\psi(\mathbf{k}) - \psi(\mathbf{k}')\right) d^3\mathbf{k}d^3\mathbf{k}'.
\end{aligned}$$

If we set without loss of generality

$$f(\mathbf{k}) = h(\mathbf{k}) \exp\left(-\frac{\mathcal{E}}{k_B T_L}\right),$$

and in analogy with the case of a simple gas we take

$$\psi(\mathbf{k}) = k_B \log h(\mathbf{k}),$$

then by using the definition of $\delta(x)$ one has

$$\begin{aligned}
k_B \int_{\mathcal{B}} \mathcal{C}[f] \log h(\mathbf{k}) d^3\mathbf{k} &= k_B \int_{\mathcal{B}\times\mathcal{B}} \mathcal{G}(\mathbf{k},\mathbf{k}')\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q) n_q \exp\left(-\frac{\mathcal{E}}{k_B T_L}\right) \\
&\left(h(\mathbf{k}') - h(\mathbf{k})\right) \left(\log h(\mathbf{k}) - \log h(\mathbf{k}')\right) d^3\mathbf{k}d^3\mathbf{k}' \leq 0.
\end{aligned} \tag{1.17}$$

Therefore along the characteristics of eq. (1.5)

$$-\int_{\mathcal{B}} \log h(\mathbf{k}) \frac{df}{dt} d^3\mathbf{k} = -\int_{\mathcal{B}} \mathcal{C}[f] \log h(\mathbf{k}) d^3\mathbf{k} \geq 0$$

holds. This implies that

$$\Psi = -\int_{\mathcal{B}} \left(\int \log h(\mathbf{k})\, df\right) d^3\mathbf{k} = -k_B \int_{\mathcal{B}} \left(f \log f - f + \frac{\mathcal{E}}{k_B T_L} f\right) d^3\mathbf{k}. \tag{1.18}$$

can be considered as a Liapunov function for the Boltzmann-Poisson system (1.5)-(1.7). The first two terms are equal to the expression of the entropy arising in the classical limit of a Fermi gas, while the last term is due to the presence of the phonons. Indeed Ψ

represent the nonequilibrium counterpart of the equilibrium Helmholtz free energy with reversed sign, divided by the lattice temperature. It is well known in thermostatics that for a body kept at constant temperature and mechanically insulated, the equilibrium states are minima for Ψ and this fact is related to determining the null space of the collision operator as explained below.

The problem of the null space of the collision operator consists of determining the solutions of the equation $\mathcal{C}(f) = 0$. The resulting distribution functions represent the equilibrium solutions. Physically one expects that, asymptotically in time, the solution to a given initial value problem will tend to such a solution.

In [69, 70] it has been proved that the solutions of $\mathcal{C}(f) = 0$ are the Fermi-Dirac distributions under the assumption that the scattering probabilities are bounded functions. However this hypothesis is not satisfied by some scattering mechanism (as with phonons, etc.).

The problem of determining the null space for the physical electron-phonon operator was tackled and solved in [60] where it is proved that the equilibrium solutions form an infinite sequence of functions of the kind

$$f(k) = \frac{1}{1 + h(\mathbf{k}) \exp \mathcal{E}(\mathbf{k})/K_B T_L} \tag{1.19}$$

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

Chapter 2

Macroscopic models

Hydrodynamical models are obtained from the moment equations of the Boltzmann transport equation suitably truncated at a certain order N. The truncation procedure requires solving the following two important problems:

i) the closure for higher order fluxes;

ii) the closure for the production terms.

The closure problem consists in finding an appropriate expression for the (N+1)-th moment which appears under the divergence operator of the N-th moment equation. Likewise, modeling the production terms consists in expressing them as suitable functions of the first N moments.

In this chapter we will present the general form of the balance equations, discuss some simple closure relations for the higher order moments as well as for the production terms and show that as limit one recovers the celebrated *drift-diffusion* model. We also treat the simple hydrodynamical models constructed by analogy with the theory of classical nonviscous heat-conducting monatomic gases, which lately has received a considerable attention by engineers and applied mathematicians. For these models the compatibility with the Onsager reciprocity relations of linear irreversible thermodynamics is investigated.

2.1 Moment equations

The macroscopic balance equations are deduced as moment equations of the Boltzmann transport equation as in gasdynamics [27]. By multiplying eq. (1.5) by a function $\psi(\mathbf{k})$ and integrating over $\mathcal{B}$, one finds the *moment equation*

$$\frac{\partial M_\psi}{\partial t} + \int_{\mathcal{B}} \psi(\mathbf{k}) v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} d^3\mathbf{k} - eE^j \int_{\mathcal{B}} \psi(\mathbf{k}) \frac{\partial}{\partial k_j} f d^3\mathbf{k} = \int_{\mathcal{B}} \psi(\mathbf{k}) \mathcal{C}[f] d^3\mathbf{k}, \tag{2.1}$$

with

$$M_\psi = \int_{\mathcal{B}} \psi(\mathbf{k}) f d^3\mathbf{k},$$

the moment relative to the weight function ψ.

Since

$$\int_{\mathcal{B}} \psi(\mathbf{k}) \frac{\partial f}{\partial k^j} d^3\mathbf{k} = \int_{\partial\mathcal{B}} \psi(\mathbf{k}) f \mathbf{n} d\sigma - \int_{\mathcal{B}} f \frac{\partial \psi(\mathbf{k})}{\partial k^j} d^3\mathbf{k},$$

with $\mathbf{n}$ outward unit normal field on the boundary $\partial\mathcal{B}$ of the domain $\mathcal{B}$ and $d\sigma$ surface element of $\partial\mathcal{B}$, eq. (2.1) becomes

$$\frac{\partial M_\psi}{\partial t} + \frac{\partial}{\partial x^i}\int_{\mathcal{B}} f\psi(\mathbf{k})v^i(\mathbf{k})d^3\mathbf{k} + eE^j\left[\int_{\mathcal{B}} f\frac{\partial\psi(\mathbf{k})}{\partial k_j}d^3\mathbf{k} - \int_{\partial\mathcal{B}}\psi(\mathbf{k})fn_j d\sigma\right] =$$
$$\int_{\mathcal{B}}\psi(\mathbf{k})\mathcal{C}(f)d^3\mathbf{k}. \tag{2.2}$$

The term

$$\int_{\partial\mathcal{B}}\psi(\mathbf{k})f\mathbf{n}d\sigma$$

vanishes either when $\mathcal{B}$ is expanded to $\mathcal{R}^3$ (because in order to guarantee the integrability condition f must tend to zero sufficiently fast as $k \mapsto \infty$) or when $\mathcal{B}$ is compact and $\psi(\mathbf{k})$ is periodic and continuous on ∂B. This latter condition is a conseguence of the periodicity of f on $\mathcal{B}$ and the symmetry of $\mathcal{B}$ with respect to the origin.

In the applications several choices of the weight function ψ can be made and they lead to different balance equations for macroscopic quantities. In [12] ψ was chosen equal to 1, $\hbar\mathbf{k}$, $\mathcal{E}$ and $\mathcal{E}\,\hbar\mathbf{k}$ in order to make a comparison with the results obtained in [50] by means of Monte Carlo simulations. However for time dependent simulation it is more useful to consider a slight different set of weight functions [13], 1, $\hbar\mathbf{k}$, $\mathcal{E}$ and $\mathcal{E}\,\mathbf{V}$ because it allows an easier implementation in numerical codes (the two choices are practically equivalent for stationary problems or for nonstationary problems in the parabolic band approximation).

By considering such expressions for ψ one obtains the continuity equation (indeed a term due to the generation-recombination mechanism should appear in the right hand side, but this effect is relevant for times of order 10^{-9} second and in most applications can be neglected because the characteristic times are of order of a fraction of picosecond), the balance equation for the crystal momentum, the balance equation for the electron energy, and the balance equation for the electron energy flux. For the sake of simplicity hereafter we neglect the boundary integral terms because only the Kane dispersion relation or the parabolic case will be considered in the sequel and then the explicit form of the macroscopic balance equations reads

$$\frac{\partial n}{\partial t} + \frac{\partial(nV^i)}{\partial x^i} = 0, \tag{2.3}$$
$$\frac{\partial(nP^i)}{\partial t} + \frac{\partial(nU^{ij})}{\partial x^j} + neE^i = nC_P^i, \tag{2.4}$$
$$\frac{\partial(nW)}{\partial t} + \frac{\partial(nS^j)}{\partial x^j} + neV_kE^k = nC_W, \tag{2.5}$$
$$\frac{\partial(nS^i)}{\partial t} + \frac{\partial(nF^{ij})}{\partial x^j} + neE_jG^{ij} = nC_W^i, \tag{2.6}$$

where

$$\begin{aligned} n &= \int_{\mathcal{B}} fd^3\mathbf{k} \quad \text{is the electron density,} \\ V^i &= \frac{1}{n}\int_{\mathcal{B}} fv^id^3\mathbf{k} \quad \text{is the average electron velocity,} \\ W &= \frac{1}{n}\int_{\mathcal{B}}\mathcal{E}(k)fd^3\mathbf{k} \quad \text{is the average electron energy,} \end{aligned}$$

$$
\begin{aligned}
S^i &= \frac{1}{n}\int_{\mathcal{B}} f v^i \mathcal{E}(k) d^3\mathbf{k} \quad \text{is the energy flux,}\\
P^i &= \frac{1}{n}\int_{\mathcal{B}} f \hbar k^i d^3\mathbf{k} \quad \text{is the average crystal momentum,}\\
U^{ij} &= \frac{1}{n}\int_{\mathcal{B}} f v^i k^j d^3\mathbf{k} \quad \text{is the flow of crystal momentum,}\\
G^{ij} &= \frac{1}{n}\int_{\mathcal{B}} \frac{1}{\hbar} f \frac{\partial}{\partial k_j}(\mathcal{E} v_i) d^3\mathbf{k},\\
F^{ij} &= \frac{1}{n}\int_{\mathcal{B}} f v^i v^j \mathcal{E}(k) d^3\mathbf{k} \quad \text{is the flux of energy flux,}\\
C_P^i &= \frac{1}{n}\int_{\mathcal{B}} \mathcal{C}[f] \hbar k^i d^3\mathbf{k} \quad \text{is the production of the crystal momentum balance equation,}\\
C_W &= \frac{1}{n}\int_{\mathcal{B}} \mathcal{C}[f] \mathcal{E}(k) d^3\mathbf{k} \quad \text{is the production of the energy balance equation,}\\
C_W^i &= \frac{1}{n}\int_{\mathcal{B}} \mathcal{C}[f] v^i \mathcal{E}(k) d^3\mathbf{k} \quad \text{is the production of the energy flux balance equation.}
\end{aligned}
$$

Analogous equations can be written for holes if a two component charge carrier model is employed.

The moment equations do not constitute a set of closed relations because of the fluxes and production terms.

In the following sections of this chapter we will discuss some of the simplest closure relations and point out their deficiencies.

2.2 The relaxation time approximation

A simplistic model approximately valid under non degenerate conditions ($f \ll 1$) and for elastic scattering [43] gives for the collision term $\mathcal{C}$ a relaxation type expression

$$\mathcal{C}(f) = -\frac{f - \hat{f}}{\tau(\mathcal{E}(\mathbf{k}))} \tag{2.7}$$

where $\hat{f}$ can be written in the following more convenient form

$$\hat{f} = \exp\left(-\frac{\mathcal{E}(\mathbf{k}) - e\phi + q\mathcal{E}_F}{k_B T}\right) \tag{2.8}$$

corresponding to the local maxwellian distribution, T is the local electron temperature (at global equilibrium $T = T_L$), ϕ the electrostatic potential and $\mathcal{E}_F$ the Fermi energy.

At global thermal equilibrium T=const and $\mathcal{E}_F$=const in space and time.

We consider time scales longer than the collision times $\tau(\mathcal{E}(\mathbf{k}))$ and therefore we can neglect $\frac{\partial f}{\partial t}$ in the Boltzmann equation (1.5). By iterating we then obtain [43] in the usual way to first order

$$f = f_{eq} - \tau(\mathcal{E}(\mathbf{k}))[\mathbf{v}(\mathbf{k}) \cdot \nabla f_{eq} - e\mathbf{E} \cdot \nabla_{\mathbf{k}} f_{eq}] \tag{2.9}$$

which,using eq.(2.8) gives

$$f = f_{eq} - \tau(\mathcal{E}(\mathbf{k}))\frac{f_{eq}}{k_B T}\left[\frac{\mathcal{E}(\mathbf{k}) - e\phi + e\mathcal{E}_F}{K_B T}\mathbf{v}(\mathbf{k}) \cdot \nabla T - q\mathbf{v}(\mathbf{k}) \cdot \nabla \mathcal{E}_F\right] \tag{2.10}$$

Let $\mathbf{J} = n\mathbf{V}$ denote the particle flux. Then by substituting eq.(2.10) into the definition of $\mathbf{V}$, one obtains

$$\mathbf{J} = -\frac{4\pi}{3m^\star k_B T}\left\{[A + Bq(\mathcal{E}_F - \phi)]\frac{\nabla T}{k_B T} - eB\nabla\mathcal{E}_F\right\} \tag{2.11}$$

where

$$A = 4\pi \int d^3\mathbf{k} f_{eq} k^4 \tau(\mathcal{E}(\mathbf{k}))\mathcal{E}(\mathbf{k})$$

$$B = 4\pi \int d^3\mathbf{k} f_{eq} k^4 \tau(\mathcal{E}(\mathbf{k}))$$

Now the particle density is given by

$$n = \int d^3\mathbf{k} f = (\pi 2m^\star k_B T)^{3/2} \exp -\frac{e\mathcal{E}_F - e\phi}{k_B T} \tag{2.12}$$

whence

$$\mathcal{E}_F = \phi - \frac{k_B T}{e}\log(\frac{n}{aT^{3/2}}) + \text{const} \tag{2.13}$$

$$\nabla\mathcal{E}_F = \nabla\phi + \nabla[\frac{k_B T}{e}\log(\frac{aT^{3/2}}{n})]$$

with

$$a = (\pi 2m^\star k_B)^{3/2}$$

From q.(2.13) we see that $\mathcal{E}_F$ plays the role of electrochemical potential (usually called, in this context, quasi-Fermi potential).

It is convenient to introduce the intrinsic concentration of electrons

$$n_i = aT^{3/2} \tag{2.14}$$

and then

$$\mathcal{E}_F = \phi - U_T \log(\frac{n}{n_i})$$

where U_T is the thermal potential

$$U_T = \frac{k_B T}{e}$$

Also, it is convenient to introduce the mobility

$$\mu_n = \frac{4\pi e B}{3m^\star k_B T n} \tag{2.15}$$

and the thermoelectric power

$$P_n = \frac{A + Be(\mathcal{E}_F - \phi)}{eBk_B T} \tag{2.16}$$

Eq.(2.11) then rewrites

$$\mathbf{J} = \mu_n n(\nabla \mathcal{E}_F - P_n \nabla T) \tag{2.17}$$

Under isothermal conditions, $T = T_L$=const, we have

$$\nabla \mathcal{E}_F = \nabla \phi - U_T \frac{\nabla n}{n}$$

whence

$$\mathbf{J} = \mu_n n \nabla \phi - D_n \nabla n \tag{2.18}$$

where

$$D_n = \mu_n U_T \tag{2.19}$$

is the diffusion coefficient and eq.(2.19) expresses the equilibrium statistical mechanics Einstein relations.

Under isothermal conditions therefore the electron system can be described by the particle continuity equation (2.3), the constitutive equation (2.18) and the Poisson equation for the self-consistent potential. Allowing for two bands (valence and conduction band) and including holes we obtain the celebrated *drift-diffusion equations*

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J}_n = G - R \tag{2.20}$$

$$\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{J}_p = G - R \tag{2.21}$$

$$\mathbf{J}_n = \mu_n n \nabla \phi - D_n \nabla n \tag{2.22}$$

$$\mathbf{J}_p = -\mu_p p \nabla \phi - D_p \nabla p \tag{2.23}$$

$$\nabla \cdot (\epsilon \nabla \phi) = e(N_A - N_D + n - p) \tag{2.24}$$

where $n, p, \mathbf{J}_n, \mathbf{J}_p$ are the particle number densities of electrons and holes and their respective fluxes, μ_n, μ_p, D_n, D_p are their mobilities and diffusivities (related by the Einstein relations), N_A, N_D the concentration of acceptors and donors and ϵ the dielectric constant. The quantities G, R are functions of n, p and represent the rates of generation and recombination respectively.

In the general case, when the temperature is not uniforn, the drift- diffusion equations must be suitably modified.

