

# Non parabolic band transport in semiconductors: closure of the moment equations

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The problem of the closure of the moment equations of the semiconductor Boltzmann equation is studied in the framework of the Kane dispersion relation (therefore avoiding the limitations of the parabolic band approximation). By using the maximum entropy ansatz for the closure one obtains, in the limit of small anisotropy, explicit constitutive relations for the stress tensor and the flux of energy flux tensor. The results obtained are in remarkable agreement with those arising from Monte Carlo simulations.

## 1 Introduction

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. Also the new concepts of MEMS (integrated electromechanical sensors) require, for an efficient CAD tool, a thorough understanding of the interaction between charged carrier transport and mechanical, thermal and magnetic effects in a semiconductor. The standard drift-diffusion models cannot cope with high-field and submicron phenomena, because they do not comprise energy as a dynamical variable and furthermore they are obtained from short mean free path expansions [1]. Therefore it is mandatory to describe these phenomena within the framework of the semiclassical Boltzmann Transport Equation (BTE). The fundamental approach is to solve the BTE, but this is a daunting task, also from the numerical viewpoint. Presently one of the most popular approaches is to solve the BTE in a stochastic sense by Monte Carlo methods and use the results as a way of determining the parameters in macroscopic models which are obtained from the BTE by suitable approximations. In the hierarchy of approximate macroscopic models beyond the drift-diffusion equations one finds the hydrodynamical models, which are obtained from the infinite set of moment equations of the Boltzmann transport equation (BTE) by a suitable truncation procedure.

It is well-known that moment systems require a closure assumption in order to lead to a closed system of evolution equation. In the case of parabolic band approximation various closure assumptions have been made for the semiconductor transport moment systems, leading to various classes of hydrodynamical models, e.g. [2, 3, 4]. However, these various closure assumptions are, at best, only phenomenological and lack a consistent physical and mathematical justification. Lately a closure assumption based on the entropy principle of extended thermodynamics [5, 6] or equivalently the method of exponential moments [7] has been applied, in the parabolic band approximation, to the semiconductor moment equations, leading to a semicon-

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ductor hydrodynamical model free from phenomenological assumptions and enjoying important mathematical properties like hyperbolicity [8, 9, 10, 11].

In this method the distribution function used to calculate the higher order moments and the productions is assumed to be that which maximizes the entropy under the constraints of the given set of moments. The resulting constitutive equations for various moments have been compared with the results obtained by Monte Carlo (MC) simulations in [12] and are very encouraging in support of the maximum entropy ansatz.

The parabolic band approximation is however not fully adequate in order to describe high energy phenomena. Short of a full band description, a widely used analytical approximation to the band structure is the Kane dispersion relation [13].

For the Kane dispersion relation the analogy between the moment system and the gas-dynamic one is not so close and depends on the choice of the appropriate weight functions in the definition of the moments. Various formulations of the moment-like equations exist, with phenomenological based closure [14, 15, 16]

In this article we extend the maximum entropy approach to semiconductor moment-like systems in the case of the Kane dispersion relation. Here we do not compute the production terms with the maximum entropy ansatz but we concentrate on the closure for the high order fluxes. The validity of the constitutive equations has been assessed by comparing them with those obtained in the stationary regime from the simulations of semiconductor devices by Monte Carlo methods.

The plan of the paper is as follows. In Sect. 2 the basic concepts concerning the energy band structure and the electron transport in semiconductors are briefly presented. In Sect. 3 macroscopic balance equations are obtained as moment equations of the Boltzmann transport equation for electrons in semiconductors. The appropriate formulation of the maximum entropy principle is given in Sect. 4 where the closure procedure is shown. The results of this section are then used for getting the closure relations in the case of Kane's dispersion relation. The limit of parabolic band approximation is recovered in Sect. 6 and in the last section a comparison with previous models is presented.

## 2 Basic concepts on the energy band structure and electron transport in semiconductors

In this section we give a brief account of the main concepts and assumptions concerning the physics of semiconductors and the charge transport inside them, mainly in order to fix the notation and make the reader acquainted with the basic concepts of solid state physics needed in the following (for a more accurate description the interested reader is referred to a standard text-book, e.g. [17]).

