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OVERVIEWS AND TUTORIALS

Hydrodynamical Modeling of Charge Carrier Transport in Semiconductors *

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Abstract. 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 must be 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. One of the earliest hydrodynamical models currently used in applications was originally put forward by Blotekjaer [1] and subsequently investigated by Baccarani and Wordeman [2] and by other authors [3]. Eventually other models have also been investigated, some including also non-parabolic effects [4–6, 8–20]. Most of the 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). 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 [21, 22]). The considerations and the results reported in the paper are exclusively concerned with silicon.

Sommario. L'estrema miniaturizzazione dei moderni dispositivi elettronici richiede una accurata modellizzazione del trasporto di energia nei semiconduttori al fine di descrivere effetti di alti campi quali elettroni caldi, ionizzazione da impatto e generazione di calore nel materiale. I modelli standard tipo drift-diffusion non possono trattare fenomeni di alto campo perché non comprendono l'energia tra le variabili di campo. Inoltre in molte applicazioni in opto-elettronica si ha bisogno di descrivere l'interazione transiente di radiazione elettromagnetica con i portatori di carica in mezzi semiconduttori complessi e, dal momento che i tempi caratteristici sono dell'ordine dei tempi di rilassamento del momento o dell'energia, alcuni momenti di ordine piú alto della funzione di distribuzione devono essere necessariamente inclusi. Quindi questi fenomeni non possono essere descritti nell'ambito delle equazioni drift-diffusion (che sono valide solo nel limite quasi-stazionario). Pertanto sono state cercate generalizzazioni delle equazioni drift-diffusion in modo da includere l'energia quale variabile dinamica e la cui validitá non sia ristretta a situazioni quasi-stazionarie. Questi modelli sono chiamati in senso generico modelli idrodinamici. Uno dei primi modelli idrodinamici, di uso corrente nelle applicazioni, è stato sviluppato da Blotekjaer [1] e successivamente investigato da Baccarani e Wordeman [2] e da altri autori (si vedano le referenze

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in [3]). Sono stati investigati anche altri modelli, alcuni di questi includenti anche effetti di non parabolicitá [4–6, 8–20]. La maggior parte dei modelli idrodinamici implementati è affetta da inconvenienti di tipo teorico dovuti al trattamento ad hoc del problema della chiusura (senza convincenti motivazioni fisiche) e della modellizzazione dei termini di produzione (usualmente assunti di tipo rilassamento, fatto che, come vedremo, comporta serie inconsistenze con le condizioni di reciprocitá di Onsager). In questa trattazione presenteremo una rassegna generale della teoria alla base dei modelli idrodinamici. In particolare investigheremo in dettaglio il problema della chiusura sia per i flussi che per i termini di produzione e presenteremo un approccio, introdotto recentemente, basato sul principio di massima entropia (fisicamente sviluppato nell'ambito della termodinamica estesa [21, 22]). Le considerazioni e i risultati riportati nell'articolo riguarderanno esclusivamente il silicio.

Key words: Continuum model, Extended thermodynamics, Microelectromechanical systems, Monte–Carlo method, Electromagneto-fluids.

1. Carrier 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 [23], 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.

$\mathcal{B}$ is said to be the first Brillouin zone if it is the Wigner-Seirg primitive cell of the reciprocal lattice $\hat{L}$. It consists 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*

$$H = -\frac{\hbar^2}{2m_e}\,\triangle - eV_{\mathrm{L}},$$

$\hbar$ being the Planck constant divided by 2π, m_e the electron mass in the vacuum and e the absolute value of the electron charge.

The bounded eigenstates have the form

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

and

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

One obtains a second order self-adjoint elliptic problem posed on a primitive cell of the crystal lattice L. It is possible to prove [23] the existence of an infinite sequence of eigenpairs (energy – wave vector)

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

$\mathcal{N}$ 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 wave vectors which differ by a reciprocal lattice vector. Therefore one can constrain the wave vector $\mathbf{k}$ 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 [23–25].

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 [23]. However, in order to describe electron transport, for most applications, a simplified description is adopted which is based on a simple analytical model.

In silicon electrons which contribute mainly to the charge transport are those with energy close to the lowest conduction band minima. In the Brillouin zone this corresponds to six equivalent ellipsoidal valleys along the main crystallographic directions Δ at about 85% from the center of the first Brilloiun zone, near the X points. For this reason these are termed as X-valleys.

In the parabolic band and effective mass approximation the energy curve is approximated by a parabola near the minimum of each valley. Then if we denote by $\mathcal{E}$ the energy of the considered conduction band measured from the band minimum, we have

$$\mathcal{E} = \frac{\hbar^2|\mathbf{k}|^2}{2m^*}, \tag{1}$$

with $\mathbf{k}$ assumed to vary in all $\mathcal{R}^3$. m^* is the effective electron mass (for silicon $m^* = 0.32\, m_e$, with m_e the electron mass in vacuum) and $\hbar\mathbf{k}$ the *crystal momentum*.

A more appropriate analytical approximation, which takes into account the non-parabolicity at high energy, is given by the Kane dispersion relation

$$\mathcal{E}(k)\,[1 + \alpha\mathcal{E}(k)] = \frac{\hbar^2 k^2}{2m^*}, \qquad \mathbf{k} \in \mathcal{R}^3, \tag{2}$$

where α is the non-parabolicity parameter (for Silicon $\alpha = 0.5$ eV^{-1} for each X-valley).

In the Monte Carlo simulations the anisotropic version of (1) and (2) are also used

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

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

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

$$v^i = \frac{\hbar k^i}{m^*}, \tag{3}$$

while in the approximation of the Kane dispersion relation

$$v^i = \frac{\hbar k^i}{m^*\,[1 + 2\alpha\mathcal{E}(k)]}. \tag{4}$$

1.2. THE SEMICLASSICAL LIOUVILLE EQUATION

In principle the motion of an ensemble of N electrons could be obtained in a quantum framework by solving the Schrödinger equation for a N-electron wave function. However, this many body problem is computationally prohibitive even in the classical case. A rather accurate way to overcome the problem is of resorting to a probabilistic description in a semiclassical kinetic framework. As in classical gas dynamics, under the assumption that external forces (electric field $\mathbf{E}^{\text{ext}}$) 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 N electrons belonging to the same energy band with wavevectors $\mathbf{k}_i, i = 1, \dots, N$, it is possible to show that the semiclassical Liouville equation for the joint probability density $f(\mathbf{x}_1 \cdots \mathbf{x}_N, \mathbf{k}_1 \cdots \mathbf{k}_N, t)$

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

must be satisfied. Then by proceeding as in the classical theory one obtains the *hierarchy BBGKY of equations* and, under the usual assumptions [26] (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. THE BOLTZMANN–POISSON EQUATIONS

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*, that is, 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*

$$\frac{\partial f}{\partial t} + v^i(\mathbf{k})\frac{\partial f}{\partial x^i} - \frac{eE^i}{\hbar}\frac{\partial f}{\partial k^i} = \mathcal{C}[f], \tag{5}$$

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

$$E_i = -\frac{\partial \phi}{\partial x_i}, \tag{6}$$

$$\epsilon \Delta \phi = -e(N_{\mathrm{D}} - N_{\mathrm{A}} - n), \tag{7}$$

N_{D} and N_{A} being the donor and acceptor density, respectively. These are fixed ions implanted in the semiconductors and their densities depend only on the position. N is the electron number density

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

The Equations (5)–(7) constitute the Boltzmann–Poisson system that is the basic semiclassical model of electron transport in semiconductors.

1.4. SCATTERING MECHANISMS

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.

After a collision the electron can remain in the same valley (intravalley scattering) or be drawn in another equivalent valley (intervalley scattering). In silicon the allowed electron–phonon scattering can be summarized as follows:

- scattering with intravalley acoustic phonon (elastic),
- scattering with intervalley acoustic phonons (inelastic),
- scattering with non-polar optical phonons (inelastic);

the values of the electron acoustic–phonon deformation potential and of the deformation potential constants as well as the silicon bulk constants are given in [24]. For the sake of completeness we summarize the physical parameters in Tables 1 and 2.

The form of the collision operator $\mathcal{C}[f]$ for each type of scattering mechanism is

$$\mathcal{C}[f] = \int_{\mathcal{B}} [P(\mathbf{k}', \mathbf{k}) f(\mathbf{k}')(1 - f(\mathbf{k})) - P(\mathbf{k}, \mathbf{k}') f(\mathbf{k})(1 - f(\mathbf{k}'))]\, \mathrm{d}^3\mathbf{k}'. \tag{8}$$

The first term in (8) represents the gain and the second one the loss. The terms $1 \pm f(\mathbf{k})$ account for the Pauli exclusion principle. $P(\mathbf{k}, \mathbf{k}')$ is the transition probability from the state $\mathbf{k}$ to the state $\mathbf{k}'$.

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

$$\mathcal{C}[f] = \int_{\mathcal{B}} [P(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') - P(\mathbf{k}, \mathbf{k}') f(\mathbf{k})]\, \mathrm{d}^3\mathbf{k}'. \tag{9}$$

At equilibrium the electron distribution must obey the Fermi–Dirac statistics

$$f_{\mathrm{eq}} = \left[\exp\left(-\frac{\mathcal{E}}{k_{\mathrm{B}} T_{\mathrm{L}}} \right) + 1 \right]^{-1},$$

k_{B} being the Boltzmannn constant and T_{L} being the lattice temperature which will be taken as constant.

Table 1. Values of the physical parameters used for silicon

m_{e}	Electron rest mass	9.1095×10^{-28} g
m^*	Effective electron mass	$0.32\, m_e$
T_{L}	Lattice temperature	300° K
ρ_0	Density	2.33 g/cm^3
v_s	Longitudinal sound speed	9.18×10^5 cm/sec
Ξ_d	Acoustic-phonon deformation potential	9 eV
α	Non-parabolicity factor	0.5 eV^{-1}
ϵ_r	Relative dielectric constant	11.7
ϵ_0	Vacuum dieletric constant	8.85×10^{-18} C/V μm

Table 2. Coupling constants and phonon energies for the inelastic scatterings in silicon

A	Z_f	$\hbar\omega$ (meV)	$D_t K\,(10^8 eV/\mathrm{cm})$
1	1	12	0.5
2	1	18.5	0.8
3	4	19.0	0.3
4	4	47.4	2.0
5	1	61.2	11
6	4	59.0	2.0

In the dilute case, one can consider the Maxwellian limit of the Fermi–Dirac distribution

$$f_{\mathrm{eq}} \approx \exp\left(-\frac{\mathcal{E}}{k_{\mathrm{B}}T_{\mathrm{L}}}\right).$$

In both cases from the principle of detailed balance [26] it follows that

$$P(\mathbf{k}', \mathbf{k}) = P(\mathbf{k}, \mathbf{k}') \exp\left(-\frac{\mathcal{E} - \mathcal{E}'}{k_{\mathrm{B}}T_{\mathrm{L}}}\right), \tag{10}$$

where $\mathcal{E} = \mathcal{E}(\mathbf{k})$ and $\mathcal{E}' = \mathcal{E}(\mathbf{k}')$.

In the elastic case

$$P(\mathbf{k}, \mathbf{k}') = \frac{k_{\mathrm{B}}T_{\mathrm{B}}\,\Xi_{\mathrm{d}}^2}{4\pi^2\hbar\rho v_{\mathrm{s}}^2}\delta(\mathcal{E} - \mathcal{E}'), \tag{11}$$

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.

In the case of inelastic scattering

$$P(\mathbf{k}, \mathbf{k}') = \frac{Z_{\mathrm{f}}(D_t K)^2}{8\pi^2\rho\omega}\left(n_{\mathrm{B}} + \frac{1}{2} \mp \frac{1}{2}\right)\delta(\mathcal{E}' - \mathcal{E} \mp \hbar\omega), \tag{12}$$

where $D_t K$ is the deformation potential for non-polar optical phonons, Z_{f} is the number of final equivalent valleys for the considered intervalley scattering, $\hbar\omega$ is the longitudinal optical phonon energy and n_{B} is the phonon equilibrium distribution according to the Bose–Einstein statistics

$$n_{\mathrm{B}} = \frac{1}{\exp(\hbar\omega/k_{\mathrm{B}}T_{\mathrm{L}}) - 1}.$$

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 [27], which is well suited for a quasi isotropic distribution function

$$\mathcal{C}_{\mathrm{imp}}[f] = -\frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau_{\mathrm{imp}}}, \tag{13}$$

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

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

with N_{imp} concentration of impurities and γ screening parameter $\gamma = \hbar^2 b^2 / 8m^* \mathcal{E}$, b being the inverse screening length. We observe that the non-parabolicity will enter only in the calculation of the moments of the impurity scattering through the elementary volume in the integrals.

1.5. H-THEOREM AND THE NULL SPACE OF THE COLLISION OPERATOR

H-theorems were obtained in [28, 29] under the assumption that the transition probabilities are bounded functions. In [30–32] 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 [33] in the parabolic case.

Here, we review the question 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. By following [34] a physical interpretation of the results is suggested.

As showed in the previous section, the transition probability from the state $\mathbf{k}$ to the state $\mathbf{k}'$ can be written as [25]

$$P(\mathbf{k}, \mathbf{k}') = \mathcal{G}(\mathbf{k}, \mathbf{k}') \left[(n_{\text{B}} + 1)\delta(\mathcal{E}' - \mathcal{E} + \hbar\omega_q) + n_{\text{B}}\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q) \right], \tag{14}$$

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 [25] and enjoys the properties

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

$\hbar\omega_q$ stands for the phonon energy.