In linear non-equilibrium thermodynamics it is customary to define the *thermodynamic heat flux* (note that it is different from the kinetic definition of heat flux) as follows

$$\mathbf{H} = \int d\mathbf{k}(\mathcal{E}(\mathbf{k}) - e\phi + e\mathcal{E}_F)\mathbf{v}(\mathbf{k}) f \tag{2.25}$$

i.e. we subtract from the total energy the Fermi energy $-e\mathcal{E}_F$ and the potential energy $e\phi$. Hence

$$\mathbf{H} = \mathbf{S} + e(\mathcal{E}_F - \phi)\mathbf{J} \tag{2.26}$$

It follows

$$\mathbf{H} = -\frac{4\pi}{3m^\star k_B T} \left\{ C \frac{\nabla T}{k_B T} - e[A + Bq(\mathcal{E}_F - \phi)] \nabla \mathcal{E}_F \right\} \tag{2.27}$$

where

$$C = 4\pi \int dk f_{eq} k^4 \tau(\mathcal{E}(\mathbf{k}))(\mathcal{E}(\mathbf{k}) - e\phi + e\mathcal{E}_F)^2$$

Eq.(2.27) can be rewritten in the form

$$\mathbf{H} = n[e\mu_n P_n k_B T \nabla \mathcal{E}_F - \frac{\lambda_n}{k_B T} \nabla T] \tag{2.28}$$

where

$$\lambda_n = \frac{4\pi C}{3m^\star k_B T n}.$$

Equations (2.11),(2.28) form the basis of the energy transport model [83]. By comparing eq.(2.28) to eq.(2.11) we see that the Onsager reciprocity principle [28] holds for the energy transport model [43, 3].

2.3 Hydrodynamical models

The drift-diffusion equations do not comprise the energy-density as a dynamical variable, hence they are not capable of describing phenomena where energy plays an important role, as hot electrons. Energy can be taken into account by including the energy equation (2.5) and the energy-flux equation (2.6). This approach dates back to the pionereeing work of Blotekjaer [23]. We shall first introduce a *simplified model* originally due to Baccarani and Wordeman [19] and extensively investigated by several authors. Because of its widespread popularity we denote this model by BBW (Blotekjaer-Baccarani-Wordeman).

We suppose the energy band of parabolic type and introduce the random component $m^\star \mathbf{c}$ and the mean value $m^\star \mathbf{u}$ of $\mathbf{k}$,

$$\mathbf{k} = m^\star(\mathbf{V} + \mathbf{c}),$$

and then decompose the tensor U^{ij} as

$$nU^{ij} = nV^i V^j + \int d^3\mathbf{k} f c^i c^j$$

The tensor

$$\hat{\theta}^{ij} = \int d^3\mathbf{k} c^i c^j f$$

is then split into an isotropic and traceless part

$$\hat{\theta}^{ij} = \frac{1}{3}\hat{\theta}^k_k \delta^{ij} + \hat{\theta}^{<ij>}$$

where

$$\hat{\theta}^k_k = \int d^3\mathbf{k} f \mathbf{c}^2.$$

Then

$$U^{ij} = nV^iV^j + \frac{1}{3}\hat{\theta}^k_k\delta^{ij} + \hat{\theta}^{<ij>} \tag{2.29}$$

In the model of Baccarani and Wordeman the anisotropic tensor $\hat{\theta}^{<ij>}$ is neglected

$$\hat{\theta}^{<ij>} = 0 \tag{2.30}$$

For the energy density one has

$$nW = \frac{m^\star}{2}(nV^2 + \hat{\theta}^k_k).$$

Now we define the electron temperature T (distinct from the lattice temperature T_L) by

$$\frac{3nk_BT}{2} = nW - \frac{nm^\star \mathbf{V}^2}{2} \tag{2.31}$$

whence

$$\hat{\theta}^k{}_k = \frac{3nk_BT}{m^\star}$$

and

$$\hat{\theta}^{ij} = \frac{nk_BT}{m^\star}\delta^{ij}.$$

Then the momentum rate of change is assumed to be of the relaxation time type

$$\mathbf{Q} = -\frac{\mathbf{J}}{\tau_p} \tag{2.32}$$

hence the momentum equation (2.4) rewrites

$$\frac{\partial(nV^i)}{\partial t} + \frac{\partial}{\partial x^j}\left[nV^iV^j + \frac{nk_BT}{m^\star}\delta^{ij}\right] + \frac{nqE^i}{m^\star} = -\frac{nV^i}{\tau_p} \tag{2.33}$$

Furthermore we can always decompose the energy flow $\mathbf{S}$ as

$$\mathbf{S} = W\mathbf{V} + k_BT\mathbf{V} + \mathbf{q} \tag{2.34}$$

where $\mathbf{q}$ is the heat flow vector

$$n\mathbf{q} = \frac{m^\star}{2}\int d^3\mathbf{k} f \mathbf{c}^2\mathbf{c} \tag{2.35}$$

In the BBW model it is assumed that *the heat flow vector is given by the Fourier law* (closure assumption)

$$\mathbf{q} = -\kappa\nabla T \tag{2.36}$$

In the original Baccarani and Wordeman model the Fourier law is simply assumed as a phenomenological law. A better justification (which however leads to a more complicated expression) has been given by several authors [43, 8, 9]. The argument runs as follows. Assume the distribution function to be very nearly isotropic, hence $F_{<ij>} = 0$ and $\theta_{<ij>} = 0$. Furthermore assume $\tilde{\mathbf{Q}}$ to be represented as relaxation term

$$\tilde{\mathbf{Q}} = -\frac{\mathbf{S}}{\tau_q}$$

with τ_q the energy flux relaxation time. Then under stationary conditions eq.(2.6) yields

$$S_i = -\tau_q \left[\frac{1}{3} \frac{\partial F_{rr}}{\partial x^i} + \frac{5qnk_B T}{2m^\star} E_i \right]$$

Now let us assume (closure assumption) that F_{rr} can be calculated as it were due to a maxwellian with temperature T (thereby neglecting the convective terms), then

$$F_{rr} = \frac{15n(k_B T)^2}{2m^\star}$$

Now the momentum equation (2.4) with the assumption

$$\mathbf{Q} = -\frac{\mathbf{J}}{\tau_p}$$

and neglecting the convective terms yields

$$\mathbf{J} = -\frac{\tau_p}{m^\star} \left[\nabla(nk_B T) + ne\mathbf{E} \right]$$

Then, from the definition of heat flow vector and still neglecting the kinetic energy contribution, one obtains

$$nq_i = -\frac{5\tau_h nk_B T}{2m^\star} \frac{\partial(k_B T)}{\partial x^i} + \frac{5nk_B T V_i}{2} \left(\frac{1}{\tau_p} - \frac{1}{\tau_q} \right) \tau_q \tag{2.37}$$

By assuming $\tau_p = \tau_q$ (also required for consistency with the Onsager reciprocity relations) one recovers the standard Fourier law.

The closure assumptions made by Baccarani and Wordeman are open to criticism. In particular the assumption that the heat flow is described by the Fourier law is rather questionable, as will be discussed in the sequel.

Modeling the relaxation times requires more care. In the original Baccarani and Wordeman formulation τ_p is determined by the following consideration. The electron mobility μ_n is defined by

$$\mu_n = \frac{e\tau_p}{m^\star}$$

Then it is assumed that the Einstein relations relating mobility to diffusivity hold also outside thermal equilibrium.

$$D_n = \frac{k_B T}{e} \mu_n$$

and that D_n is constant and equal to the low field diffusivity D_0. Hence

$$D_0 = \frac{k_B T_L}{e} \mu_{n0} = \frac{k_B T}{e} \mu_n$$

where μ_{n0} is the low field mobility, whence

$$\tau_p = \frac{m^\star \mu_{n0} T_L}{eT}$$

The relaxation time τ_w is obtained by approximating it with the corresponding expression which holds in the stationary and homogeneous case

$$\tau_w = \frac{W - W_0}{e \mid \mathbf{E} \mid V}$$

and by expressing the electric field $\mid \mathbf{E} \mid$ as a function of temperature by using the Caughey-Thomas formula for the high-field mobility [74]

$$\mu_n = \mu_{n0} \left[1 + \left(\frac{\mu_{n0} \mid \mathbf{E} \mid}{v_s} \right)^2 \right]^{-1/2}$$

where $v_s = 1.0 \times 10^7$ cm/s is the saturation velocity. Then

$$\tau_w = \frac{m^\star \mu_{n0} T_L}{2eT} + \frac{3\mu_{n0} T T_L}{2ev_s^2 (T + T_L)}$$

The modeling of the thermal conductivity coefficient is a crucial step. In the original Baccarani and Wordeman model the thermal conductivity is obtained from the Wiedemann-Franz law (which holds near thermal equilibrium)

$$\kappa = (\frac{5}{2} + c)(\frac{k_B}{e})^2 nq\mu_n T \qquad (2.38)$$

where the constant c is related to the exponent in the expression for the relaxation time

$$\tau(\mathcal{E}) = \tau_0 \left(\frac{\mathcal{E}}{\mathcal{E}_0} \right)^c$$

In the original model of Baccarani and Wordeman $c = -1$ and therefore

$$\kappa = \frac{3}{2}(\frac{k_B}{e})^2 ne\mu_n T$$

The BBW hydrodynamical model for electrons consists then of the following equations.

- continuity equation

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{V}) = 0 \qquad (2.39)$$

- momentum equation

$$\frac{\partial (nV^i)}{\partial t} + \frac{\partial}{\partial x^j} \left(nV^i V^j + \frac{nk_B T}{m^\star} \delta^{ij} \right) + \frac{nqE^i}{m^\star} = -\frac{nV^i}{\tau_p} \qquad (2.40)$$

-energy equation

$$\frac{\partial}{\partial t} \left(\frac{1}{2} nm^\star \mathbf{V}^2 + \frac{3}{2} nk_B T \right) + \nabla \cdot \left[(\frac{1}{2} nm^\star V^2 + \frac{5}{2} nk_B T)\mathbf{V} \right.$$
$$\left. - \kappa \nabla T \right] + ne\mathbf{E} \cdot \mathbf{V} = -\frac{W - W_0}{\tau_w} \qquad (2.41)$$

-Poisson's equation

$$\nabla \cdot (\epsilon \nabla \phi) = e(N_A - N_D + n - p) \tag{2.42}$$

with κ the heat conduction coefficient. These equations, were not for the collision terms, would be the same as the balance equations for a charged heat conducting fluid coupled to Poisson's equation.

Gardner,Jerome and Rose [40] and Gardner [38] numerically integrated the BBW model for the ballistic diode in the stationary case. In [38] the system of equations was discretized by using central differences (if the flow is everywhere subsonic) or the second upwind method (for transonic flow). The discretized system is then linearized by using Newton's method with a damping factor. In this way Gardner was able to show evidence for an electron shock wave in the diode. In [2] Gardner's results have been recovered by using a viscosity method.

Numerical solutions in the nonstationary case have been obtained in [31] by using an ENO scheme. The same results have been obtained in [71] by using a central scheme.

Now we pass to investigate the Onsager conditions for the BBW model.

Now let us go back to the momentum balance equation (2.40). In the stationary case it yields to the first order approximation (that is by neglecting the second order terms in the velocity)

$$\mathbf{Q} = \frac{1}{m^\star} \nabla (n k_B T) - \frac{ne}{m^\star} \nabla \phi \tag{2.43}$$

and from eq.(2.13)

$$\mathbf{Q} = \frac{n}{m^\star} \left\{ -e \nabla \mathcal{E}_F + [\frac{5}{2} + \log(\frac{a T^{3/2}}{n})] \nabla (k_B T) \right\} \tag{2.44}$$

Now we consider the energy flux equation (2.6) in the stationary case. Also in this case $F_{<ij>} = 0$ approximately, hence

$$\tilde{\mathbf{Q}} = \frac{1}{3} \nabla F_{rr} - \frac{5 q n k_B T}{m^\star} \nabla \phi$$

$$\frac{F_{rr}}{3} = \frac{5 n (k_B T)^2}{2 m^\star}$$

according to the equilibrium f_{eq}, whence

$$\tilde{\mathbf{Q}} = \frac{5}{2m^\star} \left\{ \nabla [n (k_B T)^2] - e n k_B T \nabla \phi \right\}$$

which gives, by using eq.(2.13)

$$\tilde{\mathbf{Q}} = \frac{5}{2m^\star} \left\{ -q n k_B T \nabla \mathcal{E}_F + [\frac{7}{2} + \log(\frac{a T^{3/2}}{n})] n k_B T \nabla (k_B T) \right\} \tag{2.45}$$

Now, in the BBW model one assumes the following relaxation type forms for the collision terms

$$\mathbf{Q} = -\frac{\mathbf{J}}{\tau_p} \tag{2.46}$$

$$\tilde{\mathbf{Q}} = -\frac{\mathbf{S}}{\tau_q}. \tag{2.47}$$

Then we have

$$\mathbf{J} = -\frac{n\tau_p}{m^\star}\left\{-e\nabla\mathcal{E}_F + [\frac{5}{2} + \log(\frac{aT^{3/2}}{n})]\nabla(k_BT)\right\} \tag{2.48}$$

$$\mathbf{H} = \frac{en\tau_p}{m^\star}\left\{k_BT[\frac{5\tau_q}{2\tau_p} + \log(\frac{aT^{3/2}}{n})]\nabla\mathcal{E}_F + \Lambda\nabla T\right\} \tag{2.49}$$

with

$$\Lambda = \frac{1}{e\tau_p}\left\{-\frac{5\tau_q}{2}[\frac{7}{2} + \log(\frac{aT^{3/2}}{n})]k_BT - \tau_p k_BT\log(\frac{n}{aT^{3/2}})[\frac{5}{2} + \log(\frac{aT^{3/2}}{n})]\right\}$$

Let I denote the coefficient of $\nabla(k_BT)$ in the expression for $\mathbf{J}$ and II the coefficient of $\nabla\mathcal{E}_F$ in the expression for $\mathbf{H}$. The Onsager reciprocity principle requires that [28]

$$qk_BTI = -II \tag{2.50}$$

Therefore the Onsager reciprocity relations are satisfied if and only if $\tau_p = \tau_q$, but Monte Carlo simulations show that this relationship does not hold near thermal equilibrium. [3]. This implies that the production terms must have a more general form.

A more suitable form is given by

$$\mathbf{Q} = -(a\mathbf{J} + b\mathbf{S}) \tag{2.51}$$

$$\tilde{\mathbf{Q}} = -(\tilde{a}\mathbf{J} + \tilde{b}\mathbf{S}) \tag{2.52}$$

Now

$$\mathbf{J} = \frac{1}{\Delta}(b\tilde{\mathbf{Q}} - \tilde{b}\mathbf{Q}),$$
$$\mathbf{S} = \frac{1}{\Delta}(\tilde{a}\mathbf{Q} - a\tilde{\mathbf{Q}}),$$

with

$$\Delta = a\tilde{b} - \tilde{a}b$$

and therefore eq.(64) gives

$$\frac{1}{k_B}\left\{\tilde{a} - \frac{5ak_NT}{2} + k_BT\log(\frac{n}{n_i})[\tilde{b} - \frac{5bk_NT}{2}]\right\} =$$
$$= \frac{5bk_BT}{2}[\frac{7}{2} - \log(\frac{n}{n_i})] - \tilde{b}[\frac{5}{2} - \log(\frac{n}{n_i})],$$

which can be rewritten as

$$\tilde{a} + \frac{5}{2}\tilde{b}k_BT = \frac{5}{2}k_BT(a + \frac{7}{2}bk_BT). \tag{2.53}$$

This last relation has been compared with Monte Carlo simulation in [4].

Chapter 3

The extended hydrodynamical model

In a series of articles [11, 8, 3, 14, 15, 12, 13] a general framework in which to construct solutions to the closure problem is proposed which, contrary to previous treatments, is not ad hoc but is based on the application of the entropy principle within the framework of Extended Thermodynamics [63, 49] or equivalently the maximum entropy principle. Apart from the usual balance equations for carriers density, momentum and energy, this class of models comprises evolution equations for the heat flux and shear stress.

The resulting system is hyperbolic in a suitable domain of the space of variables. In the stationary case, by linearizing the heat flux equation for small temperature gradients (*Maxwellian iteration*) one obtains an extension of the Fourier law which includes also a convective term. With the addition of this term, the Onsager relations for small deviations from thermodynamical equilibrium are verified (at variance with the BBW model). Furthermore the heat conductivity turns out to be directly related to the energy-flux relaxation time and does not contain any undetermined free parameters (at variance with the BBW model).