Charge carriers in a semiconductor move under the effect of a periodic crystal potential, due to the atomic nuclei, and under the effect of the potential due to the charges of the carriers themselves. Ideal crystals are described in terms of Bravais lattices, which are sets of vectors of the form

$$\mathcal{L} = \{i\mathbf{a}_1 + j\mathbf{a}_2 + l\mathbf{a}_3 : i, j, l \in \mathcal{Z}\}$$

where  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  are primitive lattice vectors,  $\mathcal{Z}$  being the set of relative integers. The reciprocal lattice  $\mathcal{L}^*$  of the Bravais lattice  $\mathcal{L}$  is defined by

$$\mathcal{L}^* = \{i\mathbf{a}^1 + j\mathbf{a}^2 + l\mathbf{a}^3 : i, j, l \in \mathcal{Z}\}$$

with the reciprocal lattice vectors  $\mathbf{a}^1, \mathbf{a}^2, \mathbf{a}^3$  satisfying

$$\mathbf{a}_i \cdot \mathbf{a}^j = 2\pi\delta_i^j.$$

A connected subset  $\mathcal{B} \subseteq \mathcal{R}^3$  is called a *primitive cell* of the lattice if the volume of  $\mathcal{B}$  equals  $|\mathbf{a}_1 \cdot \mathbf{a}_2 \wedge \mathbf{a}_3|$  and the whole space  $\mathcal{R}^3$  is covered by the union of translates of  $\mathcal{B}$  by the lattice vectors.

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

The quantum mechanical dynamics of an electron in the periodic potential of an ideal crystal lattice is governed by *Bloch's Theorem* whose contents we summarize below.

Consider an electron moving under the action of the potential  $V_L$  generated by the ions located at the points of the crystal lattice  $\mathcal{L}$ . Since the periodicity of the potential is on scale of the order of the de Broglie wavelength, the electron states are determined by the time independent Schrödinger equation

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

with the Hamiltonian  $H$  given by

$$H = -\frac{\hbar^2}{2m_e} \Delta - qV_L,$$

$\hbar$  being the Planck constant divided by  $2\pi$  and  $m_e$  electron mass in the vacuum.

The bounded eigenstates have the form:

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

and

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

One obtains a second order self-adjoint elliptic problem posed on a primitive cell of the crystal lattice  $\mathcal{L}$ . It is possible to prove [17] the existence of an infinite sequence of eigenpairs (energy-wave function)

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

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

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

with  $\mathbf{x} \in \mathcal{R}^3$ ,  $\mathbf{X} \in \mathcal{L}$ , it follows that the set of eigenfunctions  $\psi$  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.

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. In the sequel we neglect the hole motion and restrict ourselves to electrons, considering for the sake of clarity only one conduction band.

The energy band structure of crystals for electrons can be obtained at the expenses of intensive numerical calculations (and also semiphenomenologically) by the quantum theory of solids. However, in order to describe electron transport, for most applications, a simplified description is adopted which is based on a simple analytical model.

This is the so-called effective parabolic band and effective mass approximation, where the energy curve corresponding to a given energy band is approximated by a parabola near its minimum.  $\mathcal{B}$  is expanded to all  $\mathbf{R}^3$  and in the approximation of a single band (hereafter we omit the band index)

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

with  $m^*$  as the *effective mass* (e.g. in the case of Si  $m^* = 0.32m_e$ ) and  $\hbar\mathbf{k}$  the so-called *crystal momentum*.

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

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

where  $\alpha$  is the non parabolicity parameter ( e.g. for Silicon  $\alpha=0.5 \text{ eV}^{-1}$  while for GaAs  $\alpha=0.64 \text{ eV}^{-1}$  in the  $\Gamma$ -valley,  $\alpha=0.46$  in the  $L$ -valley and  $\alpha = 0.20$  in the  $X$ -valley).

In a semiclassical approach the velocity of the charge carriers depends on the energy  $\varepsilon$  measured from the band minimum by the relation

$$v_i(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial}{\partial k_i} \mathcal{E}(\mathbf{k}).$$

which comes from the expression of the group velocity and by assuming as localized the wave-packet describing the electron state in the quantum picture [17].

In the case of parabolic band we get, apart from a normalization factor for the electron mass, the classical relation between velocity and momentum

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

while in the case of the Kane dispersion relation one finds

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

which shows that the crystal momentum  $\hbar \mathbf{k}$  in general does not represent the electron momentum.