For the moments of the collision term with respect to the weight function $\psi(\mathbf{k})$ the following chain of identities can be proved as in [30–32]

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

By following [32] if we set without loss of generality

$$f(\mathbf{k}) = h(\mathbf{k}) \exp\left(-\frac{\mathcal{E}}{k_{\text{B}} T_{\text{L}}} \right),$$

and in analogy with the case of a simple gas if we take $\psi(\mathbf{k}) = k_{\mathrm{B}} \log h(\mathbf{k})$, then by using the definition of $\delta(x)$ one has

$$k_{\mathrm{B}} \int_{\mathcal{B}} \mathcal{C}[f] \log h(\mathbf{k})\, \mathrm{d}^3\mathbf{k} \;=\; k_{\mathrm{B}} \int_{\mathcal{B}\times\mathcal{B}} \mathcal{G}(\mathbf{k}, \mathbf{k}')\delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_q)n_q \exp\left(-\frac{\mathcal{E}}{k_{\mathrm{B}}T_{\mathrm{L}}}\right) \times$$
$$\times (h(\mathbf{k}') - h(\mathbf{k})) \left(\log h(\mathbf{k}) - \log h(\mathbf{k}')\right) \mathrm{d}^3\mathbf{k}\, \mathrm{d}^3\mathbf{k}' \leqslant 0. \quad (15)$$

Therefore along the characteristics of Equation (5)

$$-\int_{\mathcal{B}} \log h(\mathbf{k}) \frac{\mathrm{d}f}{\mathrm{d}t}\, \mathrm{d}^3\mathbf{k} = -\int_{\mathcal{B}} \mathcal{C}[f] \log h(\mathbf{k})\, \mathrm{d}^3\mathbf{k} \geqslant 0$$

holds. This implies that the opposite of

$$\Psi = -\int_{\mathcal{B}} \left(\int \log h(\mathbf{k})\, \mathrm{d}f\right) \mathrm{d}^3\mathbf{k} = -k_{\mathrm{B}} \int_{\mathcal{B}} \left(f \log f - f + \frac{\mathcal{E}}{k_{\mathrm{B}}T_{\mathrm{L}}} f\right) \mathrm{d}^3\mathbf{k}, \quad (16)$$

can be considered as a Liapunov function for the Boltzmann–Poisson system (5)–(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 non-equilibrium 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.

Strictly related there is the problem of determining the null space of the collision operator which consists in finding 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 if $E = 0$.

In [28, 29] 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 general in [32] where it is proved that the equilibrium solutions are not only the Fermi–Dirac distributions but form an infinite sequence of functions of the kind

$$f(k) = \frac{1}{1 + h(\mathbf{k}) \exp \mathcal{E}(\mathbf{k})/K_{\mathrm{B}}T_{\mathrm{L}}}, \quad (17)$$

where $h(\mathcal{E}) = h(\mathcal{E} + \hbar\omega_q)$ is a periodic function of period $\hbar\omega_q/n$, with n positive integer. 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.

2. Macroscopic Models

Macroscopic 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.

If a N-moment model is considered, the closure problem consists in finding an appropriate expression for the higher order moments and the production terms as suitable functions (constitutive relations) 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 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 [35]. By multiplying Equation (5) by a function $\psi(\mathbf{k})$ and integrating over $\mathcal{B}$, one finds the *moment equation*

$$\frac{\partial M_\psi}{\partial t} + \int_{\mathcal{B}} \psi(\mathbf{k}) v^i(\mathbf{k}) \frac{\partial f}{\partial x^i}\, \mathrm{d}^3\mathbf{k} - eE^j \int_{\mathcal{B}} \psi(\mathbf{k}) \frac{\partial}{\partial k_j} f \, \mathrm{d}^3\mathbf{k} = \int_{\mathcal{B}} \psi(\mathbf{k}) \mathcal{C}[f]\, \mathrm{d}^3\mathbf{k}, \tag{18}$$

with

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

the moment relative to the weight function ψ.

Since

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

with $\mathbf{n}$ outward unit normal field on the boundary $\partial\mathcal{B}$ of the domain $\mathcal{B}$ and $\mathrm{d}\sigma$ surface element of $\partial\mathcal{B}$, Equation (18) becomes

$$\begin{aligned} &\frac{\partial M_\psi}{\partial t} + \frac{\partial}{\partial x^i} \int_{\mathcal{B}} f \psi(\mathbf{k}) v^i(\mathbf{k})\, \mathrm{d}^3\mathbf{k} + eE^j \left[\int_{\mathcal{B}} f \frac{\partial \psi(\mathbf{k})}{\partial k_j}\, \mathrm{d}^3\mathbf{k} - \int_{\partial\mathcal{B}} \psi(\mathbf{k}) f n_j \mathrm{d}\sigma \right] \\ &\quad = \int_{\mathcal{B}} \psi(\mathbf{k}) \mathcal{C}(f)\, \mathrm{d}^3\mathbf{k}. \end{aligned} \tag{19}$$

The term

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

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 consequence of the periodicity of f on $\mathcal{B}$ and the symmetry of $\mathcal{B}$ with respect to the origin.

Various models employ different expression of $\psi(\mathbf{k})$ and number of moments. Moreover a unipolar or bipolar version can be formulated.

2.2. THE RELAXATION TIME APPROXIMATION

A simplistic model approximately valid under non-degenerate conditions ($f \ll 1$) for parabolic bands and elastic scatterings [4] is represented by the continuity equations, obtained by taking $\psi(\mathbf{k}) = 1$, coupled to the Poisson equation for the electrical potential. For a unipolar model (only the electrons are considered) these equations read

$$\frac{\partial n}{\partial t} + \frac{\partial (nV^i)}{\partial x^i} = 0, \tag{20}$$

$$\nabla \cdot (\epsilon \nabla \phi) = e(N_{\mathrm{A}} - N_{\mathrm{D}} + n), \tag{21}$$

where

$$V^i = \frac{1}{n} \int_{\mathcal{B}} f v^i \, \mathrm{d}^3\mathbf{k}$$

is the average electron velocity.

When a bipolar models is considered, a term due to the generation-recombination mechanism should appear in the RHS, even though this effect is relevant for times of order 10^{-9} s and in most applications can be neglected because the characteristic times are of order of a fraction of picosecond.

In this model the closure consists in expressing nV^i as function of n and the electric field in order to get a diffusion equation for the charge density.

The closure procedure is based on the approximation of the collision term $\mathcal{C}$ as a relaxation type expression

$$\mathcal{C}(f) = -\frac{f - \hat{f}}{\tau(\mathcal{E}(\mathbf{k}))}, \tag{22}$$

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

$$\hat{f} = \exp(-\frac{\mathcal{E}(\mathbf{k}) - e\phi + q\mathcal{E}_{\mathrm{F}}}{k_{\mathrm{B}}T}), \tag{23}$$

corresponding to the local Maxwellian distribution. T is the local electron temperature (at global equilibrium $T = T_{\mathrm{L}}$), ϕ the electrostatic potential and $\mathcal{E}_{\mathrm{F}}$ the Fermi energy.

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

We consider time scales longer than the collision times $\tau(\mathcal{E}(\mathbf{k}))$ and therefore we can neglect $\partial f/\partial t$ in the Boltzmann Equation (5). By iterating we then obtain [4] in the usual way to first order

$$f = f_{\mathrm{eq}} - \tau(\mathcal{E}(\mathbf{k}))[\mathbf{v}(\mathbf{k}) \cdot \nabla f_{\mathrm{eq}} - e\mathbf{E} \cdot \nabla_{\mathbf{k}} f_{\mathrm{eq}}], \tag{24}$$

which, using Equation (23), gives

$$f = f_{\mathrm{eq}} - \tau(\mathcal{E}(\mathbf{k}))\frac{f_{\mathrm{eq}}}{k_{\mathrm{B}}T}\left[\frac{\mathcal{E}(\mathbf{k}) - e\phi + e\mathcal{E}_{\mathrm{F}}}{K_{\mathrm{B}}T}\mathbf{v}(\mathbf{k}) \cdot \nabla T - q\mathbf{v}(\mathbf{k}) \cdot \nabla \mathcal{E}_{\mathrm{F}}\right]. \tag{25}$$

Let $\mathbf{J} = n\mathbf{V}$ denote the particle flux. Then by substituting Equation (25) into the definition of $\mathbf{V}$, one obtains

$$\mathbf{J} = -\frac{4\pi}{3m^\star k_{\mathrm{B}}T}\left\{[A + Bq(\mathcal{E}_{\mathrm{F}} - \phi)]\frac{\nabla T}{k_{\mathrm{B}}T} - eB\nabla\mathcal{E}_{\mathrm{F}}\right\}, \tag{26}$$

where

$$\begin{aligned} A &= 4\pi \int \mathrm{d}^3\mathbf{k} f_{\mathrm{eq}} k^4 \tau(\mathcal{E}(\mathbf{k}))\mathcal{E}(\mathbf{k}), \\ B &= 4\pi \int \mathrm{d}^3\mathbf{k} f_{\mathrm{eq}} k^4 \tau(\mathcal{E}(\mathbf{k})). \end{aligned}$$

Now the particle density is given by

$$n = \int \mathrm{d}^3\mathbf{k} f = (\pi 2m^\star k_\mathrm{B} T)^{3/2} \exp - \frac{e\mathcal{E}_\mathrm{F} - e\phi}{k_\mathrm{B} T}, \tag{27}$$

whence

$$\mathcal{E}_\mathrm{F} = \phi - \frac{k_\mathrm{B} T}{e} \log\left(\frac{n}{aT^{3/2}}\right) + \text{const}, \tag{28}$$

$$\nabla\mathcal{E}_\mathrm{F} = \nabla\phi + \nabla\left[\frac{k_\mathrm{B} T}{e} \log\left(\frac{aT^{3/2}}{n}\right)\right] \quad \text{with} \quad a = (\pi 2m^\star k_\mathrm{B})^{3/2}.$$

From Equation (28) we see that $\mathcal{E}_\mathrm{F}$ plays the role of electrochemical potential (usually called, in this context, quasi-Fermi potential).

It is convenient to introduce the intrinsic concentration of electrons

$$n_i = aT^{3/2} \tag{29}$$

and then

$$\mathcal{E}_\mathrm{F} = \phi - U_\mathrm{T} \log\left(\frac{n}{n_i}\right),$$

where U_T is the thermal potential

$$U_\mathrm{T} = \frac{k_\mathrm{B} T}{e}.$$

Also, it is convenient to introduce the mobility

$$\mu_n = \frac{4\pi e B}{3m^\star k_\mathrm{B} T n} \tag{30}$$

and the thermoelectric power

$$P_n = \frac{A + Be(\mathcal{E}_\mathrm{F} - \phi)}{eBk_\mathrm{B} T}. \tag{31}$$

Equation (26) then rewrites

$$\mathbf{J} = \mu_n n(\nabla\mathcal{E}_\mathrm{F} - P_n \nabla T). \tag{32}$$

Under isothermal conditions, $T = T_\mathrm{L}$=const, we have

$$\nabla\mathcal{E}_\mathrm{F} = \nabla\phi - U_\mathrm{T}\frac{\nabla n}{n},$$

whence

$$\mathbf{J} = \mu_n n \nabla\phi - D_n \nabla n, \tag{33}$$

where

$$D_n = \mu_n U_\mathrm{T}, \tag{34}$$

is the diffusion coefficient and Equation (34) expresses the equilibrium statistical mechanics Einstein relation.

Under isothermal conditions therefore the electron system can be described by the particle continuity Equation (20), the constitutive Equation (33) and the Poisson Equation for the self-consistent potential. Allowing for two bands (valence and conduction band) and including in the same way as for electrons, the equation for holes, we obtain the celebrated *drift-diffusion model*

$$\frac{\partial n}{\partial t} + \nabla\cdot\mathbf{J}_n = G - R, \tag{35}$$

$$\frac{\partial p}{\partial t} + \nabla\cdot\mathbf{J}_p = G - R, \tag{36}$$

$$\mathbf{J}_n = \mu_n n \nabla\phi - D_n \nabla n, \tag{37}$$

$$\mathbf{J}_p = \mu_p p \nabla\phi - D_p \nabla p, \tag{38}$$

$$\nabla\cdot(\epsilon\nabla\phi) = e(N_\mathrm{A} - N_\mathrm{D} + n - p), \tag{39}$$

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), $N_\mathrm{A}, N_\mathrm{D}$ 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. For a comprehensive collection of expressions for mobilities, diffusion coefficients and generation-recombination terms the interested reader can see [36]. The drift-diffusion models has received in the last decades an intensive analytical and computational investigations (for a review see [26, 37]).