In this section we show how to get a hydrodyamical model, based on a consistent theory of non-equilibrium thermodynamics, the so-called extended thermodynamics [63, 49]. First we illustrate the guideline upon which to construct the model for the case of a general energy band structure. Then specific results will be presented in the case of the Kane dispersion relation and, as limiting case, in the parabolic band approximation. The obtained constitutive equations will be compared with those derived by a fitting of Monte Carlo data in [50]

3.1 The maximum entropy principle

In this section a general energy band will be considered.

As seen in the previous sections, the set of moment equations (2.3)-(2.6) is not closed. If we assume as fundamental variables n, V^i, W and S^i, which have a direct physical interpretation, the closure problem consists in expressing P^i, U^{ij}, F^{ij} and G^{ij} and the moments of the collision term C_P^i, C_W and C_W^i as functions of n, V^i, W and S^i.

We stress that the role of the mean velocity V^i here is radically different from that played in gas dynamics. In fact, for a simple gas the explicit dependence of fluxes on the velocity can be predicted by requiring galilean invariance of the constitutive functions. Instead eqs (2.3)-(2.6) are not valid in an arbitrary galilean reference frame, but they hold only in a frame where the crystal is at rest (in the applications it can be considered as inertial and it is possible to neglect the inertial forces). Therefore V^i is the velocity relative to the crystal and the dependence on it in the constitutive functions cannot be removed by a galilean transformation.

The maximum entropy principle (hereafter MEP) leads to a systematic way for obtaining constitutive relations on the basis of information theory (see [63, 49, 53, 29] for a review).

According to the MEP if a given number of moments M_A are known, the distribution function f_{ME} which can be used to evaluate the unknown moments of f, corresponds to the extremal of the entropy functional under the constraints that it yields exactly the known moments M_A

$$\int_{\mathcal{B}} \psi_A f_{ME} d^3\mathbf{k} = M_A. \tag{3.1}$$

Since the electrons interact with the phonons describing the thermal vibrations of the ions placed at the points of the crystal lattice, in principle we should deal with a two component system (electrons and phonons). However, if one consider the phonon gas as a thermal bath at constant temperature T_L, only the electron component of the entropy must be maximized. Moreover, by considering the electron gas as sufficiently dilute, one can take for the electron gas the expression of the entropy obtained as limiting case of that arising in the Fermi statistics

$$s = -k_B \int_{\mathcal{B}} \left(f \log f - f\right) d^3\mathbf{k}. \tag{3.2}$$

If we introduce the lagrangian multipliers Λ_A, the problem to maximize s under the constraints (3.1) is equivalent to maximize

$$s' = \Lambda^A M_A - s,$$

the Legendre transform of s, without constraints,

$$\delta s' = 0.$$

This gives

$$\left[\log f + \frac{\Lambda_A \psi^A}{k_B}\right] \delta f = 0$$

Since the latter relation must hold for arbitrary δf, it follows

$$f_{ME} = \exp\left[-\frac{1}{k_B}\Lambda_A \psi^A\right]. \tag{3.3}$$

If n, V^i, W and S^i are assumed as fundamental variables,then

$$\psi^A = (1, \mathbf{v}, \mathcal{E}, \mathcal{E}\mathbf{v})$$

and

$$\Lambda_A = (\lambda, k_B\lambda_i, k_B\lambda^W, k_B\lambda_i^W)$$

with λ lagrangian multiplier relative to the density n, λ^W lagrangian multiplier relative to the energy W, λ_i lagrangian multiplier relative to the velocity V^j and λ_i^W lagrangian multiplier relative to the energy flux S^j. Therefore the maximum entropy distribution function reads

$$f_{ME} = \exp\left[-\left(\frac{1}{k_B}\lambda + \lambda^W\mathcal{E} + \lambda_i v^i + \lambda_i^W v^i\mathcal{E}\right)\right], \tag{3.4}$$

with Λ_A functions of the moments M_A. We want to stress that at variance with the monatomic gas, the problem of the integrability due to the fact that the sign of the argument of the exponential is not defined, does not arise here because the moments are obtained by integrating over the first Brillouin zone, which is a compact set of $\mathcal{R}^3$.

In order to get the dependence of the Λ_A's from the M_A, one has to invert the constraints (3.1). Then by taking the moments of f_{ME} and $\mathcal{C}[f_{ME}]$ one finds the closure relations for the fluxes and the production terms of the system (2.3)-(2.6) . On account of the analytical difficulties this can be achieved only with a numerical procedure. However, apart from the computational problems, the balance equations are now a closed set of partial differential equations and with standard considerations in extended thermodynamics [63] it is easy to show that they form a quasilinear hyperbolic system.

Let us set

$$\eta(f) = -k_B\left(f\log f - f\right).$$

The entropy balance equations is obtained multiply the equation (1.5) by $\eta'(f) = \partial_f\eta(f)$ and after integrating with respect to $\mathbf{k}$ one has

$$\frac{\partial}{\partial t}\int_{\mathcal{B}}\eta(f)d^3\mathbf{k} + \frac{\partial}{\partial x^i}\int_{\mathcal{B}}\eta(f)v^i d^3\mathbf{k} - eE^i\int_{\mathcal{B}}\eta'(f)\frac{\partial}{\partial k^j}f d^3\mathbf{k} = \int_{\mathcal{B}}\eta(f)\mathcal{C}[f]d^3\mathbf{k}.$$

By taking into account the periodicity condition of f on the first Brilluin zone, the integral

$$\int_{\mathcal{B}}\eta'(f)\frac{\partial}{\partial k^j}f d^3\mathbf{k} = \int_{\mathcal{B}}\frac{\partial\eta(f)}{\partial k^j}d^3\mathbf{k} = \int_{\partial B}\eta(f)n^i d^3\mathbf{k}$$

vanishes and the entropy balance equations assumes the usual form

$$\frac{\partial s}{\partial t} + \frac{\partial\varphi^i}{\partial x^i} = g,$$

with

$$\varphi^i = \int_{\mathcal{B}}\eta(f)v^i d^3\mathbf{k} \quad \text{entropy flux}$$

and

$$g = \int_{\mathcal{B}}\eta(f)\mathcal{C}[f]d^3\mathbf{k} \quad \text{entropy production.}$$

The electric field does not contribute neither to the entropy production nor to the entropy flux.

Let us now rewrite the balance equations (2.3)-(2.6) in the form

$$\frac{\partial M^A}{\partial t} + \frac{\partial F^{iA}}{\partial x^i} = G^A(M_B, E_j). \tag{3.5}$$

In [63] it is proved that the field equations and the entropy balance equations are related by the condition that

$$\frac{\partial s}{\partial t}+\frac{\partial \varphi^i}{\partial x^i}-g-\Lambda_A\left[\frac{\partial M^A}{\partial t}+\frac{\partial F^{iA}}{\partial x^i}-G^A(M_B,E_j)\right]=0, \tag{3.6}$$

holds for arbitrary values of the field M_A with the lagrangian multipliers Λ_A being the same as those arising by employing the maximum entropy principle. This implies [63] that

$$M_A = \frac{\partial s'}{\partial \Lambda_A}, \tag{3.7}$$

$$F^{iA} = \frac{\partial \varphi'^i}{\partial \Lambda_A}, \tag{3.8}$$

with

$$\phi'^i=\Lambda_A M^A-\phi.$$

If

$$\frac{\partial s'}{\partial \Lambda_A \partial \Lambda_B}$$

is defined in sign, one can globally invert [22] and express the moment M_A as function of the lagrangian multipliers Λ_B. As shown in [24] the previous condition is equivalent to require that

$$f'_{ME}=\frac{\partial}{\partial \chi}f_{ME}(\chi)$$

is defined in sign, with $\chi=\Lambda_A\psi^A/k_B$. One trivally gets $f'_{ME}<0$ and therefore the balance equations (2.3)-(2.6) can be rewritten in terms of the lagrangian multipliers as

$$\frac{\partial^2 s'}{\partial \Lambda_A \partial \Lambda_B}\frac{\partial \Lambda_B}{\partial t}+\frac{\partial^2 \varphi'^i}{\partial \Lambda_A \Lambda_B}\frac{\partial B}{\partial x^i}=G^A\left(\frac{\partial s'}{\partial \Lambda_C},E_j\right). \tag{3.9}$$

In this form it is immediate to recognize that the balance equations form a symmetric quasilinear hyperbolic system [47]. The main consequence of this property is that according to a theorem due to Fisher and Marsden [34] the Cauchy problem is well-posed for the system (3.9) at least in the simple case when the electric field is considered as an external field.

3.2 Closure relations for Kane's dispersion relation

As a first attempt, in order to get explicit forms of the constitutive equations and improve over the parabolic band approximation (and also to obtain a first guess for future numerical work), we shall consider hereafter the Kane dispersion relation. The price to pay for this choice is that the integrability condition is no longer guaranteed because now $\mathcal{B}$ is not a compact set but $\mathcal{B}=\mathcal{R}^3$.

However this difficulty can be circumvented and we show how to get, under reasonable assumptions, an asymptotic form of f_{ME} which enjoys the property of integrabilty also in $\mathcal{R}^3$.

At equilibrium the distribution function is isotropic

$$f_{EQ} = \exp\left[-\left(\frac{1}{k_B}\lambda_E + \frac{\mathcal{E}}{k_B T_0}\right)\right], \tag{3.10}$$

that is at equilibrium

$$\lambda_E^W = \frac{1}{k_B T_0}, \quad \lambda_E^i = 0 \quad \lambda_E^{iW} = 0.$$

Monte Carlo simulations for electron transport in Si show that the anisotropy of f is small [4, 50, 75] even far from equilibrium. The physical reason is that in Si the main scattering mechanisms, the interactions of electrons with acoustic and non-polar optical phonons, are both isotropic.

Upon such a consideration we make the ansatz of small anisotropy for f_{ME}. Formally we introduce a *small* anisotropy parameter δ, assume that the multipliers are analytic in δ and expand them around $\delta = 0$ up to second order by taking into account the representation theorems for isotropic functions,

$$\lambda = \lambda^{(0)} + \delta^2\,\lambda^{(2)}, \tag{3.11}$$

$$\lambda^W = \lambda^{W(0)} + \delta^2\,\lambda^{W(2)}, \tag{3.12}$$

$$\lambda_i = \delta\,\lambda_i^{(1)}, \tag{3.13}$$

$$\lambda_i^W = \delta\,\lambda_i^{W(1)}. \tag{3.14}$$

Therefore f_{ME} can be written as

$$f_{ME} = \exp\left(-\frac{\lambda^{(0)}}{k_B} - \lambda^{W(0)}\mathcal{E}\right)\left[1 - \delta x + \delta^2\left(\frac{x^2}{2} - \frac{\lambda^{(2)}}{k_B} - \lambda^{W(2)}\mathcal{E}\right)\right], \tag{3.15}$$

with $x = \lambda_i^{(1)} v^i + \lambda_i^{W(1)} v^i \mathcal{E}$.

We remark that $\lambda^{(0)}$ and $\lambda^{W(0)}$ are not the equilibrium part of λ and λ^W, but the part arising when f_{ME} is isotropic.

In order to get the expressions of the Λ's in terms of the M_A we have to invert the following equations:

$$n = \int_{\mathcal{B}} f_{ME}\, d^3\mathbf{k}, \tag{3.16}$$

$$nW = \int_{\mathcal{B}} \mathcal{E} f_{ME}\, d^3\mathbf{k}, \tag{3.17}$$

$$nV^i = \int_{\mathcal{B}} v^i f_{ME}\, d^3\mathbf{k}, \tag{3.18}$$

$$nS^i = \int_{\mathcal{B}} v^i \mathcal{E} f_{ME}\, d^3\mathbf{k}. \tag{3.19}$$

By retaining only the terms up to second order in δ, from the constraints (3.16)-(3.19), we get the following algebraic system (V_i and S_i are consistently considered as terms of order δ)

$$n = \exp\left[-\left(\frac{1}{k_B}\lambda^{(0)}\right)\right]\int_{\mathcal{B}} \exp\left[-\left(\lambda^{W(0)}\mathcal{E}\right)\right] d^3\mathbf{k}, \tag{3.20}$$

$$W = \exp\left[-\left(\frac{1}{k_B}\lambda^{(0)}\right)\right]\int_{\mathcal{B}} \mathcal{E}\exp\left[-\left(\lambda^{W(0)}\mathcal{E}\right)\right] d^3\mathbf{k}, \tag{3.21}$$

$$
\begin{aligned}
0 &= \int_{\mathcal{B}} \exp\left(\lambda^{W(0)}\mathcal{E}\right)\left[\frac{1}{k_B}\lambda^{(2)} + \lambda^{W(2)}\mathcal{E} - \frac{x^2}{2}\right], && (3.22)\\
0 &= \int_{\mathcal{B}} \mathcal{E}\exp\left(\lambda^{W(0)}\mathcal{E}\right)\left[\frac{1}{k_B}\lambda^{(2)} + \lambda^{W(2)}\mathcal{E} - \frac{x^2}{2}\right], && (3.23)\\
nV^i &= -\int_{\mathcal{B}} v^i \exp\left(\lambda^{W(0)}\mathcal{E}\right) x\, d^3\mathbf{k}, && (3.24)\\
nS^i &= -\int_{\mathcal{B}} v^i\,\mathcal{E}\exp\left(\lambda^{W(0)}\mathcal{E}\right) x\, d^3\mathbf{k}. && (3.25)
\end{aligned}
$$

Since $\mathcal{E}$ is a isotropic function of k, in order to solve the system for the multipliers it is computationally convenient to express $d^3\mathbf{k}$ in terms of $\mathcal{E}$ and the elementary volume of solid angle $d\Omega$,

$$
d^3\mathbf{k} = k^2\,dk\,d\Omega = \frac{m^*}{\hbar^3}\sqrt{2m^*\mathcal{E}\left(1+\alpha\mathcal{E}\right)}\left(1+2\alpha\mathcal{E}\right)d\mathcal{E}\,d\Omega.
$$

Eqs. (3.20), (3.21) decouple from the other equations and explicitly read

$$
\begin{aligned}
n &= 4\frac{\pi}{\hbar^3}\exp\left(-\frac{\lambda^{(0)}}{k_B}\right)\int_0^\infty \exp\left(-\lambda^{W(0)}\mathcal{E}\right) m^*\sqrt{2m^*\mathcal{E}\left(1+\alpha\mathcal{E}\right)}\times\\
&\quad \times\left(1+2\alpha\mathcal{E}\right)d\mathcal{E}, && (3.26)\\
W &= \frac{\int_0^\infty \mathcal{E}\sqrt{\mathcal{E}\left(1+\alpha\mathcal{E}\right)}\left(1+2\alpha\mathcal{E}\right)\exp\left(-\lambda^{W(0)}\mathcal{E}\right)d\mathcal{E}}{\int_0^\infty \sqrt{\mathcal{E}\left(1+\alpha\mathcal{E}\right)}\left(1+2\alpha\mathcal{E}\right)\exp\left(-\lambda^{W(0)}\mathcal{E}\right)d\mathcal{E}}. && (3.27)
\end{aligned}
$$

Relation (3.27) shows that $\lambda^{W(0)}$ depends only on W. The analytical inversion of equation (3.27) is rather involved and we have resorted to a numerical inversion. The results are showed in fig. 1. Near global thermal equilibrium the value of $\lambda^{W(0)}$ is the same for both the parabolic and Kane dispersion relation. When W increases, the value of $\lambda^{W(0)}$ in the Kane case is greater.

The knowledge of $\lambda^{W(0)}$ allows us to get the constitutive functions for the other lagrangian multipliers.

Relation (3.26) gives $\lambda^{(0)}$, which essentially plays the role of a normalization factor

$$
\frac{\lambda^{(0)}}{k_B} = -\log\left(\frac{\hbar^3 n}{4\pi m^*\sqrt{2m^*}d_0}\right),
$$

with

$$
d_0 = \int_0^\infty \sqrt{\mathcal{E}\left(1+\alpha\mathcal{E}\right)}\left(1+2\alpha\mathcal{E}\right)\exp\left(-\lambda^{W(0)}\mathcal{E}\right)d\mathcal{E}.
$$

The lagrangian multipliers λ_i^v and λ_i^W can be obtained by inverting the linear system represented by eq.s (3.24)-(3.25).

By taking into account the following formula [1] valid for $\mathbf{l}$ belonging to S^2, the unit sphere of $\mathbf{R^3}$,

$$
\int_{S^2} l^{i_1}\cdots l^{i_k}\,d\Omega = \begin{cases} 0 & \text{if } k \text{ is odd}\\ \frac{4\pi}{k+1}\delta^{(i_1 i_2}\cdots\delta^{i_{k-1}i_k)} & \text{if } k \text{ is even}\end{cases}
$$

[1] round brackets mean symmetrization, e.g. $A_{(ij)} = 1/2(A_{ij}+A_{ji})$.