The dynamics of an ensemble of  $M$  electrons belonging to the same energy band is a rather complicated many-body problem. For this reason a kinetic description is employed. By proceeding as in classical gas dynamics one can write (see [18] for details) a Liouville equation for the M-electron joint probability distribution function and then with the hierarchy BBGKY, a single particle semiclassical Vlasov equation is obtained

$$\frac{\partial f}{\partial t} + v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} - \frac{eE^i}{\hbar} \frac{\partial f}{\partial k^i} = 0, \quad (3)$$

for the one particle distribution function  $f(\mathbf{x}, t, \mathbf{k})$ , which gives the probability density of finding an electron, in the position  $\mathbf{x}$  and at time  $t$ , with a state belonging to a small volume of the first Brillouin zone centered at the state of wave vector  $\mathbf{k}$ . In (3)  $\mathbf{E}$  represents the self-consistent electric field due to the long range electrostatic interactions.

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 and 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 ions 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, the *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. In this way one obtains the semiclassical Boltzmann equation for electrons in semiconductors [1, 4, 13, 18]

$$\frac{\partial f}{\partial t} + v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} - \frac{eE^i}{\hbar} \frac{\partial f}{\partial k^i} = \mathcal{C}[f], \quad (4)$$

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

The electric field is calculate by solving the Poisson equation for the electric potential  $\phi$

$$E_i = -\frac{\partial \phi}{\partial x_i}, \quad (5)$$

$$\epsilon \Delta \phi = -e(N_D - N_A - n), \quad (6)$$

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

$$n = \int_{\mathcal{B}} f d^3 \mathbf{k}.$$

We do not report the expression of collision operator (the interested reader is referred to [19]). The only important point is that the phonons, describing the energy transport in the lattice, will be assumed to remain at the constant lattice temperature  $T_0$  and to obey the equilibrium Bose–Einstein statistics

$$n_q = \left[ \exp \left( \frac{\hbar \omega_q}{k_B T_0} \right) - 1 \right]^{-1}, \quad (7)$$

where  $k_B$  is the Boltzmann constant and  $\hbar \omega_q$  is the phonon energy.

The equation (4) coupled with the equations (5)–(6) is usually referred to as Boltzmann–Poisson system that constitutes the model employed in the modern analysis of submicron semiconductor device simulation.

However, the direct attempt to solve the Boltzmann–Poisson system in describing the electron transport in semiconductors is a daunting task even from a numerical point of view and practically only solutions in stochastic sense by Monte Carlo methods are available. In this article we will deduce a consistent continuum model based on Extended Thermodynamics [5, 6], by employing the maximum entropy principle, under the assumption that the energy band of electrons is given by the Kane dispersion relation (2).

### 3 Moment equations

The macroscopic balance equations are deduced as moment equations of the transport equations<sup>1</sup>. By multiplying (4) by a weight function  $\psi(\mathbf{k})$  and integrating over  $\mathcal{B}$  (from now on by assumption equal to  $\mathcal{R}^3$ ), one finds

$$\frac{\partial M_\psi}{\partial t} + \int_{\mathcal{B}} \psi(\mathbf{k}) v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} d^3 \mathbf{k} - e E^j \int_{\mathcal{B}} \psi(\mathbf{k}) \frac{\partial}{\partial k_j} f d^3 \mathbf{k} = \int_{\mathcal{B}} \psi(\mathbf{k}) \mathcal{C}[f] d^3 \mathbf{k}, \quad (8)$$

with

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

moment of  $f$  relative to the weight function  $\psi(\mathbf{k})$ .

Since

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

with  $\mathbf{n}$  as the outward unit normal field on the boundary  $\partial B$  of the domain  $B$  and  $d\sigma$  as the surface element of  $\partial B$ , (8) becomes

$$\begin{aligned} \frac{\partial M_\psi}{\partial t} + \frac{\partial}{\partial x^i} \int_{\mathcal{B}} f \psi(\mathbf{k}) v^i(\mathbf{k}) d^3 \mathbf{k} + e E^j \left[ \int_{\mathcal{B}} f \frac{\partial \psi(\mathbf{k})}{\partial k_j} d^3 \mathbf{k} - \int_{\partial B} \psi(\mathbf{k}) f n_j d\sigma \right] = \\ \int_{\mathcal{B}} \psi(\mathbf{k}) \mathcal{C}[f] d^3 \mathbf{k}. \end{aligned} \quad (9)$$

The term

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

vanishes under the assumption that  $f$  must tend to zero sufficiently fast as  $k \mapsto \infty$ .