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:

$$\mathbf{H} = \int d\mathbf{k}(\mathcal{E}(\mathbf{k}) - e\phi + e\mathcal{E}_\mathrm{F})\mathbf{v}(\mathbf{k})f \tag{40}$$

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

$$\mathbf{H} = \mathbf{S} + e(\mathcal{E}_F - \phi)\mathbf{J}. \tag{41}$$

It follows

$$\mathbf{H} = -\frac{4\pi}{3m^\star k_\mathrm{B}T}\left\{C\frac{\nabla T}{k_\mathrm{B}T} - e[A + Bq(\mathcal{E}_\mathrm{F} - \phi)]\nabla\mathcal{E}_\mathrm{F}\right\}, \tag{42}$$

where

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

Equation (42) can be rewritten in the form

$$\mathbf{H} = n \left[e\mu_n P_n k_\mathrm{B} T \nabla \mathcal{E}_\mathrm{F} - \frac{\lambda_n}{k_\mathrm{B} T} \nabla T \right], \tag{43}$$

where

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

Equations (26), (43) form the basis of the energy transport model [38]. By comparing Equation (43) to Equation (26) we see that the Onsager reciprocity principle [39] holds for the energy transport model [4, 15].

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. A way of including energy as additional variable is given by the model we will show in this subsection.

The energy bands are still assumed to be of parabolic type and in addition to the continuity equation, further moment equations are considered: the balance equations of linear momentum (particle flux) and energy

$$\frac{\partial(nV^i)}{\partial t} + \frac{\partial(nP^{ij})}{\partial x^j} + \frac{neE^i}{m^*} = nC_P^i, \tag{44}$$

$$\frac{\partial(nW)}{\partial t} + \frac{\partial(nS^j)}{\partial x^j} + neV_k E^k = nC_W, \tag{45}$$

where

$$W = \frac{1}{n}\int_\mathcal{B} \mathcal{E}(k) f \, \mathrm{d}^3\mathbf{k} \quad \text{is the average electron energy}, \tag{46}$$

$$S^i = \frac{1}{n}\int_\mathcal{B} f v^i \mathcal{E}(k) \, \mathrm{d}^3\mathbf{k} \quad \text{is the energy flux}, \tag{47}$$

$$P^{ij} = \frac{1}{n}\int_\mathcal{B} f v^i v^j \, \mathrm{d}^3\mathbf{k} \quad \text{is the pressure tensor}, \tag{48}$$

$$C_P^i = \frac{1}{n}\int_\mathcal{B} \mathcal{C}[f] v^i \, \mathrm{d}^3\mathbf{k} \quad \text{is the linear momentum production}, \tag{49}$$

$$C_W = \frac{1}{n}\int_\mathcal{B} \mathcal{C}[f] \mathcal{E}(k) \, \mathrm{d}^3\mathbf{k} \quad \text{is the energy production}. \tag{50}$$

This approach dates back to the pioneering work of Blotekjaer [1] and then of Baccarani and Wordeman [2]. Because of its widespread popularity we denote this model by BBW (Blotekjaer–Baccarani–Wordeman).

Let us 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 decompose the tensor P^{ij} as

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

The tensor

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

is then split into an isotropic and traceless part

$$\hat{\theta}^{ij} = \tfrac{1}{3}\hat{\theta}^k_k \delta^{ij} + \hat{\theta}^{\langle ij \rangle},$$

where

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

Then

$$P^{ij} = nV^i V^j + \tfrac{1}{3}\hat{\theta}^k_k \delta^{ij} + \hat{\theta}^{\langle ij \rangle}. \tag{51}$$

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

$$\hat{\theta}^{\langle ij \rangle} = 0. \tag{52}$$

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 assuming, in analogy with kinetic energy of monatomic gas, the equation of state for ideal gas

$$\frac{3nk_\mathrm{B}T}{2} = nW - \frac{nm^\star \mathbf{V}^2}{2}, \tag{53}$$

whence

$$\hat{\theta}^k{}_k = \frac{3nk_\mathrm{B}T}{m^\star} \quad \text{and} \quad \hat{\theta}^{ij} = \frac{nk_\mathrm{B}T}{m^\star}\delta^{ij}.$$

Concerning the productions, the momentum rate of change is assumed to be of the relaxation time type

$$\mathbf{Q} = -\frac{\mathbf{J}}{\tau_p}, \tag{54}$$

hence the momentum Equation (44) rewrites

$$\frac{\partial(nV^i)}{\partial t} + \frac{\partial}{\partial x^j}\left[nV^i V^j + \frac{nk_\mathrm{B}T}{m^\star}\delta^{ij}\right] + \frac{nqE^i}{m^\star} = -\frac{nV^i}{\tau_p}. \tag{55}$$

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

$$\mathbf{S} = W\mathbf{V} + k_\mathrm{B}T\mathbf{V} + \mathbf{q}, \tag{56}$$

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

$$n\mathbf{q} = \frac{m^\star}{2}\int \mathrm{d}^3\mathbf{k} f \mathbf{c}^2\mathbf{c}. \tag{57}$$

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

$$\mathbf{q} = -\kappa \nabla T. \tag{58}$$

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 [4, 14, 40]. 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 Equation (79) yields

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

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

$$F_{rr} = \frac{15n(k_{\mathrm{B}}T)^2}{2m^\star}.$$

Now the momentum Equation (44) with the assumption $\mathbf{Q} = -\mathbf{J}/\tau_p$ and neglecting the convective terms yields

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

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

$$nq_i = -\frac{5\tau_h nk_{\mathrm{B}}T}{2m^\star} \frac{\partial (k_{\mathrm{B}}T)}{\partial x^i} + \frac{5nk_{\mathrm{B}}TV_i}{2} \left(\frac{1}{\tau_p} - \frac{1}{\tau_q} \right) \tau_q. \tag{59}$$

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 for fluxes are open to criticism. In particular the assumption that the heat flow is described by the Fourier law is rather questionable [6, 7], as will be discussed in the sequel.

Modeling the relaxation times is also a rather delicate question. In the original Baccarani and Wordeman formulation τ_p is determined by the following consideration. The electron mobility μ_n is related to the momentum relaxation times by

$$\mu_n = e\tau_p/m^\star.$$

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

$D_n = k_{\mathrm{B}}T\mu_n$ and that D_n is constant and equal to the low field diffusivity D_0. Hence,

$$D_0 = k_{\mathrm{B}}T_{\mathrm{L}}\mu_{n0} = k_{\mathrm{B}}T\mu_n,$$

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

$$\tau_p = \frac{m^\star \mu_{n0} T_\mathrm{L}}{eT}.$$

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

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

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 [36]

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

where $v_\mathrm{s} = 1.0 \times 10^7$ cm/s is the saturation velocity. Since in the homogeneous case

$$V^i = \frac{\tau_p e E^i}{m^*} = \mu_n E^i,$$

then

$$\tau_w = \frac{m^\star \mu_{n0} T_\mathrm{L}}{2eT} + \frac{3k_\mathrm{B} \mu_{n0} T T_\mathrm{L}}{2ev_\mathrm{s}^2 (T + T_\mathrm{L})}.$$

The modeling of the thermal conductivity coefficient is obtained from the Wiedemann–Franz law (which holds near thermal equilibrium)

$$\kappa = \left(\frac{5}{2} + c \right) \left(\frac{k_\mathrm{B}}{e} \right)^2 nl\mu_n T, \tag{60}$$

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

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

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

$$\kappa = \frac{3}{2} \left(\frac{k_\mathrm{B}}{e} \right)^2 ne\mu_n T.$$

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

- continuity equation

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{V}) = 0, \tag{61}$$

- momentum equation

$$\frac{\partial (nV^i)}{\partial t} + \frac{\partial}{\partial x^j} \left(nV^i V^j + \frac{nk_\mathrm{B}T}{m^\star} \delta^{ij} \right) + \frac{nqE^i}{m^\star} = -\frac{nV^i}{\tau_p}, \tag{62}$$

- energy equation

$$\frac{\partial}{\partial t}\left(\frac{1}{2}nm^\star \mathbf{V}^2 + \frac{3}{2}nk_\mathrm{B}T\right) + \nabla \cdot \left[\left(\frac{1}{2}nm^\star V^2 + \frac{5}{2}nk_\mathrm{B}T\right)\mathbf{V} - \kappa \nabla T\right] + \\ + ne\mathbf{E}\cdot\mathbf{V} = -\frac{W - W_0}{\tau_w}, \tag{63}$$

- Poisson's equation

$$\nabla \cdot (\epsilon \nabla \phi) = e(N_\mathrm{A} - N_\mathrm{D} + n - p). \tag{64}$$

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 [41] and Gardner [42, 43] numerically integrated the BBW model for the ballistic diode in the stationary case. In [42] 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 [44] Gardner's results have been recovered by using a viscosity method.

Numerical solutions in the non-stationary case have been obtained in [45] by using an ENO scheme. The same results have been obtained in [46] 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 (62). In the stationary case it yields to the first order approximation (that is by neglecting the second order terms in the velocity)

$$\mathbf{Q} = \frac{1}{m^\star}\nabla(nk_\mathrm{B}T) - \frac{ne}{m^\star}\nabla\phi \tag{65}$$

and from Equation (28)

$$\mathbf{Q} = \frac{n}{m^\star}\left\{-e\nabla\mathcal{E}_\mathrm{F} + \left[\frac{5}{2} + \log\left(\frac{aT^{3/2}}{n}\right)\right]\nabla(k_\mathrm{B}T)\right\}. \tag{66}$$

Now we consider the energy flux Equation (79) in the stationary case. Also in this case $F_{<ij>} = 0$ approximately, hence

$$\tilde{\mathbf{Q}} = \frac{1}{3}\nabla F_{rr} - \frac{5qnk_\mathrm{B}T}{m^\star}\nabla\phi, \qquad \frac{F_{rr}}{3} = \frac{5n(k_\mathrm{B}T)^2}{2m^\star},$$

according to the equilibrium f_eq, whence

$$\tilde{\mathbf{Q}} = \frac{5}{2m^\star}\left\{\nabla[n(k_\mathrm{B}T)^2] - enk_\mathrm{B}T\nabla\phi\right\},$$

which gives, by using Equation (28)

$$\tilde{\mathbf{Q}} = \frac{5}{2m^\star}\left\{-qnk_\mathrm{B}T\nabla\mathcal{E}_\mathrm{F} + \left[\frac{7}{2} + \log\left(\frac{aT^{3/2}}{n}\right)\right]nk_\mathrm{B}T\nabla(k_\mathrm{B}T)\right\}. \tag{67}$$

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

$$\mathbf{Q} = -\frac{\mathbf{J}}{\tau_p}, \tag{68}$$

$$\tilde{\mathbf{Q}} = -\frac{\mathbf{S}}{\tau_q}. \tag{69}$$

Then we have

$$\mathbf{J} = -\frac{n\tau_p}{m^\star}\left\{-e\nabla\mathcal{E}_\mathrm{F} + \left[\frac{5}{2} + \log\left(\frac{aT^{3/2}}{n}\right)\right]\nabla(k_\mathrm{B}T)\right\}, \tag{70}$$

$$\mathbf{H} = \frac{en\tau_p}{m^\star}\left\{k_\mathrm{B}T\left[\frac{5\tau_q}{2\tau_p} + \log\left(\frac{aT^{3/2}}{n}\right)\right]\nabla\mathcal{E}_\mathrm{F} + \Lambda\nabla T\right\}, \tag{71}$$

with

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

Let I denote the coefficient of $\nabla(k_\mathrm{B}T)$ in the expression for $\mathbf{J}$ and II the coefficient of $\nabla\mathcal{E}_\mathrm{F}$ in the expression for $\mathbf{H}$. The Onsager reciprocity principle requires that [39]

$$qk_\mathrm{B}TI = -II. \tag{72}$$

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 [15]. This implies that the production terms must have a more general form.

A more suitable expression is given by

$$\mathbf{Q} = -(a\mathbf{J} + b\mathbf{S}), \tag{73}$$

$$\tilde{\mathbf{Q}} = -(\tilde{a}\mathbf{J} + \tilde{b}\mathbf{S}). \tag{74}$$

Now

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

with $\Delta = a\tilde{b} - \tilde{a}b$ and therefore Equation (64) gives

$$\frac{1}{k_\mathrm{B}}\left\{\tilde{a} - \frac{5ak_\mathrm{N}T}{2} + k_\mathrm{B}T\log\left(\frac{n}{n_i}\right)\left[\tilde{b} - \frac{5bk_\mathrm{N}T}{2}\right]\right\}$$
$$= \frac{5bk_\mathrm{B}T}{2}\left[\frac{7}{2} - \log\left(\frac{n}{n_i}\right)\right] - \tilde{b}\left[\frac{5}{2} - \log\left(\frac{n}{n_i}\right)\right],$$

which can be rewritten as

$$\tilde{a} + \tfrac{5}{2}\tilde{b}k_\mathrm{B}T = \tfrac{5}{2}k_\mathrm{B}T(a + \tfrac{7}{2}bk_\mathrm{B}T). \tag{75}$$

This last relation has been compared with Monte Carlo simulation in [53].

3. The Extended Hydrodynamical Model

In a series of articles [13–20, 34] a general framework for getting closure relation is proposed. At variance with previous treatments, it is not an ad hoc procedure but it is based on the application of the entropy principle within the framework of extended thermodynamics [21, 22] or equivalently the maximum entropy principle or the moment theory of Levermore [47]. 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 also includes 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).

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.

Concerning the moment equations several choices of the weight function ψ can be made and they lead to different balance equations for macroscopic quantities. In [18] 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 [8] by means of Monte Carlo simulations. However, for time dependent simulation it is more useful to consider a slight different set of weight functions [19], 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 non-stationary problems in the parabolic band approximation).