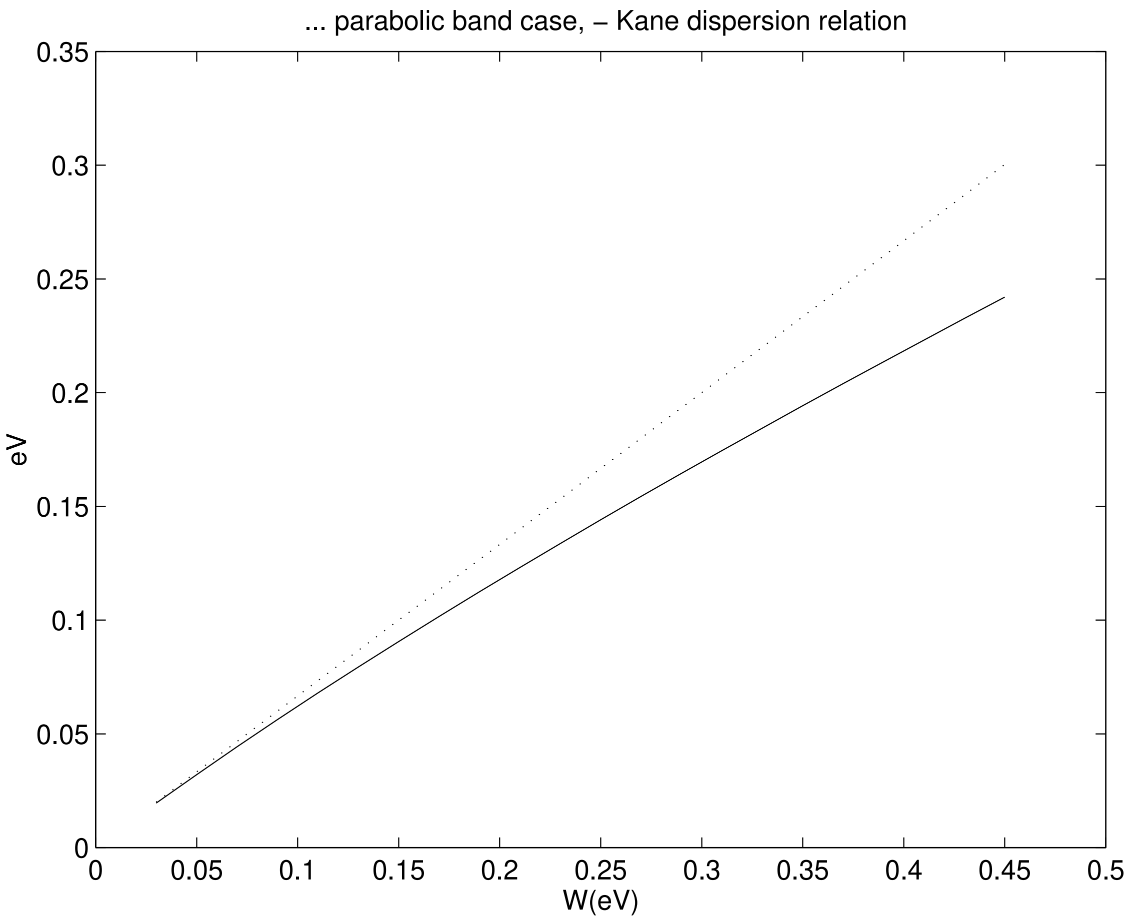

Figure 3.1: Inverse of the Lagrangian multipliers $\lambda^{W(0)}$ vs. the energy W

one finds

$$\begin{aligned} \lambda_i &= b_{11} V_i + b_{12} S_i, \\ \lambda_i^W &= b_{12} V_i + b_{22} S_i. \end{aligned}$$

The coefficients b_{ij} are given by

$$b_{11} = \frac{a_{22}}{\Delta}, \quad b_{12} = -\frac{a_{12}}{\Delta}, \quad b_{22} = \frac{a_{11}}{\Delta}$$

with

$$a_{11} = -\frac{2p_0}{3m^* d_0}, \quad a_{12} = -\frac{2p_1}{3m^* d_0}, \quad a_{22} = -\frac{2p_2}{3m^* d_0},$$

and

$$\Delta = a_{11} a_{22} - a_{12}^2,$$

d_k and p_k being

$$\begin{aligned} d_k &= \int_0^\infty \mathcal{E}^k \sqrt{\mathcal{E}\,(1+\alpha\mathcal{E})}\,(1+2\alpha\mathcal{E}) \exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E}, \\ p_k &= \int_0^\infty \frac{\left[\mathcal{E}(1+\alpha\mathcal{E})\right]^{3/2} \mathcal{E}^k}{1+2\alpha\mathcal{E}} \exp(-\lambda^{W(0)}\mathcal{E})\, d\mathcal{E}. \end{aligned}$$

Finally, the second order corrections to λ and λ^W, are obtained by solving the linear system (3.22)-(3.23).

The following expressions are found

$$\begin{aligned}
\frac{\lambda^{(2)}}{k_B} &= \alpha_1 \mathbf{V}\cdot\mathbf{V} + 2\alpha_2 \mathbf{S}\cdot\mathbf{V} + \alpha_3 \mathbf{S}\cdot\mathbf{S}, &(3.28)\\
\lambda^{W(2)} &= \alpha_4 \mathbf{V}\cdot\mathbf{V} + 2\alpha_5 \mathbf{S}\cdot\mathbf{V} + \alpha_6 \mathbf{S}\cdot\mathbf{S}, &(3.29)
\end{aligned}$$

where

$$\begin{aligned}
\alpha_1 &= \frac{3}{4}\frac{m^* d_0^2\left[d_1 p_1 (p_2^2 - p_3 p_1) - d_2 p_2 (p_1^2 - p_0 p_2)\right]}{\hat{D}}, &(3.30)\\
\alpha_2 &= \frac{3}{4}\frac{m^* d_0^2\left[d_2 p_1 (p_1^2 - p_0 p_2) - d_1 p_0 (p_2^2 - p_1 p_3)\right]}{\hat{D}}, &(3.31)\\
\alpha_3 &= \frac{3}{4}\frac{m^* d_0^2\left[(d_1 p_1 + d_2 p_0)(p_0 p_2 - p_1^2) + d_1 p_0 (p_1 p_2 - p_3 p_0)\right]}{\hat{D}}, &(3.32)\\
\alpha_4 &= -\frac{3}{4}\frac{m^* d_0^2\left[d_1 p_2 (p_2 p_0 - p_1^2) + d_0 p_1 (p_2^2 - p_1 p_3)\right]}{\hat{D}}, &(3.33)\\
\alpha_5 &= \frac{3}{4}\frac{m^* d_0^2\left[d_1 p_1 (p_2 p_0 - p_1^2) + d_0 p_0 (p_2^2 - p_1 p_3)\right]}{\hat{D}}, &(3.34)\\
\alpha_6 &= -\frac{3}{4}\frac{m^* d_0^2\left[(d_1 p_0 + p_1 d_0)(p_2 p_0 - p_1^2) + d_0 p_0 (p_1 p_2 - p_0 p_3)\right]}{\hat{D}}. &(3.35)
\end{aligned}$$

with

$$\hat{D} = (d_0 d_2 - d_1^2)(p_0 p_2 - p_1^2)^2. \tag{3.36}$$

3.3 Constitutive equations for fluxes

Once the lagrangian multipliers are expressed as functions of the fundamental variables, the constitutive equations for fluxes can be obtained by using the distribution function given by the maximum entropy principle. First we observe that by the definition of P^i, it follows

$$P^i = m^*(v^i + 2\alpha S^i), \tag{3.37}$$

while for the other tensorial quantities up to second order terms the constitutive equations are of the form

$$\begin{aligned}
U_{ij} &= U_{ij}^{(0)} + \delta^2 U_{ij}^{(2)}, &(3.38)\\
F_{ij} &= F_{ij}^{(0)} + \delta^2 F_{ij}^{(2)}, &(3.39)\\
G_{ij} &= G_{ij}^{(0)} + \delta^2 G_{ij}^{(2)}. &(3.40)
\end{aligned}$$

Concerning the tensor U^{ij} at the zero order we have

$$U^{ij(0)} = U^{(0)}\delta^{ij}, \tag{3.41}$$

with

$$U^{(0)} = \frac{2}{3d_0}\int_0^\infty \left[\mathcal{E}\,(1+\alpha\mathcal{E})\right]^{3/2} \exp\left(-\lambda^{W(0)}\mathcal{E}\right) d\mathcal{E},.$$

For $U^{ij(2)}$ we get

$$U^{ij(2)} = (\delta_1 \mathbf{V}\cdot\mathbf{V} + 2\delta_2 \mathbf{S}\cdot\mathbf{V} + \delta_3 \mathbf{S}\cdot\mathbf{S})\,\delta^{ij} + \delta_4\, V^i V^j + 2\delta_5\, V^{(i} S^{j)} + \delta_6\, S^i S^j. \quad (3.42)$$

The coefficients δ_k are given by

$$\begin{aligned}
\delta_1 &= \frac{3m^* d_0}{20\hat{D}} \Big\{ 2(d_0 d_2 - d_1^2)(b_0 p_2^2 - 2b_1 p_1 p_2 + b_2 p_1^2) + \\
&\quad 5U^{(0)} \Big[d_0 d_2 (p_2 p_1^2 - p_0 p_2^2) - d_0 d_1 (p_1 p_2^2 - p_3 p_1^2) \Big] \\
&\quad + 5R^{(0)} \Big[d_0 d_1 (p_0 p_2^2 - p_2 p_1^2) - d_0^2 (p_3 p_1^2 - p_1 p_2^2) \Big] \Big\}, && (3.43) \\
\delta_2 &= -\frac{3m^* d_0}{20\hat{D}} \Big\{ 2(d_0 d_2 - d_1^2) \Big[b_0 p_1 p_2 - b_1 (p_0 p_2 + p_1^2) + b_2 p_0 p_1 \Big] + \\
&\quad 5U^{(0)} \Big[d_0 d_2 (p_1^3 - p_0 p_1 p_2) - d_0 d_1 (p_0 p_2^2 - p_0 p_1 p_3) \Big] \\
&\quad + 5R^{(0)} \Big[d_0 d_1 (p_0 p_1 p_2 - p_1^3) - d_0^2 (p_0 p_1 p_3 - p_0 p_2^2) \Big] \Big\}, && (3.44) \\
\delta_3 &= \frac{3m^* d_0}{20\hat{D}} \Big\{ 2(d_0 d_2 - d_1^2)(b_0 p_1^2 - 2b_1 p_0 p_1 + b_2 p_0^2) + \\
&\quad 5U^{(0)} \Big[d_0 d_1 (p_1^3 - 2p_0 p_1 p_2 + p_0^2 p_3) - d_0 d_2 (p_0^2 p_2 - p_0 p_1^2) \Big] \\
&\quad + 5R^{(0)} \Big[d_0 d_1 (p_0^2 p_2 - p_0 p_1^2) - d_0^2 (p_0^2 p_3 - 2p_0 p_1 p_2 + p_1^3) \Big] \Big\}, && (3.45) \\
\delta_4 &= \frac{3m^* d_0}{5(p_0 p_2 - p_1^2)^2} \Big(b_0 p_2^2 - 2b_1 p_1 p_2 + b_2 p_1^2 \Big), && (3.46) \\
\delta_5 &= \frac{3m^* d_0}{5(p_0 p_2 - p_1^2)^2} \left[p_0 (b_1 p_2 - b_2 p_1) + p_1 (b_1 p_1 - b_0 p_2) \right], && (3.47) \\
\delta_6 &= \frac{3m^* d_0}{5(p_0 p_2 - p_1^2)^2} \Big(b_0 p_1^2 - 2b_1 p_1 p_0 + b_2 p_0^2 \Big), && (3.48)
\end{aligned}$$

with

$$b_k = \int_0^\infty \frac{\mathcal{E}^k \left[\mathcal{E}(1+\alpha\mathcal{E})\right]^{5/2}}{(1+2\alpha\mathcal{E})^2} \exp\left(-\lambda^{(0)}\mathcal{E}\right) d\mathcal{E} \quad (3.49)$$

and

$$R^{(0)} = \frac{2}{3d_0} \int_0^\infty \mathcal{E}^{5/2} (1+\alpha\mathcal{E})^{3/2} \exp\left(-\lambda^{(0)}\mathcal{E}\right) d\mathcal{E}. \quad (3.50)$$

Similar calculation can be performed for F_{ij} and G_{ij}. However in order to make a comparison with other existing models, based on a fitting procedure of Monte Carlo data, we calculate the constitutive equation for the tensor R_{ij} defined by

$$R_{ij} = \frac{1}{n} \int_{\mathcal{B}} \hbar k_i v_j f \, d^3\mathbf{k}.$$

This quantity has been introduced in [50] where the balance equation (2.6) was replaced with the equation obtained by taking the moment equation of the transport equation with the weight function

$$\psi(\mathbf{k}) = \hbar k_i v_j.$$

The advantge of this choice is that in the stationary case the number of constitutive functions is reduced to a minimum, but in the non stationary case the choice presented in the subsection 3.1 is more natural and computationally more efficient.

One has

$$R_{ij} = R_{ij}^{(0)} + R_{ij}^{(2)}.$$

For $R_{ij}^{(0)}$ one has

$$R_{ij}^{(0)} = R^{(0)}\delta_{ij},$$

with $R^{(0)}$ given by (3.50), while for $R^{ij(2)}$, we find

$$\begin{aligned} R^{ij(2)} &= (\gamma_1\,\mathbf{V}\cdot\mathbf{V} + 2\gamma_2\,\mathbf{S}\cdot\mathbf{V} + \gamma_3\,\mathbf{S}\cdot\mathbf{S})\,\delta^{ij} + \gamma_4\,V^iV^j + 2\gamma_5\,V^{(i}S^{j)} + \\ &\quad \gamma_6\,S^iS^j, \end{aligned} \tag{3.51}$$

where

$$\begin{aligned} \gamma_1 &= -\frac{3m^*d_0}{20\hat{D}}\Big\{2(d_1^2 - d_0d_2)(b_1p_2^2 - 2b_2p_1p_2 + b_3p_1^2) + \\ &\quad 5R^{(0)}\Big[d_0d_1(p_1p_2^2 - p_1^2p_3) + d_0d_2(p_0p_2^2 - p_2p_1^2)\Big] + \\ &\quad 5Q^{(0)}\Big[d_0^2(p_3p_1^2 - p_1p_2^2) + d_0d_1(p_2p_1^2 - p_0p_2^2)\Big]\Big\}, \end{aligned} \tag{3.52}$$

$$\begin{aligned} \gamma_2 &= \frac{3m^*d_0}{20\hat{D}}\Big\{2(d_1^2 - d_0d_2)\Big[b_1p_1p_2 - b_2(p_0p_2 + p_1^2) + b_3p_0p_1\Big] + \\ &\quad 5R^{(0)}\Big[d_0d_1(p_0p_2^2 - p_0p_1p_3) + d_0d_2(p_0p_1p_2 - p_1^3)\Big] + \\ &\quad 5Q^{(0)}\Big[d_0^2(p_0p_1p_3 - p_0p_2^2) + d_0d_1(p_1^3 - p_0p_1p_2)\Big]\Big\}, \end{aligned} \tag{3.53}$$

$$\begin{aligned} \gamma_3 &= \frac{3m^*d_0}{20\hat{D}}\Big\{2(d_0d_2 - d_1^2)(b_1p_1^2 - 2b_2p_0p_1 + b_3p_0^2) \\ &\quad 5R^{(0)}\Big[d_0d_1(p_1^3 - 2p_0p_1p_2 + p_0^2p_3) + d_0d_2(p_0p_1^2 - p_0^2p_2)\Big] + \\ &\quad 5Q^{(0)}\Big[d_0d_1(p_0^2p_2 - p_0p_1^2) - d_0^2(p_0^2p_3 - 2p_0p_1p_2 + p_1^3)\Big]\Big\}, \end{aligned} \tag{3.54}$$

$$\gamma_4 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2}\Big(b_1p_2^2 - 2b_2p_1p_2 + b_3p_1^2\Big), \tag{3.55}$$

$$\gamma_5 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2}\left[p_0(b_2p_2 - b_3p_1) + p_1(b_2p_1 - b_1p_2)\right], \tag{3.56}$$

$$\gamma_6 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2}\Big(b_1p_1^2 - 2b_2p_1p_0 + b_3p_0^2\Big), \tag{3.57}$$

$Q^{(0)}$ being

$$Q^{(0)} = \frac{2}{3d_0}\int_0^\infty \mathcal{E}^{7/2}(1+\alpha\mathcal{E})^{3/2}\exp\Big(-\lambda^{(0)}\mathcal{E}\Big)\,d\mathcal{E}.$$

3.4 Parabolic band approximation

In this section we shall consider the limiting case $\alpha \mapsto 0$. The aim is twofold. On one hand we will be able to get explicit formulas for the coefficients appearing in the constitutive equations, on the other hand it will be possible to have a comparison with previous hydrodynamical models. Moreover, since the difference of the results between the parabolic and Kane's dispersion relation should be small, at least at low energies, the results presented here can be useful to check the numerical evaluation of the previously obtained constitutive equations.

In the parabolic band approximation, it is possible to calculate the terms d_k, p_k and b_k by taking into account that for $a, \nu > 0$

$$\int_0^\infty x^{\nu-1} \exp(-ax)dx = \frac{1}{a^\nu}\Gamma(\nu),$$

with $\Gamma(\nu)$ the special Gamma function, and the property valid for positive integers p

$$\Gamma\left(p+\frac{1}{2}\right) = \frac{\sqrt{\pi}}{2^p}(2p-1)!!.$$

Concerning the lagrangian multipliers one has

$$\begin{aligned}
\frac{\lambda}{k_B} &= -\log\frac{n}{\left(\frac{4}{3}\pi m^* W\right)^{3/2}} + \frac{9m^*}{4W^2}\mathbf{V}\cdot\mathbf{S} - \frac{27m^*}{20W^3}\mathbf{S}\cdot\mathbf{S}, && (3.58)\\
\lambda^W &= \frac{3}{2W} + \frac{21m^*}{8W^2}\mathbf{V}\cdot\mathbf{V} - \frac{9m^*}{2W^3}\mathbf{V}\cdot\mathbf{S} + \frac{81m^*}{40W^4}\mathbf{S}\cdot\mathbf{S}, && (3.59)\\
\lambda_i &= -\frac{21m^*}{4W}V_i + \frac{9m^*}{4W^2}S_i, && (3.60)\\
\lambda_i^W &= \frac{9m^*}{4W^2}V_i - \frac{27m^*}{20W^3}S_i. && (3.61)
\end{aligned}$$

The distribution function given by the maximum entropy principle in this case reads

$$\begin{aligned}
f^P_{ME} = {} & \frac{n\exp(-\lambda^{W(0)}\mathcal{E})}{\left(\frac{4}{3}\pi m^* W\right)^{3/2}} \times \\
& \left\{1 - \left(-\frac{21m^*}{4W}V_i + \frac{9m^*}{4W^2}S_i\right)v^i - \left(\frac{9m^*}{4W^2}V_i - \frac{27m^*}{20W^3}S_i\right)\mathcal{E}v^i\right. \\
& +\frac{1}{2}\left[\left(-\frac{21m^*}{4W}V_i + \frac{9m^*}{4W^2}S_i\right)v^i + \left(\frac{9m^*}{4W^2}V_i - \frac{27m^*}{20W^3}S_i\right)\mathcal{E}v^i\right]^2 \\
& - \left(\frac{9m^*}{4W^2}\mathbf{V}\cdot\mathbf{S} - \frac{27m^*}{20W^3}\mathbf{S}\cdot\mathbf{S}\right) \\
& \left.- \left(\frac{21m^*}{8W^2}\mathbf{V}\cdot\mathbf{V} - \frac{9m^*}{2W^3}\mathbf{V}\cdot\mathbf{S} + \frac{81m^*}{40W^4}\mathbf{S}\cdot\mathbf{S}\right)\mathcal{E}\right\} \qquad (3.62)
\end{aligned}$$

and the constitutive equations become

$$\begin{aligned}
U^P_{ij} &= \frac{2}{3}W\delta_{ij} + \left(-\frac{7}{6}m^*\mathbf{V}\cdot\mathbf{V} + \frac{7m^*}{5W}\mathbf{S}\cdot\mathbf{V} - \frac{27m^*}{50W^2}\mathbf{S}\cdot\mathbf{S}\right)\delta^{ij} + \\
&\quad \frac{7}{2}m^*V^iV^j - \frac{21m^*}{5W}V^{(i}S^{j)} + \frac{81m^*}{50W^2}S^iS^j, && (3.63)\\
R^P_{ij} &= \frac{10}{9}W^2\delta_{ij} + \left(-\frac{7}{18}m^*W\mathbf{V}\cdot\mathbf{V} + \frac{m^*}{15}\mathbf{S}\cdot\mathbf{V} - \frac{9m^*}{50W}\mathbf{S}\cdot\mathbf{S}\right)\delta^{ij} + \\
&\quad \frac{77}{6}m^*WV^iV^j - \frac{91m^*}{5}V^{(i}S^{j)} + \frac{357m^*}{50W}S^iS^j. && (3.64)
\end{aligned}$$

In order to compare the results with those obtained for the monatomic gas and the hydrodynamical models of semiconductors presented in [8, 3, 68, 16], we observe that

$$\mathcal{E} = \frac{1}{2} m^* v^2 = \frac{1}{2} m^* (V_k + c_k)(V^k + c^k).$$

Therefore, by defining the electron temperature through

$$3nk_B T = 3p = m^* \int_{\mathcal{B}} c_k c^k f d^3\mathbf{k}$$

and introducing the heat flux

$$nq_i = \frac{1}{2} m^* \int_{\mathcal{B}} c_i c_k c^k f d^3\mathbf{k},$$

and the shear tensor

$$n\sigma_{ij} = m^* \int_{\mathcal{B}} c_{<i} c_{j>} f d^3\mathbf{k},$$

we have up to second order terms

$$\begin{aligned} W^{(P)} &= \frac{1}{2} m^* V^2 + \frac{3}{2} k_B T, \\ S^{i(P)} &= \frac{5}{2} k_B T V^i + \sigma^{ik} V_k + q^i. \end{aligned}$$

Then the lagrangian multipliers read

$$\begin{aligned} \frac{\lambda}{k_B} &= -\log \frac{n}{(2\pi m^* k_B T)^{3/2}} + \frac{m^* \mathbf{V}\cdot\mathbf{V}}{2k_B T} - \frac{m^*}{(k_B T)^2} \mathbf{V}\cdot\mathbf{q} - \frac{2}{5} \frac{m^*}{(k_B T)^3} \mathbf{q}\cdot\mathbf{q}, \\ \lambda^W &= \frac{1}{k_B T} + \frac{2}{3} \frac{m^* \mathbf{V}\cdot\mathbf{q}}{(k_B T)^3} + \frac{2}{5} \frac{m^* \mathbf{q}\cdot\mathbf{q}}{(k_B T)^4}, \\ \lambda_i &= -\frac{m^*}{k_B T} V_i + \frac{m^*}{(k_B T)^2} q_i, \\ \lambda_i^W &= -\frac{2}{5} \frac{m^*}{(k_B T)^3} q_i, \end{aligned}$$

which are the same as those obtained for a monatomic gas in the inviscid case. This shows that according to the results presented in [68], the explicit dependence of the multipliers on the velocity is the same as that found for a monatomic gas by operating the decomposition of the lagrangian multipliers into convective and non convective parts (compare the previous expressions for the $\Lambda' s$ with that reported in [56, 18]).

The constitutive equations (3.63),(3.64) become [2]

$$U_{ij}^{(P)} = m^* V_i V_j + k_B T \delta_{ij} + \frac{4m^*}{5k_B T} V_{<i} q_{j>} + \frac{18 m^*}{25 (k_B T)^2} q_{<i} q_{j>}, \tag{3.65}$$

$$\begin{aligned} R_{ij}^{(P)} = &\left(\frac{1}{2} m^* V^2 k_B T + \frac{5}{2} (k_B T)^2 - \frac{8}{15} m^* \mathbf{V}\cdot\mathbf{q} - \frac{3}{25} \frac{m^* q^2}{k_B T} \right) \delta_{ij} + \\ &\frac{7}{2} m^* k_B T V_i V_j + \frac{28}{5} m^* V_{(i} q_{j)} + \frac{119}{25} \frac{m^* q_i q_j}{k_B T}. \end{aligned} \tag{3.66}$$

[2] $< A_{ij} >$ means deviatoric part of A_{ij}, that is $< A_{ij} >= \frac{1}{2}(A_{ij} + A_{ji}) - 1/3 A_l^l \delta_{ij}$

By comparing the relation (3.65) with the analogous expression $U_{ij}^{(MG)}$ in the case of a monoatomic gas [56]

$$U_{ij}^{(MG)} = m^* V_i V_j + k_B T \delta_{ij} + \sigma_{ij},$$

we may make the identification

$$\sigma_{ij} = \frac{4m^*}{5k_B T} V_{<i} q_{j>} + \frac{18m^*}{25(k_B T)^2} q_{<i} q_{j>}. \tag{3.67}$$

Now, if such an expression for σ_{ij} is inserted into the expression for R_{ij} for the monatomic gas [56], $R_{ij}^{(MG)}$, with quadratic correction we obtain (we neglect the term of higher order than the second in V_k and the second order terms involving the shear because they are of the third order in V_i and q_j)

$$\begin{aligned} R_{ij}^{(MG)} &= \left(\frac{1}{2} m^* k_B T V^2 + \frac{5}{2}(k_B T)^2 + \frac{36 m^* q^2}{50 k_B T} \right) \delta_{ij} \\ &+ \frac{3}{2} m^* k_B T V_i V_j + \frac{7 k_B T}{2} \sigma_{ij} \\ &+ 2m^* k_B T V^k V_{(j} \delta_{ki)} + \frac{6}{5} q_{(i} \delta_{jk)} V^k + 2m^* V_{(i} q_{j)} + \frac{112 m^*}{50 k_B T} q_i q_j. \end{aligned}$$

This is the same expression (3.66).

3.5 Closure of the production terms

The problem of the closure of the production terms has been tackled in different ways. In [4] a relaxation time approximation was introduced and the relaxation times were considered as functions of the electron density whose behaviour was obtained by fitting the results obtained with the Monte Carlo simulations. In other works [15] a more justifiable model has been proposed but the functional form was again based on the Monte Carlo data. Here we present, in the case of the Kane dispersion relation and parabolic band approximation, a self-consistent treatment based on the distribution function satisfying the maximum entropy principle which gives closed relations apart from the values of few material parameters which must be considered as fitting parameters as in the case of Monte Carlo simulations.

3.5.1 Acoustic phonon scattering

If we set

$$K_{ac} = \frac{k_B T_L \Xi_d^2}{4\pi^2 \hbar \rho v_s^2},$$

the collision term for acustic phonon scattering reads

$$\begin{aligned} &\mathcal{C}[f] \approx \mathcal{C}[f_{ME}] = \\ &\frac{n K_{ac}}{d_0} \sqrt{\mathcal{E}(1+\alpha\mathcal{E})}(1+2\alpha\mathcal{E}) \exp\left(-\lambda^{(0)}\mathcal{E}\right) \left[a^4 + \frac{c^4}{3} - \frac{2}{3}\delta a^2 c^2 (\lambda_k + \lambda_k^W \mathcal{E}) v^k \right] - \\ &\frac{4\pi K_{ac} \sqrt{2}(m^*)^{3(/2}}{\hbar^3} \sqrt{\mathcal{E}(1+\alpha\mathcal{E})}(1+2\alpha\mathcal{E}) \left(a^4 + \frac{c^4}{3} \right) f_{ME}. \end{aligned}$$

Since the scattering is elastic one gets

$$C_W = 0.$$

Concerning the production terms of crystal momentum and energy flux, we can write

$$\begin{aligned} C^i &= c_{11}^{(ac)}(W)V_i + c_{12}^{(ac)}(W)S_i, & (3.68)\\ C_W^i &= c_{21}^{(ac)}(W)V_i + c_{22}^{(ac)}(W)S_i. & (3.69)\end{aligned}$$

The production matrix

$$C^{(ac)} = \begin{pmatrix} c_{11}^{(ac)} & c_{12}^{(ac)} \\ c_{21}^{(ac)} & c_{22}^{(ac)} \end{pmatrix},$$

is given by

$$C^{(ac)} = A^{(ac)}B.$$

The matrix

$$B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

has been obtained in section 3.2, while the coefficients of $A^{(ac)}$ read

$$\begin{aligned} a_{11}^{(ac)} &= \frac{\overline{K}_{ac}}{d_0}\int_0^\infty \mathcal{E}^2\,(1+\alpha\mathcal{E})^2\,(1+2\alpha\mathcal{E})\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\mathcal{H}\,d\mathcal{E}, & (3.70)\\ a_{12}^{(ac)} &= \frac{\overline{K}_{ac}}{d_0}\int_0^\infty \mathcal{E}^3\,(1+\alpha\mathcal{E})^2\,(1+2\alpha\mathcal{E})\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\mathcal{H}\,d\mathcal{E}, & (3.71)\\ a_{21}^{(ac)} &= \frac{\overline{K}_{ac}}{m^*d_0}\int_0^\infty \mathcal{E}^3\,(1+\alpha\mathcal{E})^2\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\mathcal{H}\,d\mathcal{E}, & (3.72)\\ a_{22}^{(ac)} &= \frac{\overline{K}_{ac}}{m^*d_0}\int_0^\infty \mathcal{E}^4\,(1+\alpha\mathcal{E})^2\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\mathcal{H}\,d\mathcal{E}, & (3.73)\end{aligned}$$

where

$$\overline{K}_{ac} = \frac{8\pi\sqrt{2}(m^*)^{3/2}K_{ac}}{3\hbar^3}$$

and

$$\mathcal{H} = \left(a^4 - \frac{2}{3}a^2c^2 + \frac{c^4}{3}\right).$$

3.5.2 Non polar optical phonon scattering

For the non polar optical phonon scattering the collision term becomes

$$\mathcal{C}[f] \approx \mathcal{C}[f_{ME}] = \mathcal{C}_G[f_{ME}] - \mathcal{C}_L[f_{ME}].$$

If we set

$$K_{np} = \frac{(D_tK)^2}{8\pi^2\rho\omega_{np}},$$

the gain part can be written as

$$\mathcal{C}_G[f_{ME}] = \frac{4\pi\sqrt{2}(m^*)^{3/2}K_{np}}{\hbar^3}\exp\left(-\frac{\lambda^{(0)}}{k_B}\right)\left(n_B+\frac{1}{2}\pm\frac{1}{2}\right)\mathcal{N}_\pm \exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L}\right)$$
$$\exp\left[-\lambda^{W(0)(\mathcal{E}\pm\hbar\omega_{np})}\right]$$
$$\left\{\left[(aa_\pm)^2+\frac{1}{3}(cc_\pm)^2\right]-\frac{2}{3}\delta aa_\pm cc_\pm\left[|\lambda\cdot\mathbf{v}_\pm|+(\mathcal{E}\pm\hbar\omega_{np})|\lambda^W\cdot\mathbf{v}_\pm|\right]\right\}, \qquad (3.74)$$

where

$$\mathcal{N}_\pm = \sqrt{(\mathcal{E}\pm\hbar\omega_{np})[1+\alpha(\mathcal{E}\pm\hbar\omega_{np})]}[1+2\alpha(\mathcal{E}\pm\hbar\omega_{np})],$$

and $v_\pm$ is the velocity evaluated for energy $\mathcal{E}\pm\hbar\omega_{np}$. The loss term can be expressed as

$$\mathcal{C}_L[f_{ME}] = \frac{4\pi\sqrt{2}(m^*)^{3/2}K_{np}}{\hbar^3}\left(n_B+\frac{1}{2}\mp\frac{1}{2}\right)\mathcal{N}_\pm\mathcal{F}_\pm f_{ME},$$

where

$$\mathcal{F}_\pm = (aa_\pm)^2+\frac{1}{3}(cc_\pm)^2.$$

At variance with the case of acoustic phonon scattering, energy is not conserved because non polar optical phonon scattering is not elastic. One finds up to the first order in δ

$$C_W = \frac{3}{2}\frac{\overline{K}_{np}}{d_0}\left(n_B+\frac{1}{2}\mp\frac{1}{2}\right)\left[\exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L}\mp\lambda^{W(0)}\hbar\omega_{np}\right)-1\right]\eta^\pm. \qquad (3.75)$$

with

$$\eta^\pm = \int_{\hbar\omega H(1\pm1)}^{\infty}\mathcal{E}\mathcal{N}_\pm\mathcal{F}_\pm\sqrt{\mathcal{E}(1+\alpha\mathcal{E})}(1+2\alpha\mathcal{E})\exp\left(-\lambda^{W(0)\mathcal{E}}\right)d\,\mathcal{E}$$

and

$$\overline{K}_{np} = \frac{8\pi\sqrt{2}(m^*)^{3/2}K_{np}}{3\hbar^3}.$$

H is the Heviside function.