By considering such expressions for ψ one obtains the continuity equation (we recall that, as said above, indeed a term due to the generation-recombination mechanism should appear in the RHS, 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

$$\frac{\partial n}{\partial t} + \frac{\partial (nV^i)}{\partial x^i} = 0, \tag{76}$$

$$\frac{\partial (nP^i)}{\partial t} + \frac{\partial (nU^{ij})}{\partial x^j} + neE^i = nC_P^i, \tag{77}$$

$$\frac{\partial (nW)}{\partial t} + \frac{\partial (nS^j)}{\partial x^j} + neV_kE^k = nC_W, \tag{78}$$

$$\frac{\partial (nS^i)}{\partial t} + \frac{\partial (nF^{ij})}{\partial x^j} + neE_jG^{ij} = nC_W^i, \tag{79}$$

where

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

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

As remarked several times above in these lectures, the moment equations do not constitute a set of closed relations because of the fluxes and production terms. Now we will present a physically well-sounded procedure for getting the required closure relations.

3.1. THE MAXIMUM ENTROPY PRINCIPLE

In this subsection a general energy band will be considered.

If we assume n, V^i, W and S^i as fundamental variables, 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 terms 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 role 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 Equations (76)–(79) 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 [21, 22, 47, 48] 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

$$\int_{\mathcal{B}} \psi_A f_{ME} \, \mathrm{d}^3\mathbf{k} = M_A. \tag{80}$$

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

$$s = -k_\mathrm{B} \int_{\mathcal{B}} (f \log f - f) \, \mathrm{d}^3\mathbf{k}. \tag{81}$$

If we introduce the lagrangian multipliers Λ_A, the problem to maximize s under the constraints (80) is equivalent to maximize $s' = \Lambda^A M_A - s$, the Legendre transform of s, without constraints, $\delta s' = 0$.

This gives

$$\left[\log f + \frac{\Lambda_A \psi^A}{k_\mathrm{B}} \right] \delta f = 0.$$

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

$$f_{ME} = \exp\left[-\frac{1}{k_\mathrm{B}} \Lambda_A \psi^A \right]. \tag{82}$$

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

$$\psi^A = (1, \mathbf{v}, \mathcal{E}, \mathcal{E}\mathbf{v}) \quad \text{and} \quad \Lambda_A = (\lambda, k_\mathrm{B}\lambda_i, k_\mathrm{B}\lambda^W, k_\mathrm{B}\lambda_i^W),$$

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

$$f_{ME} = \exp\left[-\left(\frac{1}{k_\mathrm{B}}\lambda + \lambda^W \mathcal{E} + \lambda_i v^i + \lambda_i^W v^i \mathcal{E} \right) \right], \tag{83}$$

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 M_A, one has to invert the constraints (80). 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 (76)–(79) . 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 [21] it is easy to show that they form a quasilinear hyperbolic system.

Let us set

$$\eta(f) = -k_{\mathrm{B}}(f \log f - f).$$

The entropy balance equations is obtained multiply the Equation (5) by $\eta'(f) = \partial_f \eta(f)$ and after integrating with respect to $\mathbf{k}$ one has

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

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

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

vanishes and the entropy balance equations assumes the usual form

$$\frac{\partial s}{\partial t} + \frac{\partial \varphi^i}{\partial x^i} = g, \quad \text{with} \quad \varphi^i = \int_{\mathcal{B}} \eta(f) v^i\, \mathrm{d}^3\mathbf{k} \quad \text{entropy flux}$$

and

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

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

Let us now rewrite the balance Equations (76)–(79) in the form

$$\frac{\partial M^A}{\partial t} + \frac{\partial F^{iA}}{\partial x^i} = G^A(M_{\mathrm{B}}, E_j). \tag{84}$$

In [21] it is proved that the field equations and the entropy balance equations are related by the condition that

$$\frac{\partial s}{\partial t} + \frac{\partial \varphi^i}{\partial x^i} - g - \Lambda_A \left[\frac{\partial M^A}{\partial t} + \frac{\partial F^{iA}}{\partial x^i} - G^A(M_{\mathrm{B}}, E_j)\right] = 0, \tag{85}$$

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 [21] that

$$M_A = \frac{\partial s'}{\partial \Lambda_A}, \tag{86}$$

$$F^{iA} = \frac{\partial \varphi'^i}{\partial \Lambda_A}, \tag{87}$$

with $s' = \Lambda_A M^A - s$ and with $\varphi'^i = \Lambda_A F^{iA} - \varphi^i$.

If $\partial^2 s'/\partial\Lambda_A \partial\Lambda_{\mathrm{B}}$ is defined in sign, one can globally invert [49] and express the moment M_A as function of the lagrangian multipliers Λ_{B}. As shown in [50] the previous condition is equivalent to require that

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

is defined in sign, with $\chi = \Lambda_A \psi^A / k_\mathrm{B}$. One trivally gets $f'_{ME} < 0$ and therefore the balance Equations (76)-(79) can be rewritten in terms of the lagrangian multipliers as

$$\frac{\partial^2 s'}{\partial \Lambda_A \partial \Lambda_\mathrm{B}} \frac{\partial \Lambda_\mathrm{B}}{\partial t} + \frac{\partial^2 \varphi'^i}{\partial \Lambda_A \Lambda_\mathrm{B}} \frac{\partial \Lambda_B}{\partial x^i} = G^A \left(\frac{\partial s'}{\partial \Lambda_C}, E_j \right). \tag{88}$$

In this form it is immediate to recognize that the balance Equations form a symmetric quasi-linear hyperbolic system [51]. The main consequence of this property is that according to a theorem due to Fisher and Marsden [52] the Cauchy problem is well posed for the system (88) at least in 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

$$f_\mathrm{eq} = \exp\left[- \left(\frac{1}{k_\mathrm{B}} \lambda_E + \frac{\mathcal{E}}{k_\mathrm{B} T_0} \right) \right], \tag{89}$$

that is at equilibrium

$$\lambda_E^W = \frac{1}{k_\mathrm{B} T_0}, \quad \lambda_E^i = 0, \quad \lambda_E^{i\,W} = 0.$$

Monte Carlo simulations for electron transport in Si show that the anisotropy of f is small [6, 8, 53] 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 with a good approximation.

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,

$$\lambda = \lambda^{(0)} + \delta^2 \lambda^{(2)}, \tag{90}$$

$$\lambda^W = \lambda^{W(0)} + \delta^2 \lambda^{W(2)}, \tag{91}$$

$$\lambda_i = \delta \lambda_i^{(1)}, \tag{92}$$

$$\lambda_i^W = \delta \lambda_i^{W(1)}. \tag{93}$$

Therefore, f_{ME} can be written as

$$f_{ME} = \exp\left(- \frac{\lambda^{(0)}}{k_\mathrm{B}} - \lambda^{W(0)} \mathcal{E} \right) \left[1 - \delta x + \delta^2 \left(\frac{x^2}{2} - \frac{\lambda^{(2)}}{k_\mathrm{B}} - \lambda^{W(2)} \mathcal{E} \right) \right], \tag{94}$$

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:

$$n = \int_{\mathcal{B}} f_{ME} \, \mathrm{d}^3\mathbf{k}, \tag{95}$$

$$nW = \int_{\mathcal{B}} \mathcal{E} f_{ME} \, \mathrm{d}^3\mathbf{k}, \tag{96}$$

$$nV^i = \int_{\mathcal{B}} v^i f_{ME} \, \mathrm{d}^3\mathbf{k}, \tag{97}$$

$$nS^i = \int_{\mathcal{B}} v^i \mathcal{E} f_{ME} \, \mathrm{d}^3\mathbf{k}. \tag{98}$$

By retaining only the terms up to second order in δ, from the constraints (95)–(98), we get the following algebraic system (V_i and S_i are consistently considered as terms of order δ)

$$n = \exp\left[-\left(\frac{1}{k_{\mathrm{B}}}\lambda^{(0)}\right)\right] \int_{\mathcal{B}} \exp\left[-\left(\lambda^{W(0)}\mathcal{E}\right)\right] \mathrm{d}^3\mathbf{k}, \tag{99}$$

$$W = \exp\left[-\left(\frac{1}{k_{\mathrm{B}}}\lambda^{(0)}\right)\right] \int_{\mathcal{B}} \mathcal{E} \exp\left[-\left(\lambda^{W(0)}\mathcal{E}\right)\right] \mathrm{d}^3\mathbf{k}, \tag{100}$$

$$0 = \int_{\mathcal{B}} \exp\left(\lambda^{W(0)}\mathcal{E}\right) \left[\frac{1}{k_{\mathrm{B}}}\lambda^{(2)} + \lambda^{W(2)}\mathcal{E} - \frac{x^2}{2}\right], \tag{101}$$

$$0 = \int_{\mathcal{B}} \mathcal{E} \exp\left(\lambda^{W(0)}\mathcal{E}\right) \left[\frac{1}{k_{\mathrm{B}}}\lambda^{(2)} + \lambda^{W(2)}\mathcal{E} - \frac{x^2}{2}\right], \tag{102}$$

$$nV^i = -\int_{\mathcal{B}} v^i \, \exp\left(\lambda^{W(0)}\mathcal{E}\right) \, x \, \mathrm{d}^3\mathbf{k}, \tag{103}$$

$$nS^i = -\int_{\mathcal{B}} v^i \, \mathcal{E} \exp\left(\lambda^{W(0)}\mathcal{E}\right) \, x \, \mathrm{d}^3\mathbf{k}. \tag{104}$$

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

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

Equations (99) and (100) decouple from the other equations and explicitly read

$$n = 4\frac{\pi}{\hbar^3} \exp\left(-\frac{\lambda^{(0)}}{k_{\mathrm{B}}}\right) \int_0^{\infty} \exp(-\lambda^{W(0)}\mathcal{E}) m^* \sqrt{2m^*\mathcal{E}(1+\alpha\mathcal{E})} \times (1+2\alpha\mathcal{E})\,\mathrm{d}\mathcal{E}, \tag{105}$$

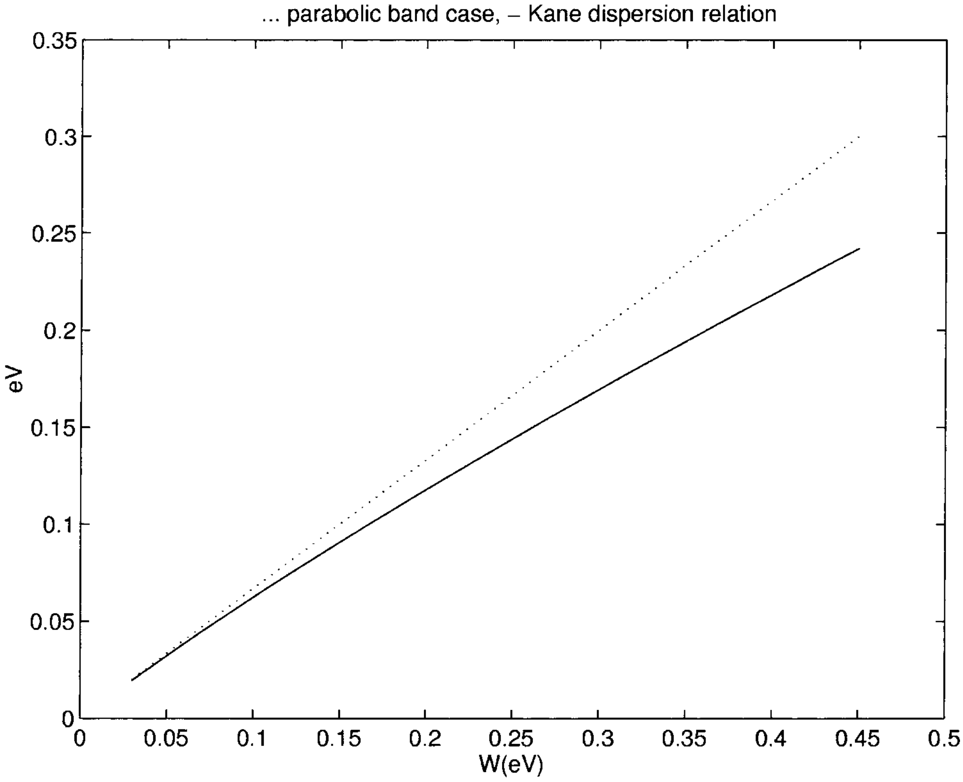

Figure 1. Inverse of the lagrangian multipliers $\lambda^{W(0)}$ vs. the energy W.

$$W = \frac{\int_0^\infty \mathcal{E}\sqrt{\mathcal{E}(1+\alpha\mathcal{E})}(1+2\alpha\mathcal{E})\exp(-\lambda^{W(0)}\mathcal{E})\,\mathrm{d}\mathcal{E}}{\int_0^\infty \sqrt{\mathcal{E}(1+\alpha\mathcal{E})}(1+2\alpha\mathcal{E})\exp(-\lambda^{W(0)}\mathcal{E})\,\mathrm{d}\mathcal{E}}. \tag{106}$$

Relation (106) shows that $\lambda^{W(0)}$ depends only on W. The analytical inversion of Equation (106) is rather involved and we have resorted to a numerical inversion. The results are showed in Figure 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 (105) 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

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

The lagrangian multipliers λ_i^v and λ_i^W can be obtained by inverting the linear system represented by Equations (103) and (104).

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

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

one finds $\lambda_i = b_{11} V_i + b_{12} S_i$, $\lambda_i^W = b_{12} V_i + b_{22} S_i$. The coefficients b_{ij} are given by

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

with

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

and

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

d_k and p_k being

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

Finally, the second order corrections to λ and λ^W, are obtained by solving the linear system (101) and (102).

The following expressions are found:

$$\frac{\lambda^{(2)}}{k_B} = \alpha_1 \mathbf{V} \cdot \mathbf{V} + 2\alpha_2 \mathbf{S} \cdot \mathbf{V} + \alpha_3 \mathbf{S} \cdot \mathbf{S}, \tag{107}$$

$$\lambda^{W(2)} = \alpha_4 \mathbf{V} \cdot \mathbf{V} + 2\alpha_5 \mathbf{S} \cdot \mathbf{V} + \alpha_6 \mathbf{S} \cdot \mathbf{S}. \tag{108}$$

The coefficients α_i are given in [18].

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

$$P^i = m^*(v^i + 2\alpha S^i), \tag{109}$$

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

$$U_{ij} = U_{ij}^{(0)} + \delta^2 U_{ij}^{(2)}, \tag{110}$$

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

$$F_{ij} = F_{ij}^{(0)} + \delta^2 F_{ij}^{(2)}, \tag{111}$$

$$G_{ij} = G_{ij}^{(0)} + \delta^2 G_{ij}^{(2)}. \tag{112}$$

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

$$U^{ij(0)} = U^{(0)} \delta^{ij}, \tag{113}$$

with

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

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

$$U^{ij(2)} = (\delta_1 \mathbf{V}\cdot\mathbf{V} + 2\delta_2 \mathbf{S}\cdot\mathbf{V} + \delta_3 \mathbf{S}\cdot\mathbf{S})\delta^{ij} + \delta_4 V^i V^j + 2\delta_5 V^{(i} S^{j)} + \delta_6 S^i S^j. \tag{114}$$

Similar calculation can be performed for F_{ij} and G_{ij}. One finds

$$F^{ij(0)} = F^{(0)} \delta^{ij}, \tag{115}$$

$$G^{ij(0)} = G^{(0)} \delta^{ij}, \tag{116}$$

where

$$F^{(0)} = \frac{2}{3m^* d_0} \int_0^\infty \exp(\lambda^{W(0)}\mathcal{E}) \frac{\mathcal{E}[\mathcal{E}(1+\alpha\mathcal{E})]^{3/2}}{1+\alpha\mathcal{E}}\, \mathrm{d}\mathcal{E}, \tag{117}$$

$$G_{(0)} = \frac{1}{nm^* d_0} \int_0^\infty \exp(-\lambda^{W(0)}\mathcal{E}) \left(1 + \frac{2}{3(1+2\alpha\mathcal{E})}\right) \mathcal{E}^{3/2}\sqrt{1+\alpha\mathcal{E}}\, \mathrm{d}\mathcal{E}. \tag{118}$$

The quadratic corrections are given by

$$F^{ij(2)} = (\varphi_1 \mathbf{V}\cdot\mathbf{V} + 2\varphi_2 \mathbf{S}\cdot\mathbf{V} + \varphi_3 \mathbf{S}\cdot\mathbf{S})\, \delta^{ij} + \varphi_4 V^i V^j + 2\varphi_5 V^{(i} S^{j)} + \varphi_6 S^i S^j,$$

$$G^{ij(2)} = (\eta_1 \mathbf{V}\cdot\mathbf{V} + 2\eta_2 \mathbf{S}\cdot\mathbf{V} + \eta_3 \mathbf{S}\cdot\mathbf{S})\, \delta^{ij} + \eta_4 V^i V^j + 2\eta_5 V^{(i} S^{j)} + \eta_6 S^i S^j.$$

The coefficients δ_i, φ_i and η_i are reported in [18, 19].

3.4. PARABOLIC BAND APPROXIMATION

In this section we shall consider the limiting case $\alpha \mapsto 0$. The aim is two fold. 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 $a, \nu > 0$

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

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

$$\frac{\lambda}{k_{\mathrm{B}}}=-\log\frac{n}{\left(\frac{4}{3}\pi m^*W\right)^{3/2}}+\frac{9m^*}{4W^2}\mathbf{V}\cdot\mathbf{S}-\frac{27m^*}{20W^3}\mathbf{S}\cdot\mathbf{S}, \tag{119}$$

$$\lambda^W=\frac{3}{2W}+\frac{21m^*}{8W^2}\mathbf{V}\cdot\mathbf{V}-\frac{9m^*}{2W^3}\mathbf{V}\cdot\mathbf{S}+\frac{81m^*}{40W^4}\mathbf{S}\cdot\mathbf{S}, \tag{120}$$

$$\lambda_i=-\frac{21m^*}{4W}V_i+\frac{9m^*}{4W^2}S_i, \tag{121}$$

$$\lambda_i^W=\frac{9m^*}{4W^2}V_i-\frac{27m^*}{20W^3}S_i. \tag{122}$$

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

$$\begin{aligned} f_{ME}^P = {} & \frac{n\exp(-\lambda^{W(0)}\mathcal{E})}{(\frac{4}{3}\pi m^*W)^{3/2}}\times \\ & \times\left\{1-\left(-\frac{21m^*}{4W}V_i+\frac{9m^*}{4W^2}S_i\right)v^i-\left(\frac{9m^*}{4W^2}V_i-\frac{27m^*}{20W^3}S_i\right)\mathcal{E}v^i+\right. \\ & +\frac{1}{2}\left[\left(-\frac{21m^*}{4W}V_i+\frac{9m^*}{4W^2}S_i\right)v^i+\left(\frac{9m^*}{4W^2}V_i-\frac{27m^*}{20W^3}S_i\right)\mathcal{E}v^i\right]^2- \\ & -\left(\frac{9m^*}{4W^2}\mathbf{V}\cdot\mathbf{S}-\frac{27m^*}{20W^3}\mathbf{S}\cdot\mathbf{S}\right)- \\ & \left.-\left(\frac{21m^*}{8W^2}\mathbf{V}\cdot\mathbf{V}-\frac{9m^*}{2W^3}\mathbf{V}\cdot\mathbf{S}+\frac{81m^*}{40W^4}\mathbf{S}\cdot\mathbf{S}\right)\mathcal{E}\right\} \end{aligned} \tag{123}$$

and the constitutive equations become

$$\begin{aligned} U_{ij}^P = {} & \frac{2}{3}W\delta_{ij}+\left(-\frac{7}{6}m^*\mathbf{V}\cdot\mathbf{V}+\frac{7m^*}{5W}\mathbf{S}\cdot\mathbf{V}-\frac{27m^*}{50W^2}\mathbf{S}\cdot\mathbf{S}\right)\delta^{ij}+ \\ & +\frac{7}{2}m^*V^iV^j-\frac{21m^*}{5W}V^{(i}S^{j)}+\frac{81m^*}{50W^2}S^iS^j, \end{aligned} \tag{124}$$

$$\begin{aligned} m^*F_{ij}^P = {} & \frac{10}{9}W^2\delta_{ij}+\left(-\frac{7}{18}m^*W\mathbf{V}\cdot\mathbf{V}+\frac{m^*}{15}\mathbf{S}\cdot\mathbf{V}-\frac{9m^*}{50W}\mathbf{S}\cdot\mathbf{S}\right)\delta^{ij}+ \\ & +\frac{77}{6}m^*WV^iV^j-\frac{91m^*}{5}V^{(i}S^{j)}+\frac{357m^*}{50W}S^iS^j, \end{aligned} \tag{125}$$

$$G_{ij}=\frac{1}{m^*}(U_{ij}+W\delta_{ij}). \tag{126}$$

In order to compare the results with those obtained for the monatomic gas and the hydrodynamical models of semiconductors presented in [14, 15, 54, 55], we observe that

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

Therefore, by defining the electron temperature through

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

and introducing the heat flux

$$n q_i = \tfrac{1}{2} m^* \int_{\mathcal{B}} c_i c_k c^k f \, \mathrm{d}^3\mathbf{k},$$

and the shear tensor

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

we have up to second order terms

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

Then the lagrangian multipliers read

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

which are same as those obtained for a monatomic gas in the inviscid case. This shows that according to the results presented in [54], 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 nonconvective parts (compare the previous expressions for the $\Lambda' s$ with that reported in [56, 57]).

The constitutive Equations (124),(125) become[2]

$$U_{ij}^{(P)} = m^* V_i V_j + k_{\mathrm{B}} T \delta_{ij} + \frac{4 m^*}{5 k_{\mathrm{B}} T} V_{<i} q_{j>} + \frac{18 m^*}{25 (k_{\mathrm{B}} T)^2} q_{<i} q_{j>}, \tag{127}$$

$$\begin{aligned} m^* F_{ij}^{(P)} = & \left(\frac{1}{2} m^* V^2 k_{\mathrm{B}} T + \frac{5}{2} (k_{\mathrm{B}} T)^2 - \frac{8}{15} m^* \mathbf{V}\cdot\mathbf{q} - \frac{3}{25} \frac{m^* q^2}{k_{\mathrm{B}} T} \right) \delta_{ij} + \\ & + \frac{7}{2} m^* k_{\mathrm{B}} T V_i V_j + \frac{28}{5} m^* V_{(i} q_{j)} + \frac{119}{25} \frac{m^* q_i q_j}{k_{\mathrm{B}} T}. \end{aligned} \tag{128}$$

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

By comparing the relation (127) with the analogous expression $U_{ij}^{(\mathrm{MG})}$ in the case of a monoatomic gas [56]

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

we may make the identification

$$\sigma_{ij} = \frac{4m^*}{5k_{\mathrm{B}}T} V_{\langle i} q_{j\rangle} + \frac{18m^*}{25(k_{\mathrm{B}}T)^2} q_{\langle i} q_{j\rangle}. \tag{129}$$

Now, if such an expression for σ_{ij} is inserted into the expression for R_{ij} for the monatomic gas [56], $R_{ij}^{(\mathrm{MG})}$, 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)

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

This is the same expression (128).

3.5. CLOSURE OF THE PRODUCTION TERMS

The problem of the closure of the production terms has been tackled in different ways. In [53] 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 [17] 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.

3.6. ACOUSTIC PHONON SCATTERING

If we set

$$K_{\mathrm{ac}} = \frac{k_{\mathrm{B}} T_{\mathrm{L}} \Xi_{\mathrm{d}}^2}{4\pi^2 \hbar \rho v_s^2},$$

the collision term for acoustic phonon scattering becomes

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

Since the scattering is elastic, one gets $C_W = 0$. Concerning the production terms of crystal momentum and energy flux, we can write

$$C_P^i = c_{11}^{(\mathrm{ac})}(W) V_i + c_{12}^{(\mathrm{ac})}(W) S_i, \tag{130}$$

$$C_W^i = c_{21}^{(\mathrm{ac})}(W) V_i + c_{22}^{(\mathrm{ac})}(W) S_i. \tag{131}$$

The production matrix

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

is given by $C^{(\mathrm{ac})} = A^{(\mathrm{ac})} B$. 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 $A^{(\mathrm{ac})}$ read

$$a_{11}^{(\mathrm{ac})} = \frac{\overline{K}_{ac}}{d_0} \int_0^{\infty} \mathcal{E}^2 \left(1 + \alpha\mathcal{E}\right)^2 \left(1 + 2\alpha\mathcal{E}\right) \exp\left(-\lambda^{W(0)}\mathcal{E}\right) \, \mathrm{d}\mathcal{E}, \tag{132}$$

$$a_{12}^{(\mathrm{ac})} = \frac{\overline{K}_{\mathrm{ac}}}{d_0} \int_0^{\infty} \mathcal{E}^3 \left(1 + \alpha\mathcal{E}\right)^2 \left(1 + 2\alpha\mathcal{E}\right) \exp\left(-\lambda^{W(0)}\mathcal{E}\right) \, \mathrm{d}\mathcal{E}, \tag{133}$$

$$a_{21}^{(\mathrm{ac})} = \frac{\overline{K}_{\mathrm{ac}}}{m^* d_0} \int_0^{\infty} \mathcal{E}^3 \left(1 + \alpha\mathcal{E}\right)^2 \exp\left(-\lambda^{W(0)}\mathcal{E}\right) \, \mathrm{d}\mathcal{E}, \tag{134}$$

$$a_{22}^{(\mathrm{ac})} = \frac{\overline{K}_{\mathrm{ac}}}{m^* d_0} \int_0^{\infty} \mathcal{E}^4 \left(1 + \alpha\mathcal{E}\right)^2 \exp\left(-\lambda^{W(0)}\mathcal{E}\right) \, \mathrm{d}\mathcal{E}, \tag{135}$$

where

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

3.7. NON-POLAR OPTICAL PHONON SCATTERING

For the non polar optical phonon scattering the collision term becomes

$$\mathcal{C}[f] \approx \mathcal{C}[f_{ME}] = \mathcal{C}_{\mathrm{G}}[f_{ME}] - \mathcal{C}_{\mathrm{L}}[f_{ME}].$$