The quadratic correction is given by

$$4\pi K_{np}\left(n_B+\frac{1}{2}\pm\frac{1}{2}\right)\int_0^\infty \mathcal{E}\mathcal{N}_\pm\exp\left(-\lambda^{W(0)\mathcal{E}}\right)\left\{\exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L}\mp\lambda^{W(0)}\hbar\omega_{np}\right)\times\right.$$
$$\left[-\frac{\lambda^{(2)}}{k_B}-\lambda^{W(2)}\mathcal{E}+\frac{1}{6}v_\pm^2(\underline{\lambda}+\underline{\lambda}^W(\mathcal{E}\pm\hbar\omega_{np}))^2\right]$$
$$\left.-\mathcal{F}_\pm\left[-\frac{\lambda^{(2)}}{k_B}-\lambda^{W(2)}\mathcal{E}+\frac{1}{6}v_\pm^2(\underline{\lambda}+\underline{\lambda}^W\mathcal{E})^2\right]\right\}d\mathcal{E}. \qquad (3.76)$$

At thermal equilibrium $\lambda^{W(0)} = 1/k_B T_L$ and the zeroth order term for energy production vanishes, while the second order correction can be neglected because for low energy the parabolic band approximation is valid and in such a case $\mathcal{F}_\pm \approx 1$.

The production terms of crystal momentum and energy flux have again the form

$$C^i = c_{11}^{(np)}(W)V_i + c_{12}^{(np)}(W)S_i, \qquad (3.77)$$
$$C_W^i = c_{21}^{(np)}(W)V_i + c_{22}^{(np)}(W)S_i. \qquad (3.78)$$

The production matrix

$$C^{(np)} = \begin{pmatrix} c_{11}^{(np)} & c_{12}^{(np)} \\ c_{21}^{(np)} & c_{22}^{(np)} \end{pmatrix},$$

is given by

$$C^{(np)} = A^{(np)} B$$

and the components of the matrix $A^{(np)}$ read

$$\begin{aligned} a_{11}^{np} &= \frac{\overline{K}_{np}}{d_0}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right)\left\{-\frac{2}{3}\exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L} \mp \lambda^{W(0)}\hbar\omega_{np}\right) \times \right. \\ & \int_{\hbar\omega H(1\pm 1)}^{\infty} \mathcal{E}(1+\alpha\mathcal{E})\sqrt{(\mathcal{E}\pm\hbar\omega_{np})[1+\alpha(\mathcal{E}\pm\hbar\omega_{np})]}aa_{\pm}cc_{\pm}\mathcal{N}_{\pm}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E} \\ & \left. + \int_{\hbar\omega H(1\pm 1)}^{\infty} \mathcal{F}_{\pm}\mathcal{N}_{\pm}\mathcal{E}^{3/2}(1+\alpha\mathcal{E})^{3/2}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E}\right\}, \end{aligned} \tag{3.79}$$

$$\begin{aligned} a_{12}^{np} &= \frac{\overline{K}_{np}}{d_0}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right)\left\{-\frac{2}{3}\exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L} \mp \lambda^{W(0)}\hbar\omega_{np}\right) \times \right. \\ & \int_{\hbar\omega H(1\pm 1)}^{\infty} (\mathcal{E}\pm\hbar\omega_{np})\mathcal{E}(1+\alpha\mathcal{E})\sqrt{(\mathcal{E}\pm\hbar\omega_{np})[1+\alpha(\mathcal{E}\pm\hbar\omega_{np})]}aa_{\pm}cc_{\pm}\mathcal{N}_{\pm}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E} \\ & \left. + \int_{\hbar\omega H(1\pm 1)}^{\infty} \mathcal{F}_{\pm}\mathcal{N}_{\pm}\mathcal{E}^{5/2}(1+\alpha\mathcal{E})^{3/2}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E}\right\}, \end{aligned} \tag{3.80}$$

$$\begin{aligned} a_{21}^{np} &= \frac{\overline{K}_{np}}{m^* d_0}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right)\left\{-\frac{2}{3}\exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L} \mp \lambda^{W(0)}\hbar\omega_{np}\right) \times \right. \\ & \int_{\hbar\omega H(1\pm 1)}^{\infty} \frac{\mathcal{E}^2(1+\alpha\mathcal{E})}{1+2\alpha(\mathcal{E}\pm\hbar\omega_{np}}\sqrt{(\mathcal{E}\pm\hbar\omega_{np})[1+\alpha(\mathcal{E}\pm\hbar\omega_{np})]}aa_{\pm}cc_{\pm}\mathcal{N}_{\pm}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E} \\ & \left. + \int_{\hbar\omega H(1\pm 1)}^{\infty} \mathcal{F}_{\pm}\mathcal{N}_{\pm}\frac{\mathcal{E}^{5/2}(1+\alpha\mathcal{E})^{3/2}}{1+2\alpha\mathcal{E}}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E}\right\}, \end{aligned} \tag{3.81}$$

$$\begin{aligned} a_{22}^{np} &= \frac{\overline{K}_{np}}{m^* d_0}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right)\left\{-\frac{2}{3}\exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L} \mp \lambda^{W(0)}\hbar\omega_{np}\right) \times \right. \\ & \int_{\hbar\omega H(1\pm 1)}^{\infty} \frac{\mathcal{E}^2(\mathcal{E}\pm\hbar\omega_{np})(1+\alpha\mathcal{E})}{1+2\alpha(\mathcal{E}\pm\hbar\omega_{np}}\sqrt{(\mathcal{E}\pm\hbar\omega_{np})[1+\alpha(\mathcal{E}\pm\hbar\omega_{np})]}aa_{\pm}cc_{\pm}\mathcal{N}_{\pm}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E} \\ & \left. + \int_{\hbar\omega H(1\pm 1)}^{\infty} \mathcal{F}_{\pm}\mathcal{N}_{\pm}\frac{\mathcal{E}^{7/2}(1+\alpha\mathcal{E})^{3/2}}{1+2\alpha\mathcal{E}}\exp\left(-\lambda^{W(0)}\mathcal{E}\right)\, d\mathcal{E}\right\}. \end{aligned} \tag{3.82}$$

At variance with the acoustic phonon scattering, the electron in the interaction with the non polar acoustic phonon can gain a quantum of energy $\hbar\omega_{np}$ which can drive it into another optical valley.

The generalization of the previous formulas to the case of intervalley interactions is straightforward and it is recovered from the formulas (3.75) and (3.79)-(3.82) with the substitution

$$\hbar\omega_{np} \mapsto \hbar\omega_{AB} \mp \Delta_{AB},$$

where Δ_{AB} is the difference between the bottom of the A and the B valley and $\hbar\omega_{AB}$ is the exchanged energy.

3.5.3 Scattering with impurities

The scattering with the impurities is elastic

$$C_W = 0.$$

The production terms of crystal momentum and energy flux are calculated as

$$\begin{aligned} C^i &= c_{11}^{(imp)}(W)V_i + c_{12}^{(imp)}(W)S_i, && (3.83)\\ C_W^i &= c_{21}^{(imp)}(W)V_i + c_{22}^{(imp)}(W)S_i. && (3.84) \end{aligned}$$

The production matrix decomposes as

$$C^{(imp)} = A^{(imp)}B$$

and the components of the matrix $A^{(imp)}$ read

$$\begin{aligned} a_{11}^{(imp)} &= \frac{K_{imp}}{d_0}\int_0^\infty \frac{(1+\alpha\mathcal{E})^{3/2}(1+2\alpha\mathcal{E})}{\sqrt{\mathcal{E}}}\left(\log\frac{1+\gamma}{\gamma}+\frac{1}{1+\gamma}\right)\times\\ &\quad \exp\left(-\lambda^{W(0)}\mathcal{E}\right)\,d\mathcal{E}, && (3.85)\\ a_{12}^{(imp)} &= \frac{K_{imp}}{d_0}\int_0^\infty (1+\alpha\mathcal{E})^{3/2}(1+2\alpha\mathcal{E})\sqrt{\mathcal{E}}\left(\log\frac{1+\gamma}{\gamma}+\frac{1}{1+\gamma}\right)\times\\ &\quad \exp\left(-\lambda^{W(0)}\mathcal{E}\right)\,d\mathcal{E}, && (3.86)\\ a_{21}^{(imp)} &= \frac{K_{imp}}{m^*d_0}\int_0^\infty \sqrt{\mathcal{E}}(1+\alpha\mathcal{E})^{3/2}\left(\log\frac{1+\gamma}{\gamma}+\frac{1}{1+\gamma}\right)\times\\ &\quad \exp\left(-\lambda^{W(0)}\mathcal{E}\right)\,d\mathcal{E}, && (3.87)\\ a_{22}^{(imp)} &= \frac{K_{imp}}{m^*d_0}\int_0^\infty \mathcal{E}^{3/2}(1+\alpha\mathcal{E})^{3/2}\left(\log\frac{1+\gamma}{\gamma}+\frac{1}{1+\gamma}\right)\times\\ &\quad \exp\left(-\lambda^{W(0)}\mathcal{E}\right)\,d\mathcal{E}, && (3.88) \end{aligned}$$

where

$$K_{imp} = \frac{\pi e^4 Z^2 N_{imp}}{3\mathcal{E}_0^2}.$$

3.5.4 Parabolic band limit

The parabolic band limit of the closures for the production terms is recovered from the results obtained in the case of the Kane dispersion relation as $\mathcal{E} \mapsto 0$.

For the acustic phonon scattering one finds

$$\begin{aligned} a_{11}^{(ac)} &= \frac{32}{3}\frac{\sqrt{2\pi}K_{ac}}{\hbar^3}(m^*)^{3/2}\left(\frac{2}{3}W\right)^{3/2}, && (3.89)\\ a_{12}^{(ac)} &= 32\frac{\sqrt{2\pi}K_{ac}}{\hbar^3}(m^*)^{3/2}\left(\frac{2}{3}W\right)^{5/2}, && (3.90)\\ a_{21}^{(ac)} &= \frac{a_{12}^{(ac)}}{m^*}, && (3.91)\\ a_{22}^{(ac)} &= 128\frac{\sqrt{2\pi m^*}K_{ac}}{\hbar^3}\left(\frac{2}{3}W\right)^{7/2}. && (3.92) \end{aligned}$$

Concerning the non polar optical phonon scattering it is also possible to get an analytical expression for the production in terms of the Bessel functons of second kind

$$K_\nu = \frac{\sqrt{\pi}(z/2)^\nu}{\Gamma\left(\nu+\frac{1}{2}\right)} \int_0^\infty \exp(-z\cosh t)\sinh^{2\nu} t\, dt, \quad z,\nu > 0, \tag{3.93}$$

with Γ the Gamma function.

After some algebra one obtains the following expressions

$$\begin{aligned}
C_W &= \left(\frac{2}{3}W\right)^{-1/2} \frac{2\sqrt{2\pi}(m^*)^{3/2}(\hbar\omega_{np})^2}{\hbar^3} K_{np}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right) e^{\pm\zeta} \times \\
&\quad \left[\exp\left(\pm\frac{\hbar\omega_{np}}{k_B T_L} \mp 2\zeta\right) - 1\right] \left[K_2(\zeta) \mp K_1(\zeta)\right], && (3.94)\\
a_{11}^{(np)} &= \frac{4}{3}\left(\frac{2}{3}W\right)^{-1/2} \frac{\sqrt{2\pi}(m^*)^{3/2}(\hbar\omega_{np})^2}{\hbar^3} K_{np}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right) e^{\pm\zeta} \times \\
&\quad \left[K_2(\zeta) \mp K_1(\zeta)\right], && (3.95)\\
a_{12}^{(np)} &= \frac{4}{3}\sqrt{\frac{2}{3}W} \frac{\sqrt{2\pi}(m^*)^{3/2}(\hbar\omega_{np})^2}{\hbar^3} K_{np}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right) e^{\pm\zeta} \times \\
&\quad \left\{3K_2(\zeta) + \zeta\left[K_1(\zeta) \mp K_2(\zeta)\right]\right\}, && (3.96)\\
a_{21}^{(np)} &= \frac{a_{12}^{(np)}}{m^*}, && (3.97)\\
a_{22}^{(np)} &= \frac{4}{3}\left(\frac{2}{3}W\right)^{3/2} \frac{\sqrt{2\pi m^*}(\hbar\omega_{np})^2}{\hbar^3} K_{np}\left(n_B + \frac{1}{2} \mp \frac{1}{2}\right) e^{\pm\zeta} \times \\
&\quad \left[K_2(\zeta)\left(12 \pm 3\zeta + \zeta^2\right) + K_1(\zeta)\left(\zeta \pm (2\zeta)^2\right)\right], && (3.98)
\end{aligned}$$

with

$$\zeta = \frac{3\hbar\omega_{np}}{4W}.$$

Unfortunately analytical expressions are not available for the scattering with impurities. In this case one has to resort to a numerical evaluation of the coefficient of the production matrix.

3.6 Comparison with previous models

Other hydrodynamical models for carrier transport in semiconductors have been proposed in the case of Kane's dispersion relation. In particular Tang et al. [50] proposed a model by considering the same moment equations (2.3)-(2.6) in the stationary case. The constitutive equations have been derived from the analysis of the Monte Carlo (MC) simulations of silicon devices in the stationary regime by considering the Kane dispersion relation for the energy bands.

In [50] the authors have simulated three n^+-n-n^+ silcon diodes with different doping profile and applied voltage of 2 Volt.

If we plots the values of H_i, U_{ij} and R_{ij} obtained from the MC simulations as function of W, or V_i or S_i, we do not get in general a single-valued function but a hysteresis loop appears. The appropriate forms of the constitutive functions are then obtained by minimizing the residue of the hysteresis loop in order to get a single-valued function.

The tensor U_{ij} has been modelled as

$$U_{ij} = U\,\delta_{ij} + m^* V_i V_j + 2\alpha m^* V_i S_j \tag{3.99}$$

and the analysis of the MC data shows that the isotropic part of U^{ij}, U, can be considered with good approximation a single-valued function of the energy W

$$U = \frac{2}{3} W + g(W) \sum_{k=0}^{4} u_k W^k.$$

where

$$u_0 = -1.01 \times 10^{-4}, \quad u_1 = 0.004, \quad u_2 = -0.415,$$
$$u_3 = 0.399, \quad u_4 = -0.175$$

and

$$g(W) = \begin{cases} 0 & \text{if } W \leq W_0 = 3/2 k_B T_0 \\ 1 - \exp\left[-\left(\frac{W}{W_0} - 1 \right) \right], & \text{otherwise} \end{cases}$$

In fig. 2 we compare the values of U of the fitting of the MC data given in [50] with the values of $U^{(0)}$ obtained with the maximum entropy principle in the case of parabolic band approximation and in the case of the Kane dispersion relation.

The agreement between the fitting of the MC data and the results given by the ME is highly satisfactory. Moreover it is clear that the higher the energy the less accurate the parabolic band approximation becomes.

Concerning the anisotropic part, we observe that although the definition implies that U_{ij} must be symmetric for Kane's dispersion relation, the expression proposed in [50] is not symmetric. Moreover in the approach of Tang et al. [50] there is the *a priori* assumption that the coefficients of the terms $S_i V_j$ is zero and the isotropic part does not contain second order corrections.