If we set

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

the gain part can be written as

$$\begin{aligned}\mathcal{C}_{\mathrm{G}}[f_{ME}] \;=\; & \frac{4\pi\sqrt{2}(m^*)^{3/2}K_{\mathrm{np}}}{\hbar^3}\exp\left(-\frac{\lambda^{(0)}}{k_{\mathrm{B}}}\right)\left(n_{\mathrm{B}}+\frac{1}{2}\pm\frac{1}{2}\right)\mathcal{N}_{\pm}\exp\left(\pm\frac{\hbar\omega_{\mathrm{np}}}{k_{\mathrm{B}}T_0}\right)\times \\ & \times\,\exp\left[-\lambda^{W(0)(\mathcal{E}\pm\hbar\omega_{\mathrm{np}})}\right], \end{aligned} \tag{136}$$

where

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

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

$$\mathcal{C}_{\mathrm{L}}[f_{ME}] = \frac{4\pi\sqrt{2}(m^*)^{3/2}K_{\mathrm{np}}}{\hbar^3}\left(n_{\mathrm{B}}+\frac{1}{2}\mp\frac{1}{2}\right)\mathcal{N}_{\pm}f_{ME}.$$

At variance with the case of acoustic phonon scattering, energy is not conserved because non-polar optical phonon scattering is not elastic. Moreover, the effects of intervalley interaction must be taken into account. One finds up to the first order in δ

$$C_W = \sum_{A=1}^{6} C_{W_A},$$

where for each valley

$$C_{W_A} = \frac{3}{2}\frac{\overline{K}_{\mathrm{np}}}{d_0}\left(n_{\mathrm{B}}+\frac{1}{2}\mp\frac{1}{2}\right)\left[\exp\left(\pm\frac{\hbar\omega_{\mathrm{np}}}{k_{\mathrm{B}}T_0}\mp\lambda^{W(0)}\hbar\omega_{\mathrm{np}}\right)-1\right]\eta^{\pm}. \tag{137}$$

with

$$\eta^{\pm} = \int_0^{\infty}\mathcal{E}\mathcal{N}_{\pm}\sqrt{\mathcal{E}(1+\alpha\mathcal{E})}(1+2\alpha\mathcal{E})\exp\left(-\lambda^{W(0)\mathcal{E}}\right)\,\mathrm{d}\mathcal{E}$$

and

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

For the quadratic correction see [19].

At thermal equilibrium $\lambda^{W(0)} = 1/k_{\mathrm{B}}T_0$ and the zeroth-order term for energy production vanishes.

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

$$C_P^i = c_{11}^{(\mathrm{np})}(W)V_i + c_{12}^{(\mathrm{np})}(W)S_i, \tag{138}$$

$$C_W^i \;=\; c_{21}^{(\mathrm{np})}(W)V_i + c_{22}^{(\mathrm{np})}(W)S_i. \tag{139}$$

The production matrix

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

is given by

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

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

$$\begin{aligned}
a_{11}^{\mathrm{np}} &= \frac{\overline{K}_{\mathrm{np}}}{d_0} \sum_{\pm} \left(n_{\mathrm{B}} + \frac{1}{2} \mp \frac{1}{2} \right) \int_{\hbar\omega_{\mathrm{np}} H(1\mp 1)}^{\infty} \mathcal{N}_{\pm} \mathcal{E}^{3/2} (1+\alpha\mathcal{E})^{3/2} \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E}, \\
a_{12}^{\mathrm{np}} &= \frac{\overline{K}_{\mathrm{np}}}{d_0} \sum_{\pm} \left(n_{\mathrm{B}} + \frac{1}{2} \mp \frac{1}{2} \right) \int_{\hbar\omega_{\mathrm{np}} H(1\mp 1)}^{\infty} \mathcal{N}_{\pm} \mathcal{E}^{5/2} (1+\alpha\mathcal{E})^{3/2} \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E}, \\
a_{21}^{\mathrm{np}} &= \frac{\overline{K}_{\mathrm{np}}}{m^* d_0} \sum_{\pm} \left(n_{\mathrm{B}} + \frac{1}{2} \mp \frac{1}{2} \right) \int_{\hbar\omega_{\mathrm{np}} H(1\mp 1)}^{\infty} \mathcal{N}_{\pm} \frac{\mathcal{E}^{5/2} (1+\alpha\mathcal{E})^{3/2}}{1+2\alpha\mathcal{E}} \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E}, \\
a_{22}^{\mathrm{np}} &= \frac{\overline{K}_{\mathrm{np}}}{m^* d_0} \sum_{\pm} \left(n_{\mathrm{B}} + \frac{1}{2} \mp \frac{1}{2} \right) \int_{\hbar\omega_{\mathrm{np}} H(1\mp 1)}^{\infty} \mathcal{N}_{\pm} \frac{\mathcal{E}^{7/2} (1+\alpha\mathcal{E})^{3/2}}{1+2\alpha\mathcal{E}} \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E}.
\end{aligned}$$

3.8. 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

$$C_P^i = c_{11}^{(\mathrm{imp})}(W) V_i + c_{12}^{(\mathrm{imp})}(W) S_i, \tag{140}$$

$$C_W^i = c_{21}^{(\mathrm{imp})}(W) V_i + c_{22}^{(\mathrm{imp})}(W) S_i. \tag{141}$$

The production matrix decomposes as

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

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

$$\begin{aligned}
a_{11}^{(\mathrm{imp})} &= \frac{K_{\mathrm{imp}}}{d_0} \int_0^{\infty} \frac{(1+\alpha\mathcal{E})^{3/2}(1+2\alpha\mathcal{E})}{\sqrt{\mathcal{E}}} \left(\log \frac{1+\gamma}{\gamma} + \frac{1}{1+\gamma} \right) \times \\
&\quad \times \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E},
\end{aligned} \tag{142}$$

$$\begin{aligned}
a_{12}^{(\mathrm{imp})} &= \frac{K_{\mathrm{imp}}}{d_0} \int_0^{\infty} (1+\alpha\mathcal{E})^{3/2}(1+2\alpha\mathcal{E}) \sqrt{\mathcal{E}} \left(\log \frac{1+\gamma}{\gamma} + \frac{1}{1+\gamma} \right) \times \\
&\quad \times \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E},
\end{aligned} \tag{143}$$

$$\begin{aligned}
a_{21}^{(\mathrm{imp})} &= \frac{K_{\mathrm{imp}}}{m^* d_0} \int_0^{\infty} \sqrt{\mathcal{E}} (1+\alpha\mathcal{E})^{3/2} \left(\log \frac{1+\gamma}{\gamma} + \frac{1}{1+\gamma} \right) \times \\
&\quad \times \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E},
\end{aligned} \tag{144}$$

$$\begin{aligned}
a_{22}^{(\mathrm{imp})} &= \frac{K_{\mathrm{imp}}}{m^* d_0} \int_0^{\infty} \mathcal{E}^{3/2} (1+\alpha\mathcal{E})^{3/2} \left(\log \frac{1+\gamma}{\gamma} + \frac{1}{1+\gamma} \right) \times \\
&\quad \times \exp\left(-\lambda^{W(0)} \mathcal{E}\right) \, \mathrm{d}\mathcal{E},
\end{aligned} \tag{145}$$

where

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

3.9. PARABOLIC BAND LIMIT

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

For the acoustic phonon scattering one finds

$$a_{11}^{(\text{ac})} = \frac{32}{3}\frac{\sqrt{2\pi}K_{\text{ac}}}{\hbar^3}(m^*)^{3/2}\left(\frac{2}{3}W\right)^{3/2}, \tag{146}$$

$$a_{12}^{(\text{ac})} = 32\frac{\sqrt{2\pi}K_{\text{ac}}}{\hbar^3}(m^*)^{3/2}\left(\frac{2}{3}W\right)^{5/2}, \tag{147}$$

$$a_{21}^{(\text{ac})} = \frac{a_{12}^{(\text{ac})}}{m^*}, \tag{148}$$

$$a_{22}^{(\text{ac})} = 128\frac{\sqrt{2\pi m^*}K_{\text{ac}}}{\hbar^3}\left(\frac{2}{3}W\right)^{7/2}. \tag{149}$$

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

$$K_\nu = \frac{\sqrt{\pi}(z/2)^\nu}{\Gamma\left(\nu + \frac{1}{2}\right)}\int_0^\infty \exp(-z\cosh t)\sinh^{2\nu} t\, \mathrm{d}t, \quad z, \nu > 0, \tag{150}$$

with Γ the Gamma function.

After some algebra (the details are reported in Appendix A) one obtains up to first order the following expressions

$$\begin{aligned} C_W = {} & \left(\frac{2}{3}W\right)^{-1/2}\frac{2\sqrt{2\pi}(m^*)^{3/2}(\hbar\omega_{\text{np}})^2}{\hbar^3}K_{\text{np}}\sum_{\pm}\left(n_{\text{B}} + \frac{1}{2} \mp \frac{1}{2}\right)e^{\pm\zeta} \times \\ & \times \left[\exp\left(\pm\frac{\hbar\omega_{\text{np}}}{k_{\text{B}}T_{\text{L}}} \mp 2\zeta\right) - 1\right][K_2(\zeta) \mp K_1(\zeta)], \end{aligned} \tag{151}$$

$$\begin{aligned} a_{11}^{(\text{np})} = {} & \frac{4}{3}\left(\frac{2}{3}W\right)^{-1/2}\frac{\sqrt{2\pi}(m^*)^{3/2}(\hbar\omega_{\text{np}})^2}{\hbar^3}K_{\text{np}}\sum_{\pm}\left(n_{\text{B}} + \frac{1}{2} \mp \frac{1}{2}\right)e^{\pm\zeta} \times \\ & \times [K_2(\zeta) \mp K_1(\zeta)], \end{aligned} \tag{152}$$

$$\begin{aligned} a_{12}^{(\text{np})} = {} & \frac{4}{3}\sqrt{\frac{2}{3}W}\frac{\sqrt{2\pi}(m^*)^{3/2}(\hbar\omega_{\text{np}})^2}{\hbar^3}K_{\text{np}}\sum_{\pm}\left(n_{\text{B}} + \frac{1}{2} \mp \frac{1}{2}\right)e^{\pm\zeta} \times \\ & \times \{3K_2(\zeta) + 2\zeta[K_1(\zeta) \mp K_2(\zeta)]\}, \end{aligned} \tag{153}$$

$$a_{21}^{(\mathrm{np})} = \frac{a_{12}^{(\mathrm{np})}}{m^*}, \tag{154}$$

$$\begin{aligned} a_{22}^{(\mathrm{np})} = {} & \frac{4}{3}\left(\frac{2}{3}W\right)^{3/2} \frac{\sqrt{2\pi m^*}(\hbar\omega_{\mathrm{np}})^2}{\hbar^3} K_{\mathrm{np}} \sum_{\pm} \left(n_{\mathrm{B}} + \frac{1}{2} \mp \frac{1}{2}\right) e^{\pm\zeta} \times \\ & \times \left[K_2(\zeta)\left(12 \mp 9\zeta + 4\zeta^2\right) + K_1(\zeta)\left(3\zeta \mp 4\zeta^2\right)\right], \end{aligned} \tag{155}$$

with $\zeta = 3\hbar\omega_{\mathrm{np}}/(4W)$.

The quadratic correction to C_W is given by

$$c_W^{(1)}\mathbf{V}\cdot\mathbf{V} + 2c_W^{(2)}\mathbf{V}\cdot\mathbf{S} + c_W^{(3)}\mathbf{S}\cdot\mathbf{S}. \tag{156}$$

For the coefficients $c_W^{(i)}$ the interested reader is referred to [19].

Finally no analytical expressions are available for the scattering with impurities and one has to resort to a numerical evaluation of the coefficients of the production matrix.

4. Numerical Methods for Hydrodynamical Models of Semiconductors and Simulation of Electron Devices

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 non-linear 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 non-physical 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 [58, 59]). 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 [60]. 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 a numerical scheme enjoying such a property, well suited for the hydrodynamical models presented in the previous chapter.

The scheme has been proposed by Nessyahu and Tadmor (NT) [61]. 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 only for homogeneous systems. An extension of the method to systems that contain production terms has been formulated for one-dimensional problems in [62] and applied to semiconductors in [16, 17, 46].

In the following sections we briefly present the scheme 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 [63]. An alternative valid scheme has been also considered in [64, 65]. 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

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = G(U, E), \tag{157}$$

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),

$$\frac{\mathrm{d}U}{\mathrm{d}t} = G(U, E), \tag{158}$$

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

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0. \tag{159}$$

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 [16, 17, 46] for details). The electric potential is computed by solving with standard procedure the tridiagonal system

$$\epsilon(\phi_{j+1} - 2\phi_j + \phi_{j-1}) = -(\Delta x)^2 \left(N_{\mathrm{D}} - N_{\mathrm{A}} - n_i^n\right)$$

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

$$U^n_{j+1/2} = \tfrac{1}{2}(U^{n+1}_j + U^n_{j+1}) + \tfrac{1}{8}(U'_j - U'_{j+1}) - \lambda[F(U^{n+1/2}_{j+1}) - F(U^{n+1/2}_j)], \tag{160}$$

$$U^{n+1/2}_j = U^n_j - \tfrac{\lambda}{2} F'_j, \tag{161}$$

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

$$\lambda \cdot \max \rho(A(U(x, t))) < \tfrac{1}{2}, \tag{162}$$

where $\rho(A(U(x, t)))$ is the spectral radius of the Jacobian matrix, $A = \partial F/\partial U$.

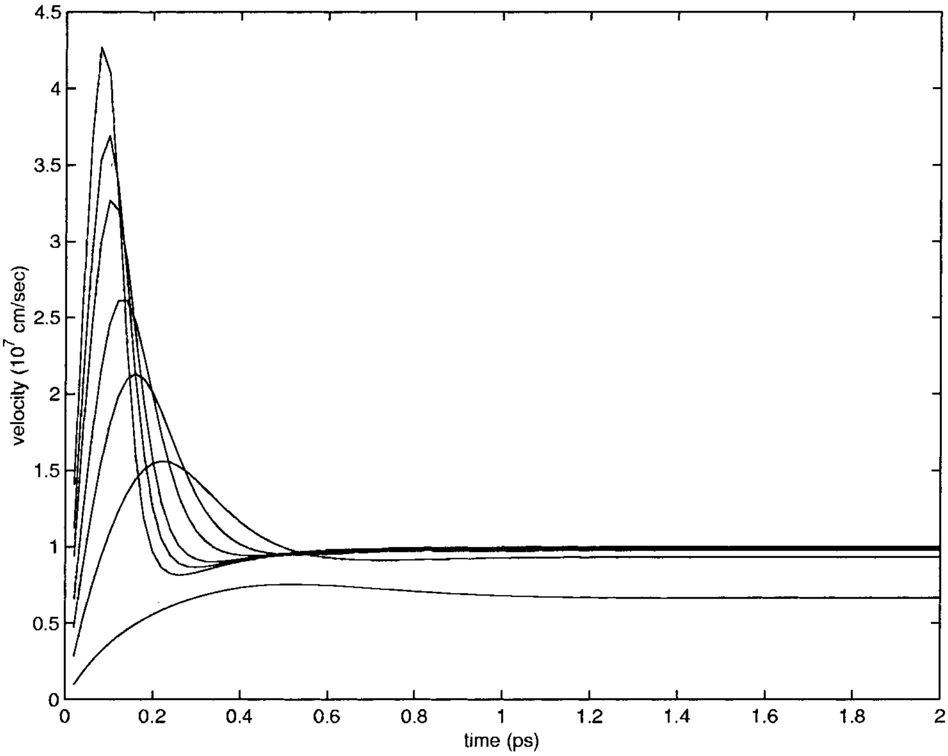

Figure 2. Velocity (cm/s) vs. time (ps) for $E = 10\,\text{kV/cm}, 30\,\text{kV/cm}, 50\,\text{kV/cm}, 70\,\text{kV/cm}, 100\,\text{kV/cm}, 120\,\text{kV/cm}, 150\,\text{kV/cm}$.

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 [60]),

$$U_j' = \text{MM}(d_{j-1/2}U + \tfrac{1}{2}\text{MM}(D_{j-1}, D_j), d_{j+1/2}U - \tfrac{1}{2}\text{MM}(D_j, D_{j+1})), \tag{163}$$

where $D_j = U_{j+1} - 2U_j + U_{j-1}$, $d_{j+1/2} = U_{j+1} - U_j$ and

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

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 [62, 66].

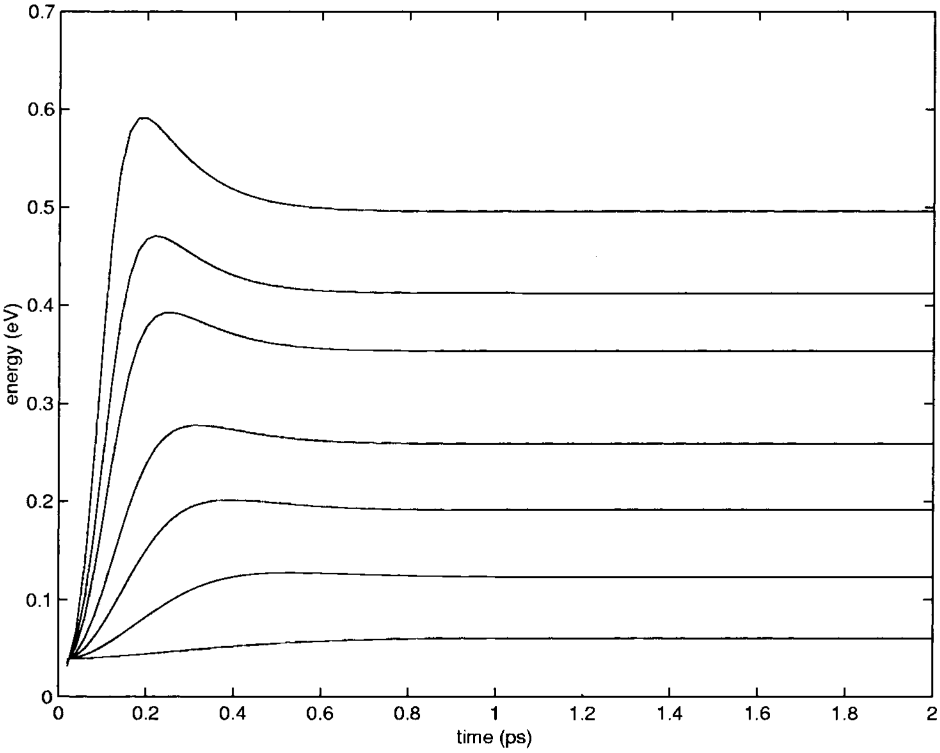

Figure 3. Energy (eV) versus time (ps) for the same values electric field as in Figure 2.

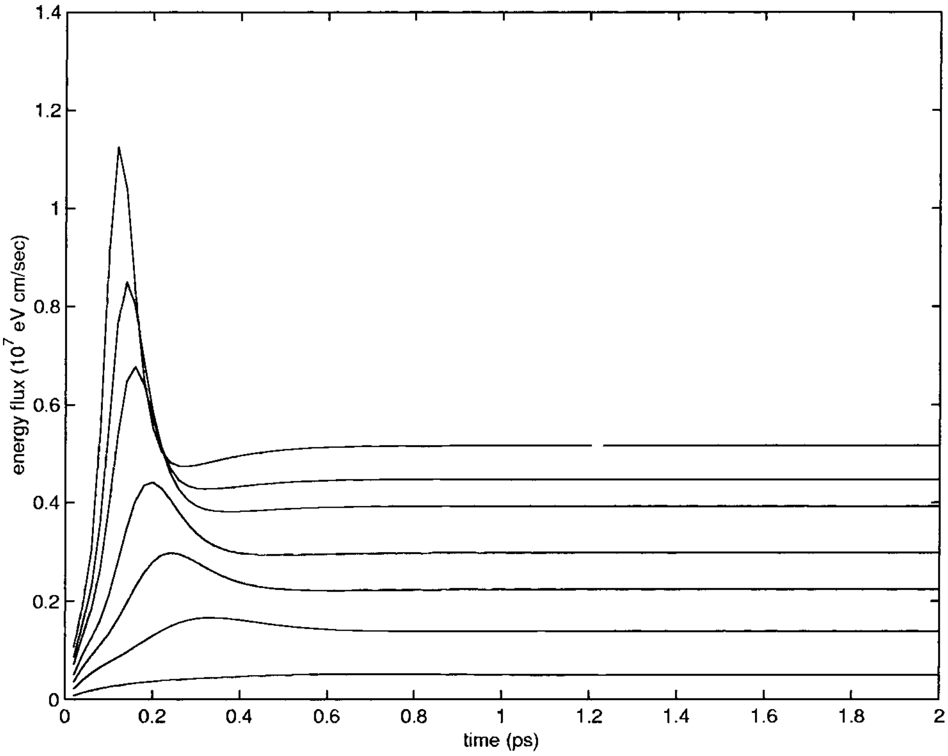

Figure 4. Energy flux (eV cm/sec) versus time (ps) for the same values of the electric field as in Figure 2.

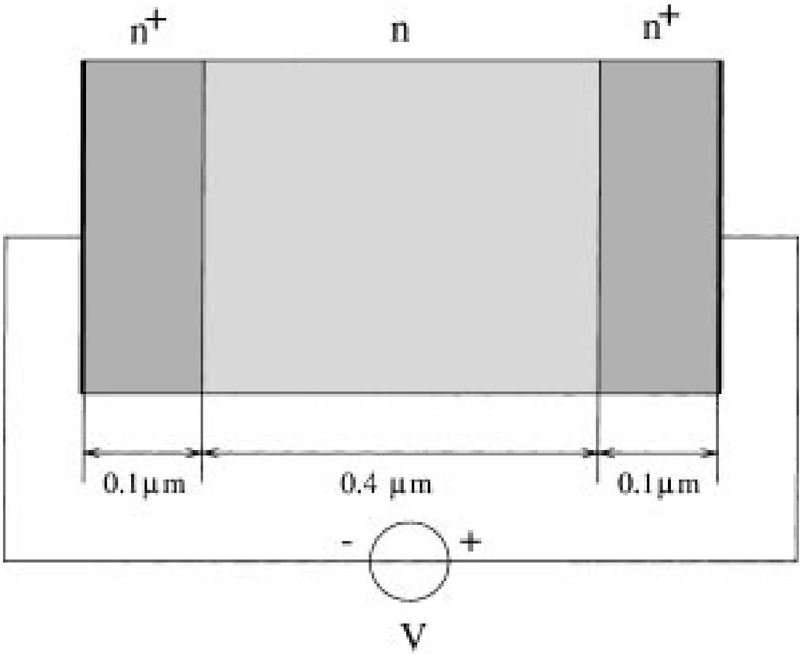

Figure 5. Schematic representation of a $n^+ - n - n^+$ silicon diode.

Table 3. Length of the channel, doping concentration and applied voltage in the test cases for the diode

Test #	Channel length L_c (μm)	N_D^+ ($\times 10^{17}$ cm^{-3})	N_D ($\times 10^{17}$ cm^{-3})	V_b (Volt)
1	0.4	5	0.02	2
2	0.3	10	0.1	1
3	0.2	10	0.1	1

Given the field at time t_n, (U^n, E^n), the field at time $t_{n+1/2}$ is obtained by

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

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. NUMERICAL RESULTS

In this section we test the hydrodynamical model presented in the previous section for silicon semiconductors by considering first the problem of the overshoot and saturation velocity in the bulk case and then by simulating a $n^+ - n - n^+$ silicon diode that models the channel of a MOSFET.

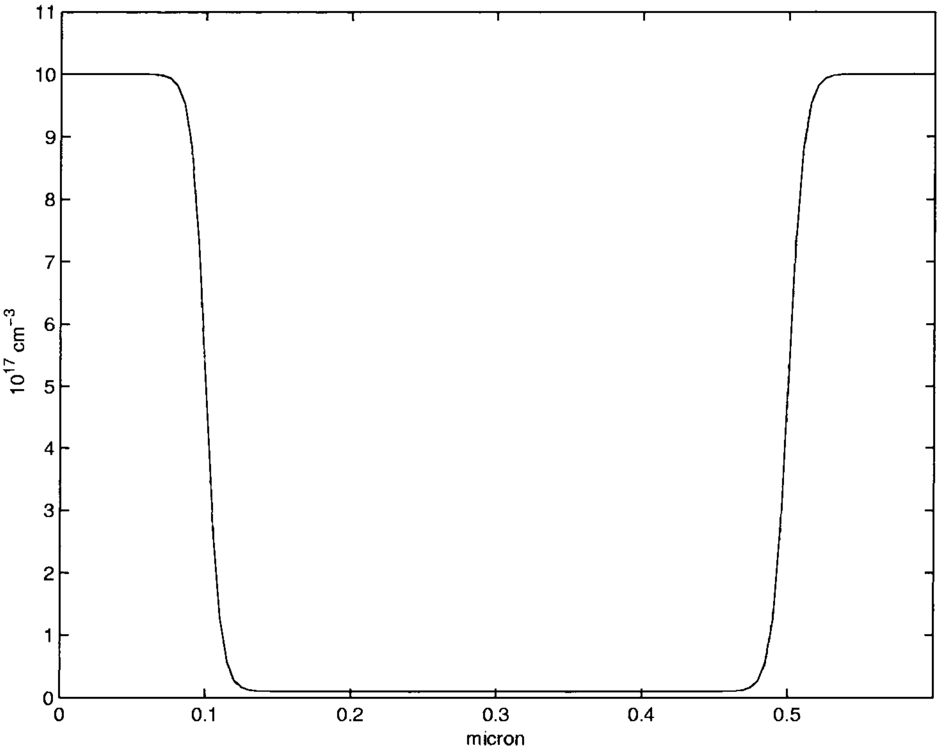

Figure 6. Doping profile for the test case 1.

We have implemented (see [20]) only the linear model, up to first order in δ, but the results are quite satisfactory and some problems of regularity of the solution, related to the quadratical closure moles, are avoided.

4.3. APPLICATION TO BULK SILICON

The physical situation is represented by a silicon semiconductor with a uniform doping concentration, we assume sufficiently low so that the scatterings with impurities can be neglected. On account of the symmetry with respect to translations, the solution does not depend on the spatial variables. The continuity equation gives $n =$ constant and from the Poisson equation one finds that $\mathbf{E}$ is also constant. Therefore the remaining balance equations reduce to the following set of ODEs for the motion along the direction of the electric field

$$\frac{\mathrm{d}}{\mathrm{d}t}V = -\frac{eE}{m^*} + \frac{2\alpha eEG}{m^*} + \left(\frac{c_{11}}{m^*} - 2\alpha c_{21}\right) V + \left(\frac{c_{12}}{m^*} - 2\alpha c_{22}\right) S, \tag{164}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}W = -eVE + C_W, \tag{165}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}S = -eEG^{(0)} + c_{21}V + c_{22}S, \tag{166}$$

where V and S are the component of $\mathbf{V}$ and $\mathbf{S}$ along the electric field.