The tensor R_{ij} was modelled in [50] as

$$R_{ij} = R\,\delta_{ij} + (S_i - 3.8 W V_i)(V_j + 2\alpha m^* S_j)$$

and for R a fitting formula similar to that for U was used

$$R = \frac{10}{9} W^2 + g(W) \sum_{k=0}^{4} r_k W^k, \tag{3.100}$$

where

$$r_0 = -5.3 \times 10^{-3}, \quad r_1 = 0.129, \quad r_2 = -0.259,$$
$$r_3 = -0.539, \quad r_4 = 0.326.$$

Again there is the problem that the last expression for R_{ij} is not symmetric and the second order terms in the isotropic part are missing. At variance with U the comparison between R and $R^{(0)}$ (fig. 3) shows that the agreement, although acceptable, does not present the same accuracy. The qualitative behaviour is good in the case of the Kane dispersion relation, but there is a certain quantitative discrepancy. Instead the

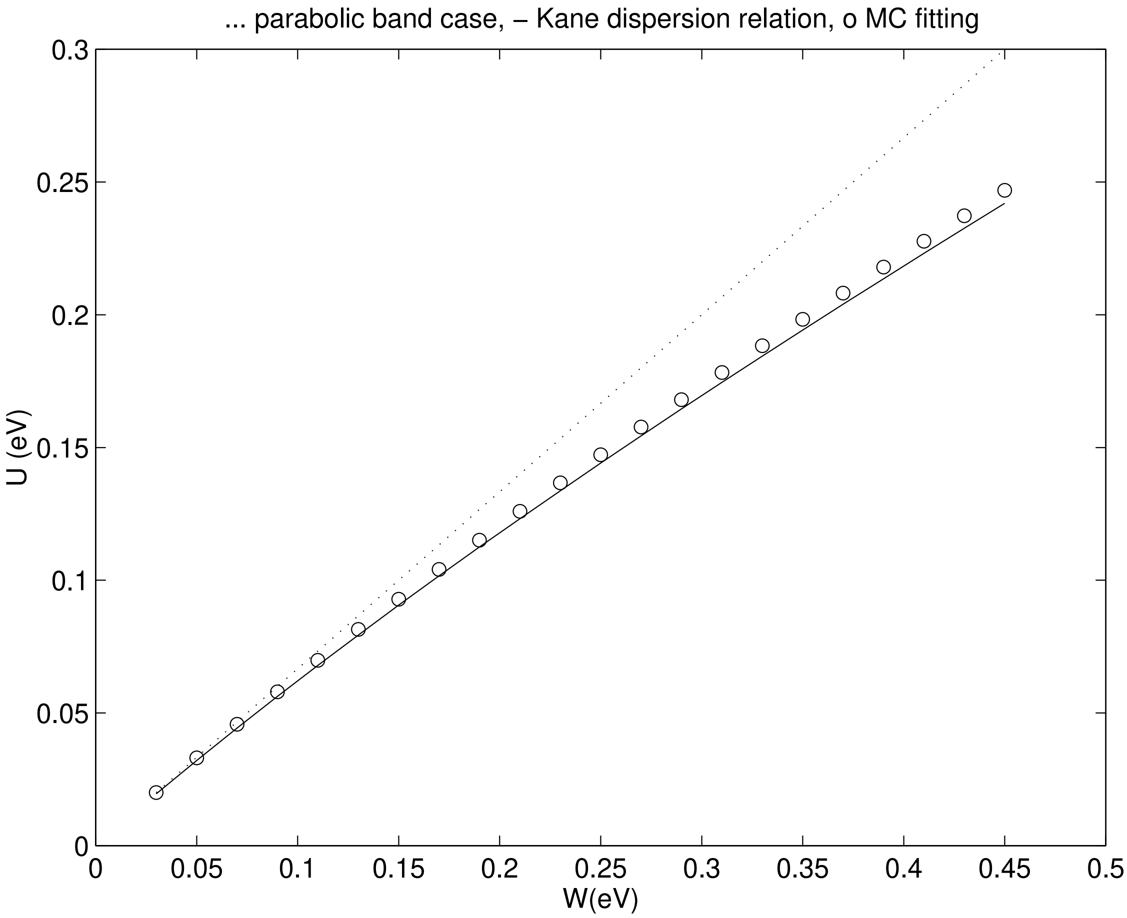

Figure 3.2: $U^{(0)}$ obtained with the maximum entropy principle in the parabolic band case (dotted line), with the Kane dispersion relation (continuous lines) and the MC simulation [50] vs. the energy W

parabolic approximation presents a little different profile, but the agreement is better. This looks as a mere coincidence.

We note that MC closure relations have been determined from one dimensional results and therefore the inferred 3D constitutive equations could not be fully appropriate. Therefore a comparison between the expressions for U_{ij} and R_{ij} proposed in [50] and those obtained by using the ME principle cannot be performed by a direct comparison of the coefficients δ_k and γ_k. Probably only an analysis of the results of numerical simulations of electron devices in one and two dimensions can asses the validity of the models.

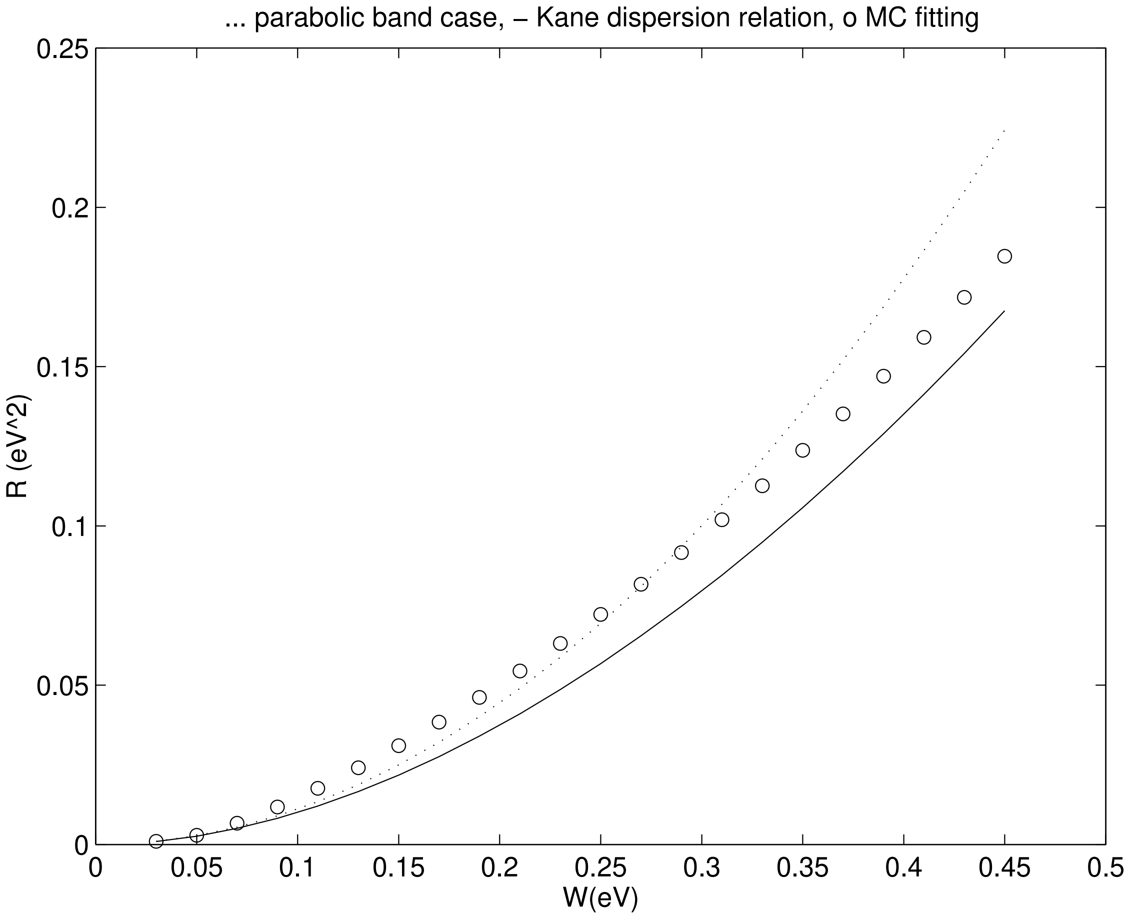

Figure 3.3: $R^{(0)}$ obtained with the maximum entropy principle in the parabolic band case (dotted line), with the Kane dispersion relation (continuous lines) and the MC simulation [50] vs. the energy W

Chapter 4

Numerical methods for hydrodynamical models of semiconductors

The hydrodynamical model presented in the previous chapter is constituted by a hyperbolic system of balance equations coupled with the Poisson equation for the electric potential. The modelling of a realistic device introduces strong gradients in the initial electron density at the junctions. The subsequent evolution of the system gives rise to nonlinear waves, before reaching a steady state. Then, the methods employed for the numerical solution of the governing equations must have certain qualities to ensure that the *correct* weak solution is captured at the correct point in space and time. Moreover the numerical schemes should not introduce spurious features, like unphysical oscillations in the vicinity of strong gradients.

The computational strategies followed to get numerical solutions of such a set of equations, solve at each time level the Poisson equation and then the hyperbolic part by considering during the time step the electric field as a given external field. The main computational efforts are due to the hyperbolic part of the set of equations representing the model because for the Poisson equation standard schemes can be used.

Numerical integration of quasi-linear hyperbolic systems represents by itself an active research area (see [51, 81]). It is well known that the solutions of quasi-linear systems suffer loss of regularity and formation of shocks. In the last decade accurate shock capturing schemes have been developed, such as ENO schemes [44]. However, high order upwind-based shock capturing schemes require the explicit knowledge of the characteristic speeds of the hyperbolic system. In the case of the model presented in the previous section, it is not possible to obtain analytical expressions for the eigenvalues and eigenvectors of the system, and it is therefore not practical to use upwind-based ENO schemes.

It is almost mandatory to resort to schemes that do not require an explicit analytical expression of the solution of the Riemann problem. Here we present two numerical schemes enjoying such a property, well suited for the hydrodynamical models presented in the previous chapter.

The first scheme was proposed by Nessyahu and Tadmor (NT) [65]. It uses Lax-Friedrichs scheme as building block, corrected by MUSCL-type interpolation so that it becomes second order accurate in smooth regions. NT scheme has been developed for homogeneous systems. An extension of the method to systems that contain production terms has been formulated in [54] and applied to semiconductors in [71, 14, 15].

The second method uses the the FLIC (flux limiter centred) method and the SLIC (slope limiter centred) [81] for the homogeneous part of the evolution equations, while various conventional methods are employed for the solution of the forcing terms. Applications to the semiconductor equations have been reported in [6, 7] .

In the following sections we briefly present the schemes for one dimensional problems. Examples of numerical results are reported in the last section. The new features of these approaches is that they use methods suitable for hyperbolic systems with source terms and in this particular case study the solution is evolved as an unsteady problem marched to steady state, preserving time as well as space accuracy. Therefore these codes could be used to investigate the transient behaviour of the system from an academic and an engineering point of view.

Other numerical simulations have been performed by using a kinetic scheme and compared with those obtained with the NT scheme in [1]. However these latter results will not be reported here.

4.1 The Nessyahu-Tadmor scheme and its extension to non homogenous hyperbolic systems

Let us consider a system of the form

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = G(U, E), \tag{4.1}$$

with $U \in \mathbf{R}^m$ and $F : \mathbf{R}^m \to \mathbf{R}^m$.

The basic idea is to integrate first the relaxation system (relaxation step),

$$\frac{dU}{dt} = G(U, E), \tag{4.2}$$

and then the homogeneous system (convection step), using the output of the previous step as initial condition

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0. \tag{4.3}$$

For the relaxation step an unconditionally stable second order scheme can be obtained by analytical integration of the linearized relaxation equation, where linearization is obtained by *freezing* the coefficients and the electric field at time t_n (see [71, 14, 15] for details). The electric potential is computed by solving with standard procedure the tridiagonal system

$$\epsilon(\phi_{j+1} - 2\phi_j + \phi_{j-1}) = -(\Delta x)^2 \left(N_D - N_A - n_i^n\right)$$

and the electric field is obtained by the electric potential using finite differences.

NT scheme with a staggered grid is used for the convection step.

Each convection step has the form of predictor-corrector scheme:

$$U_{j+1/2}^{n+1/2} = \frac{1}{2}(U_j^{n+1} + U_{j+1}^n) + \frac{1}{8}(U_j' - U_{j+1}') - \lambda\left[F(U_{j+1}^{n+1/2}) - F(U_j^{n+1/2})\right], \tag{4.4}$$

$$U_j^{n+1/2} = U_j^n - \frac{\lambda}{2}F_j'. \tag{4.5}$$

where $\lambda = \Delta t/\Delta x$. The time step Δt must satisfy a stability condition

$$\lambda \cdot \max \rho(A(U(x,t)) < \frac{1}{2} \tag{4.6}$$

where $\rho(A(U(x,t))$ is the spectral radius of the Jacobian matrix,

$$A = \frac{\partial F}{\partial U}.$$

This condition will ensure that the generalized Riemann problems with piecewise smooth data at time t_n will not interfere during the time step Δt.

The values of $U_j'/\Delta x$ and $F_j'/\Delta x$ are a first order approximation of the space derivatives of the field and of the flux, computed from cell averages by using Uniform Non Oscillatory reconstruction (UNO, see [44]),

$$U_j' = \mathrm{MM}\left(d_{j-\frac{1}{2}}U + \frac{1}{2}\mathrm{MM}(D_{j-1}, D_j), d_{j+\frac{1}{2}}U - \frac{1}{2}\mathrm{MM}(D_j, D_{j+1})\right) \tag{4.7}$$

where

$$D_j = U_{j+1} - 2U_j + U_{j-1},$$

$$d_{j+1/2} = U_{j+1} - U_j.$$

and

$$\mathrm{MM}(x,y) = \begin{cases} \mathrm{sign}(x) \cdot \min(|x|,|y|) & \text{if } \mathrm{sign}(x) = \mathrm{sign}(y) \\ 0 & \text{otherwise.} \end{cases}$$

A similar procedure is used for computing F_j'.

In order to couple the convection step with the relaxation step, it is convenient to make two convection steps of step size $\Delta t/2$, so that the solution is computed on the same grid. A complete convection step of step size Δt is obtained as a sequence of two intermediate steps of step size $\Delta t/2$.

The splitting technique presented above is first order in time. It is possible to obtain second order accuracy in time by combining the two steps according to the following scheme [26, 54]. Given the field at time t_n, (U^n, E^n), the field at time $t_{n+1/2}$ is obtained by

$$\begin{aligned} U_1 &= U^n - R(U_1, E^n, \Delta t), \\ U_2 &= \frac{3}{2}U^n - \frac{1}{2}U_1, \\ U_3 &= U_2 - R(U_3, E^n, \Delta t), \\ U_4 &= \mathcal{C}_{\Delta t} U_3, \\ E^{n+1} &= \mathcal{P}(U_4), \\ U^{n+1} &= U_4 - R(U^{n+1}, E^{n+1}, \Delta t/2) \end{aligned}$$

where R represents the discrete operator corresponding to the relaxation step, $\mathcal{C}_{\Delta t}$ is the discrete operator corresponding to NT scheme, and $\mathcal{P}(U)$ gives the solution to Poisson's equation.

4.2 FLIC-SLIC Methods

In this section we discuss the application of a family of schemes known as *high resolution* (see for example the textbooks [51, 81]).

A great number of upwind, high resolution schemes use the solution of the Riemann problem to evaluate the intercell fluxes. However, when the solution of the Riemann problem is not known, it is possible to construct *centred* schemes which do not compromise the qualities of the high resolution family. This scheme has a low computational cost, is easy to implement and it can be used for multi-dimensional discretisations on domains of arbitrary geometry.

The homogeneous part of the model is solved using the FLIC scheme, which belongs to the high resolution schemes, while various conventional methods are employed for the solution of the forcing terms.

4.3 Brief exposition of FLIC schemes

A one-dimensional system of the form:

$$U_t + F(U)_x = 0 \tag{4.8}$$

where U and $F(U)$ are the vectors of the conserved variables and the fluxes respectively could be discretized using the formula [81]

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x}[F_{i-1/2} - F_{i+1/2}] \tag{4.9}$$

where U_i^{n+1}, and U_i^n are the solutions at the next and current time-levels, $n+1$ and n, respectively. $F_{i-1/2}$, $F_{i+1/2}$ are the numerical fluxes[1] at the interfaces of the computational cells of the discretised space. For a given cell width and timestep, the values of the numerical fluxes need to be evaluated in formula (4.9) in order to compute the conserved variables at the next time level.

Centred schemes are based on the TVD flux concept. Recall that the latter is:

$$F_{i+1/2}^{TVD} = F_{i+1/2}^{LO} + \phi_{i+1/2}\left[F_{i+1/2}^{HI} - F_{i+1/2}^{LO}\right]. \tag{4.10}$$

In [81] it has been proposed to construct a Flux Limiter Centred (FLIC) scheme, where the low and the high order fluxes are given by the FORCE (First Order Centred) and the Richtmyer ones respectively:

$$F_{i+1/2}^{LO} \equiv F^{force}, \quad F_{i+1/2}^{HI} \equiv F^{Ri}$$

See the textbook by Toro for the appropriate form of popular flux limiters which can be used within this context.

The flux of the FORCE scheme [81] is a combination of the Lax-Friedrichs and the Richtmyer ones. In particular, considering an equation of the form

$$U_t + F(U)_x = 0$$

[1] The numerical fluxes are approximations to the physical fluxes.

the flux at the interface of two states U_L, U_R is:

$$F_{i+1/2}^{force} \equiv F_{i+1/2}^{force}(U_L, U_R) = 0.5\left[F_{i+1/2}^{LF}(U_L, U_R) + F_{i+1/2}^{Ri}(U_L, U_R)\right] \tag{4.11}$$

In the above expressions, the first-order Lax-Friedrichs flux, F^{LF} is given by:

$$F_{i+1/2}^{LF} \equiv F_{i+1/2}^{LF}(U_L, U_R) = 0.5\,[F(U_L) + F(U_R)] + 0.5\frac{\Delta x}{\Delta t}[U_L + U_R]$$

The second-order Richtmyer scheme (which computes a numerical flux by first defining an intermediate state) is:

$$U_{i+1/2}^{Ri} \equiv U_{i+1/2}^{Ri}(U_L, U_R) = 0.5(U_L + U_R) + 0.5\frac{\Delta t}{\Delta x}[F(U_L) - F(U_R)]$$

and then setting $F^{Ri} = F(U_{i+1/2}^{Ri})$.