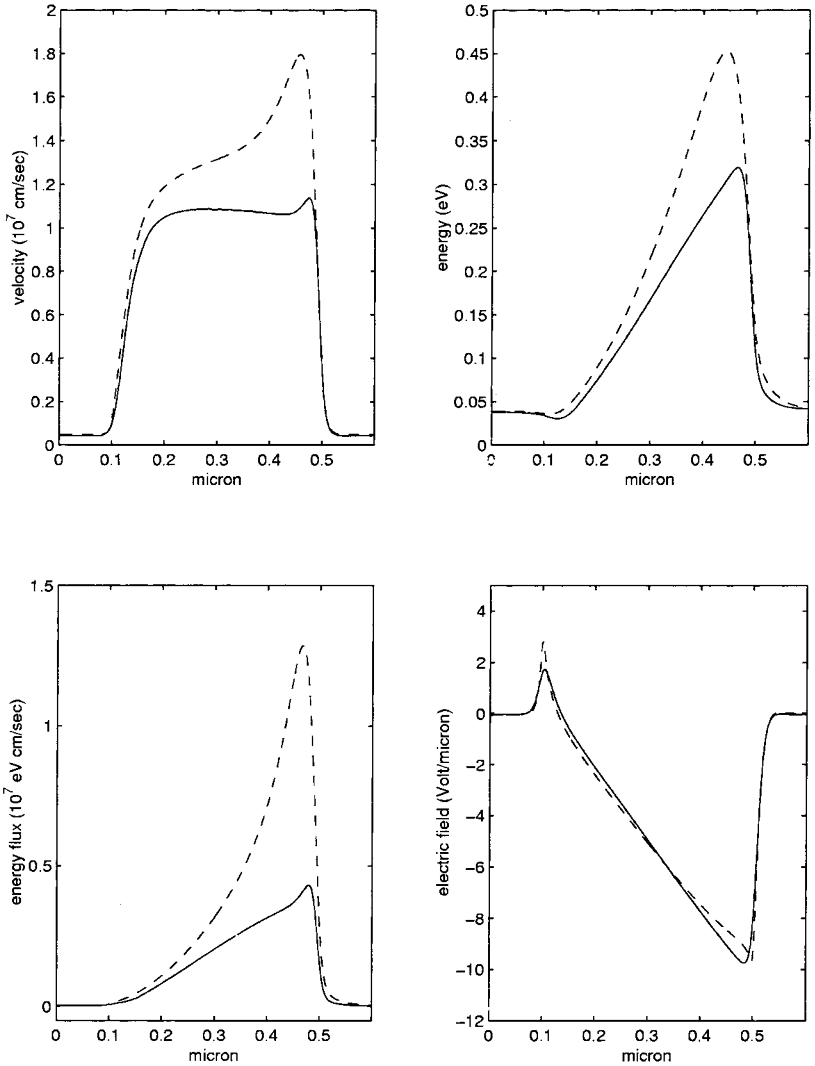

Figure 7. Numerical results of the test case 1 after 5 ps in the parabolic band case (dashed line) and for the Kane dispersion relation (continuous line).

As initial conditions for (164)–(166) we take

$$V(0) = 0, \tag{167}$$

$$W(0) = \tfrac{3}{2} k_{\mathrm{B}} T_{\mathrm{L}}, \tag{168}$$

$$S(0) = 0. \tag{169}$$

The stationary regime is reached in a few picoseconds.

The solutions of (164)–(166) for several values of the electric field are reported in Figures 2 (velocity), 3 (energy) and 4 (energy flux).

The typical phenomena of overshoot and saturation velocity are both qualitatively and quantitatively well described (see [67] fig. 3.22 for a comparison with the results obtained by MC simulations).

Similar results were reported in [19], but there a different modeling of the collision terms has been considered and, moreover, instead to take into account all the intervalley and in-

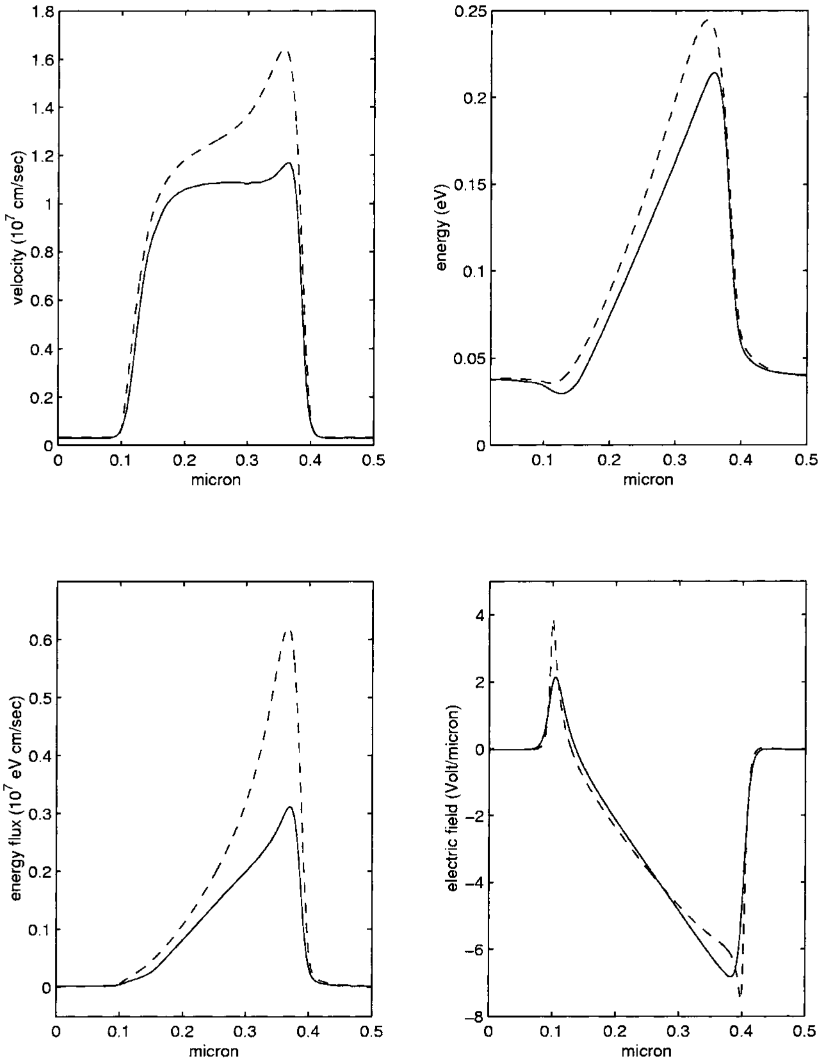

Figure 8. Numerical results of the test case 2 after 5 ps in the parabolic band case (dashed line) and for the Kane dispersion relation (continuous line).

travalley scatterings, mean values of the coupling constant Ξ and $D_t K$ have been introduced. The inclusion of all the scattering (intervalley and intravalley) mechanisms improve notably the results.

4.4. APPLICATION TO $n^+ - n - n^+$ SILICON DIODE

As second problem we simulate a ballistic $n^+ - n - n^+$ silicon diode (see Figure 5).

The n^+ regions are 0.1 μm long while the channel has different length. Moreover several doping profiles will be considered according to the Table 3.

Initially the electron energy is that of the lattice in thermal equilibrium at the temperature T_L, the charges are at rest and the density is equal to the doping concentration

$$n(x,0) = n_0(x), \quad W(x,0) = \tfrac{3}{2} k_B T_L, \quad V(x,0) = 0, \quad S(x,0) = 0.$$

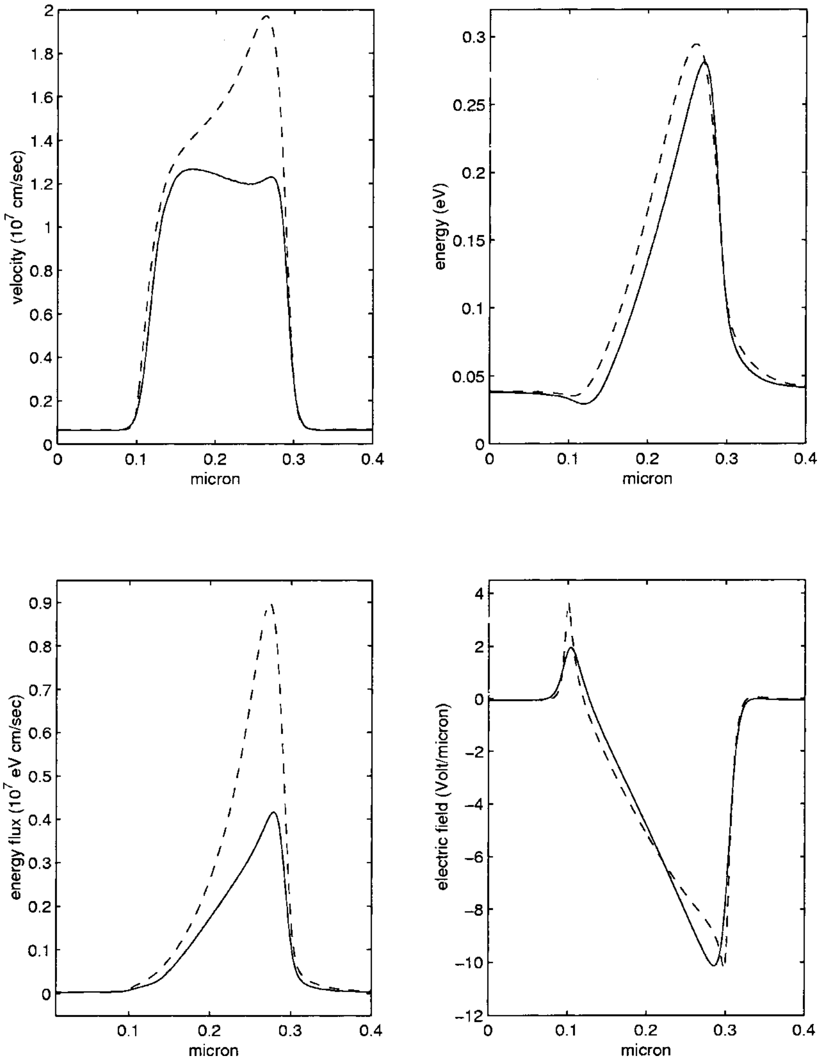

Figure 9. Numerical results of the test case 3 after 5-ps in the parabolic band case (dashed line) and for the Kane dispersion relation (continuous line).

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, we impose, in analogy with similar cases [16, 45] a double number of boundary conditions. More precisely, we give conditions for all the variables in each boundary, located at $x = 0$ and $x = L$,

$$n(0,t) = n(L,t) = N_D^+, \tag{170}$$

$$\frac{\partial}{\partial x} W(0,t) = \frac{\partial}{\partial x} W(L,t) = 0, \tag{171}$$

$$\frac{\partial}{\partial x} V(0,t) = \frac{\partial}{\partial x} V(L,t) = 0, \tag{172}$$

$$\frac{\partial}{\partial x} S(0,t) = \frac{\partial}{\partial x} S(L,t) = 0, \tag{173}$$

$$\phi(0) = 0 \quad \text{and} \quad \phi(L) = V_b, \tag{174}$$

where V_b is the applied bias voltage. In all the numerical solutions there is no sign of spurious oscillations near the boundary, indicating that the conditions (170)–(173) are in fact compatible with the solution of the problem.

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 $s = 0.01\,\mu\text{m}$, $n_0 = n_0(0)$, $d_0 = n_0(1 - N_D/N_D^+)/2$, $x_1 = 0.1\,\mu\text{m}$, and $x_2 = x_1 + L_c$ with L_c channel length. The total length of the device is $L = L_c + 0.2\,\mu\text{m}$. In Figure 6 the doping profile for the test case 1 is plotted.

A grid with 400 nodes has been used. The stationary solution is reached within a few picoseconds (about five), after a short transient with wide oscillations.

As first case we consider the test problem 1 (length of the channel 0.4 micron) with $V_b =$ 2 Volts. In Figure 7 (continuous line) the stationary solution (after 5 ps) is plotted. At variance with the numerical results obtained in [16] for the parabolic case by using a quadratic closure in δ, our numerical solutions do not present irregularities. This can be probably ascribed to the absence of the nonlinearities in the dissipative variables.

If we compare the results with those reported in [9] (Figures 1–4) and obtained by solving with Monte Carlo method the Boltzmann–Poisson system, there is a good agreement in all the variables W, V and S.

The simulation for the parabolic band approximation is also shown (Figure 7 dashed line), but it is evident, like in the bulk case, that the results are rather poor.

The other test cases have been numerically integrated with $V_b = 1$ Volt (Figures 8, 9). For these cases Monte Carlo data is not at our disposal, but the behaviour of the solution looks again physically reasonable and encouraging: the spurious spike across the second junction is here less apparent than several other hydrodynamical models. The results with the parabolic band are again rough when compared with those obtained in the non-parabolic case.

Acknowledgements

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