Not all of the upwind information is lost when we construct schemes for nonlinear laws of this form, because the timestep is still governed by the CFL condition.

The adopted scheme is based on finite differences and solved with a Strang splitting technique. The Poisson equation is solved with the same technique as in the previous section. The evolution equations are:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = S(U, E), \tag{4.12}$$

and they are coupled with the Poisson equation.

The splitting scheme is based on the solution of the two steps:

convection step:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial U} = 0,$$

relaxation step:

$$\frac{\partial U}{\partial t} = S(U).$$

Each convection step is solved by FLIC (**F**lux **L**imiter **C**entred), scheme. The relaxation step takes care of the relaxation and drift effects and is solved by using a Runge Kutta second order explicit scheme.

Calling with R the relaxation step operator, with C the convection step operator and with P the Poisson operator, the Strang splitting is:

$$U^{n+1} = R(\triangle t/2)P(\triangle t/2)C(\triangle t)P(\triangle t)R(\triangle t/2)U^n$$

4.4 Numerical results

In [14, 15] the NT method has been applied to the following hydrodynamical model for carrier transport in semiconductors in the parabolic band approximation.

The equations are of the form

$$U_t + F(U)_x = S(U)$$

where the vectors $U, F(U)$ and $S(U)$ are:

$$U = \left[\begin{array}{l} n \\ nv \\ nv^2 + 3p/m^* \\ \frac{2}{3}nv^2 + \sigma/m^* \\ nv^3 + 5vp/m^* + 2\sigma v/m^* + 2q/m^* \end{array} \right], \tag{4.13}$$

$$F(U) = \left[\begin{array}{l} nv \\ nv^2 + p/m^* + \sigma/m^* \\ nv^3 + 5vp/m^* + 2\sigma v/m^* + 2q/m^* \\ \frac{2}{3}nv^3 + \frac{4}{3}vp/m^* + \frac{7}{3}v\sigma/m^* + \frac{8}{15}q/m^* \\ nv^4 + 5p^2/n(m^*)^2 + 7\sigma p/n(m^*)^2 + \frac{32}{5}qv/m^* + \\ \qquad v^2(8p/m^* + 5\sigma/m^*) + \frac{148}{25}q^2/m^*p \end{array} \right] \tag{4.14}$$

$$S(U) = \left[\begin{array}{l} 0 \\ -nv/\tau_p - neE/m^* \\ -2(W - W_0)/m^*\tau_W - 2nevE/m^* \\ -1/m^*\tau_\sigma(nv^2 + \sigma/m^*) - 4nevE/3/m^* \\ 1/\tau_q(nv^3 + 5vp/m^* + 2\sigma v/m^* + 2q/m^*) \\ \qquad -eE/m^*(3nv^2 + 5p/m^* + 2\sigma/m^*) \end{array} \right] \tag{4.15}$$

Here n is the electron density, v is the electron velocity, p is the elctron fluid pressure, m^* is the effective electron mass (taken to be 0.32 me), σ is the anisotropic stress, q is the heat flux, τ_p is the relaxation time for momentum, τ_w is the relaxation time for energy, τ_σ for anisotropic stresses, τ_q is the relaxation time for the energy flux, e is the absolute value of the electron charge, E is the electric field, W is the energy density, $W = (1/2)m^*v^2 + (3/2)$ and W_0 is the thermal equilibrium energy density.

In the application done by [14, 15] the relaxation times are obtained from fitting to MC simulations by using the following representation

$$\begin{aligned} \tau_p^{-1} &= c_1 + c_2\frac{S}{J} + c_3\frac{S^2}{J^2}, \\ \tau_q^{-1} &= \tilde{c}_1 + \tilde{c}_2\frac{S}{J} + \tilde{c}_3\frac{S^2}{J^2}, \end{aligned}$$

while for the energy relaxation time we use $\tau_w = 0.47$ ps. The values of the constants c_i and $\tilde{c}_i$ are the following

$$\begin{aligned} c_1 &= 0.32 \quad \mathrm{ps}^{-1}, \\ c_2 &= 77.586 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-1}, \\ c_3 &= -80.092 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-2}, \\ \tilde{c}_1 &= 0.458 \quad \mathrm{ps}^{-1}, \\ \tilde{c}_2 &= 91.138 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-1}, \\ \tilde{c}_3 &= -87.866 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-2}. \end{aligned}$$

In [6, 7] the FLIC method has b,een applied to the above hydrodynamical equations [14, 15]. Relaxation times τ_W, τ_p τ_q, respectively of energy, momentum, and energy flux, have been obtained by a fitting of the results of Monte Carlo simulations [64]. They can be expressed as function of the total energy per electron, by the following formulas

$$\tau_A = a + b(\overline{\mathcal{E}} - 1) + c\exp(-d(\overline{\mathcal{E}} - 1)),$$

where $\tau_A = \tau_p, \tau_w, \tau_q$, with

$$\overline{\mathcal{E}} = \frac{\text{energy per electron in eV}}{0.025\text{eV}}$$

Coefficients a, b, c, d are reported in the following table.

Table 4.1: Coefficients for the fitting of relaxation times

	τ_p	τ_W	τ_q
a	0.0681	0.1731	0.0471
b	-0.0023	0.0313	-0.0007
c	0.2051	0.2382	0.1330
d	0.9547	0.5167	0.6911

Both approaches consider as test problem a ballistic diode $n^+ - n - n^+$, which models a MOSFET channel. The diode is made of silicon, and the bulk temperature is supposed to be 300°K. The n^+ regions are $0.1\mu m$ long. The channel length we consider is 0.4 mu and the doping profile is $N_D^+ = 5 \cdot 10^{17} cm^{-3}$ and $N_D = 2 \cdot 10^{15} cm^{-3}$

For the electron effective mass in the approximation of parabolic band we use $m^* = 0.32\ m_e$ when m_e is the electron mass [82]. Silicon dielectric constant is given by $\epsilon = \epsilon_r \epsilon_0$, where ϵ_r =11.7 is the relative dielectric constant and $\epsilon_0 = 8.85 \times 10^{-18} C/V\mu m$ is the dielectric constant of vacuum.

The initial electron temperature is the lattice temperature $T_0 = 300$°K and the charges are at rest. A bias voltage of 1 Volt is applied, and this determines a charge flux in the semiconductor.

The initial conditions for the system are;

$$n(x,0) = n_0(x), \quad T(x,0) = 300°\text{K}, \quad v(x,0) = 0, \quad q(x,0) = 0, \quad \sigma(x,0) = 0.$$

Regarding the boundary conditions, in principle the number of independent conditions on each boundary should be equal to the number of characteristics entering the domain. However, in the highly doped regions one is close to thermodynamic equilibrium, therefore in that part of the device the nonlinear effects are negligible and the results should be very close to those obtained for IT model [2]. Numerical results show that in the latter the solution is flat near the boundary. In the NT approach the following boundary conditions are used.

$$n(0,t) = n(L,t) = N_D^+ \tag{4.16}$$

$$\frac{\partial}{\partial x} v(0,t) = \frac{\partial}{\partial x} v(L,t) = 0, \tag{4.17}$$

$$\frac{\partial}{\partial x}T(0,t) = \frac{\partial}{\partial x}T(L,t) = 0, \tag{4.18}$$

$$e\phi(0) = T_0 \ln\left(\frac{n(0)}{n_i}\right), \qquad e\phi(L) = T_0 \ln\left(\frac{n(L)}{n_i}\right) + eV_b, \tag{4.19}$$

where $n_i = 1.4\times 10^{10}$ cm^{-3} is electron intrinsic concentration, and V_b is the applied bias voltage.

From the continuity equation, and from conditions (4.16, 4.17, 4.18) it follows

$$\begin{aligned}
\frac{\partial J}{\partial x}(0,t) &= \frac{\partial J}{\partial x}(L,t) = 0\\
\frac{\partial W}{\partial x}(0,t) &= \frac{\partial W}{\partial x}(L,t) = 0\\
\frac{\partial S}{\partial x}(0,t) &= \frac{\partial S}{\partial x}(L,t) = 0
\end{aligned}$$

In the FLIC approach the only variant is that purely transmissive boundary conditions are used.

The doping profile is regularized according to the function

$$n_0(x) = n_0 - d_0\left(\tanh\frac{x - x_1}{s} - \tanh\frac{x - x_2}{s}\right),$$

where $s = 0.01\mu$m, $n_0 = n_0(0)$, $d_0 = n_0(1 - N_D/N_D^+)/2$, $x_1 = 0.1\mu$m, and $x_2 = x_1 + L_c$ with L_c channel length. The total length of the device is $L = L_c + 0.2\mu$m.

In both approaches there is no sign of spurious oscillations near the boundary, indicating that the boundary conditions are in fact compatible with the solution of the problem.

The stationary solution is reached within a few picoseconds (about five). In the calculactions of [14, 15] the number of grid points is 120 and s $=0.01$ μ. In the calculations of [6] the number of grid points is 600 and s $= 0.001$ μ. The numerical results found for the stationary case

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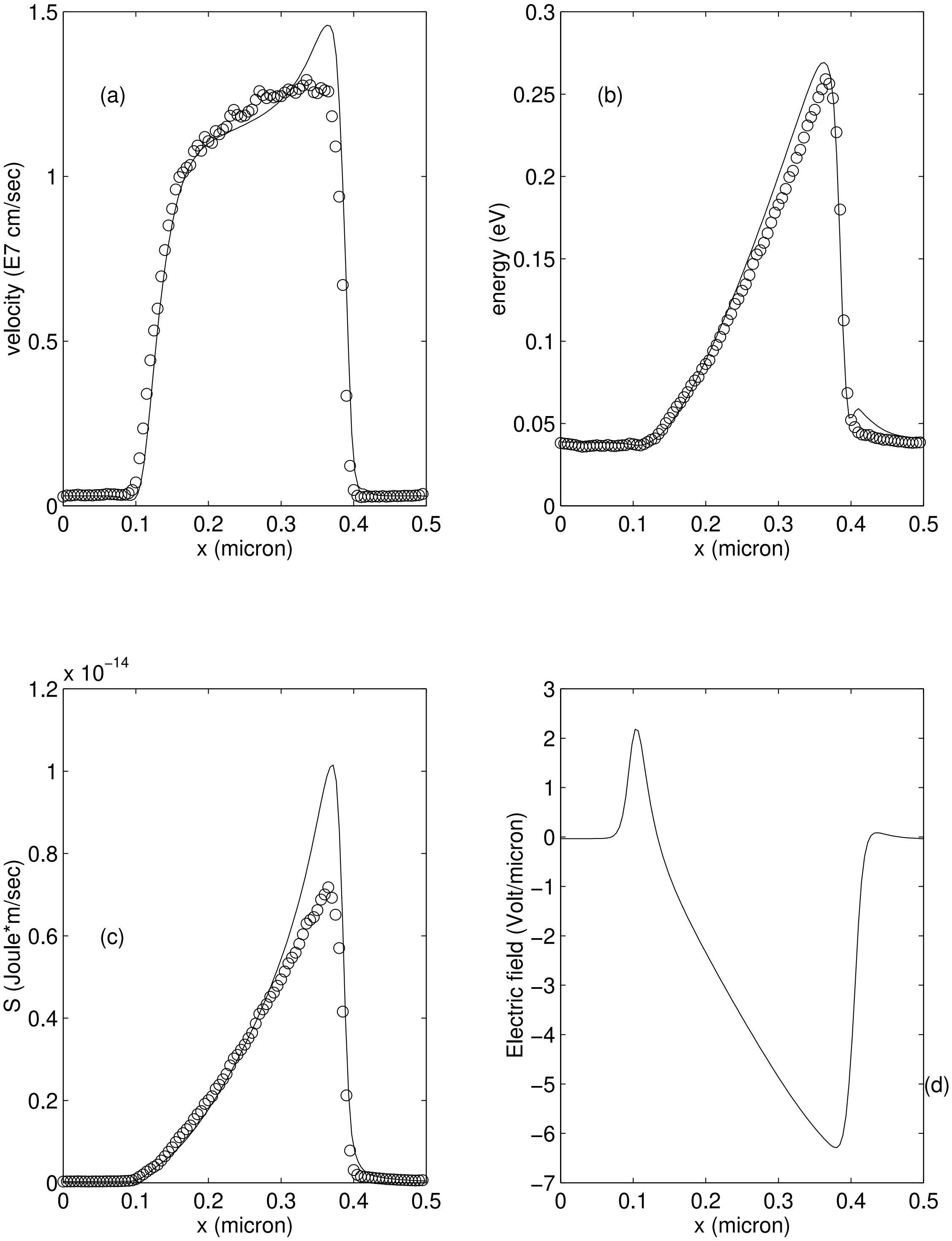

Figure 4.1: Numerical results obtained with the modified Tadmor scheme in the case of n region of length 0.3μm with 120 grid points. For completeness also the results obtained by Monte Carlo simulations are reported (circles).

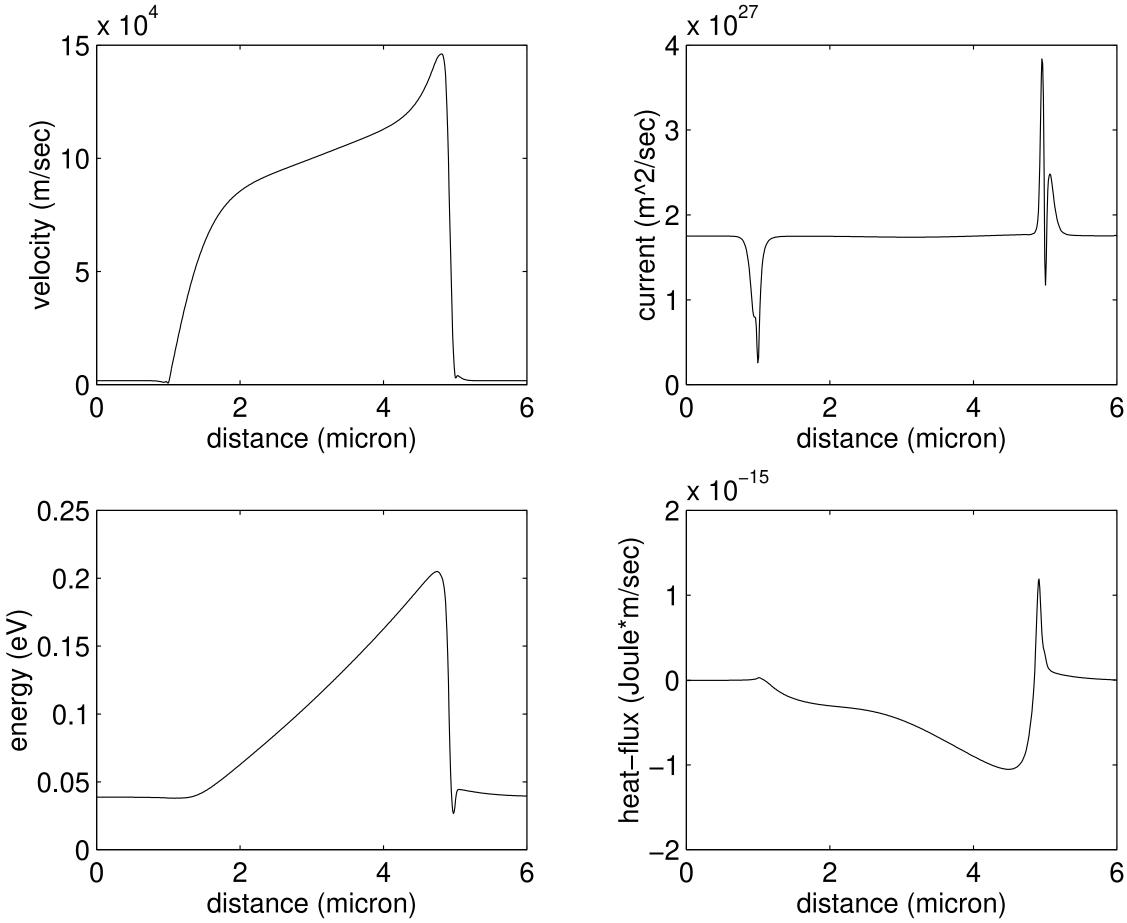

Figure 4.2: Numerical results obtained with the SLIC method in the case of n region of length 0.4 μm with 600 grid points.

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