As in [16] we choose  $\psi(\mathbf{k})$  equal to 1,  $\mathbf{k}$ ,  $\mathcal{E}(k)$  and  $\mathbf{k}\mathcal{E}(k)$  because this choice gives the minimum number of constitutive equations needed to close the corresponding moment equations.

Then we obtain the following moment equations

<sup>1</sup> Hereafter we use units such that  $\hbar = 1$

$$\frac{\partial n}{\partial t} + \frac{\partial(nV^i)}{\partial x^i} = 0, \quad (10)$$

$$\frac{\partial(nP^i)}{\partial t} + \frac{\partial(nU^{ij})}{\partial x^j} + neE^i = nC_P^i, \quad (11)$$

$$\frac{\partial(nW)}{\partial t} + \frac{\partial(nS^j)}{\partial x^j} + neV_k E^k = nC_W, \quad (12)$$

$$\frac{\partial(nN^i)}{\partial t} + \frac{\partial(nR^{ij})}{\partial x^j} + neE_j (U^{ij} + W\delta^{ij}) = nC_N^i, \quad (13)$$

where

$$\begin{aligned} n &= \int_{\mathcal{B}} f d^3\mathbf{k} \quad \text{is the electron density,} \\ V^i &= \frac{1}{n} \int_{\mathcal{B}} f v^i d^3\mathbf{k} \quad \text{is the average electron velocity,} \\ P^i &= \frac{1}{n} \int_{\mathcal{B}} f k^i d^3\mathbf{k} \quad \text{is the average crystal momentum,} \\ W &= \frac{1}{n} \int_{\mathcal{B}} \mathcal{E}(k) f d^3\mathbf{k} \quad \text{is the average electron energy,} \\ U^{ij} &= \frac{1}{n} \int_{\mathcal{B}} f v^i k^j d^3\mathbf{k} \quad \text{is the flux of crystal momentum,} \\ S^i &= \frac{1}{n} \int_{\mathcal{B}} f v^i \mathcal{E}(k) d^3\mathbf{k} \quad \text{is the flux of energy,} \\ N^i &= \frac{1}{n} \int_{\mathcal{B}} f k^i \mathcal{E}(k) d^3\mathbf{k} \quad \text{is the } N\text{-vector,} \\ R^{ij} &= \frac{1}{n} \int_{\mathcal{B}} f v^i k^j \mathcal{E}(k) d^3\mathbf{k} \quad \text{is the } R\text{-tensor,} \end{aligned}$$

while

$$\begin{aligned} C_P^i &= \frac{1}{n} \int_{\mathcal{B}} \mathcal{E}[f] k^i d^3\mathbf{k}, \\ C_W &= \frac{1}{n} \int_{\mathcal{B}} \mathcal{E}[f] \mathcal{E}(k) d^3\mathbf{k}, \\ C_N^i &= \frac{1}{n} \int_{\mathcal{B}} \mathcal{E}[f] k^i \mathcal{E}(k) d^3\mathbf{k}. \end{aligned}$$

are the moments of the collision term.

The average crystal momentum  $P^i$  and the flux of average crystal momentum  $U^{ij}$  reduce to the average electron momentum and flux of average electron momentum only in the parabolic band approximation. Moreover we observe that for a general dispersion relation the flux of crystal momentum and the R-tensor are not symmetric. However, if  $\mathcal{E}$  is an isotropic function of  $\mathbf{k}$  as in the parabolic band approximation and Kane's dispersion relation, then

$$U^{ij} = U^{ji}, \quad R^{ij} = R^{ji}.$$

We remark that in [16] only the stationary case is considered and the N-vector is not introduced.

Of course other choices for the functions  $\psi(\mathbf{k})$  are possible. In analogy with gas dynamics, one can set  $\psi(\mathbf{k})$  equal to 1,  $v_i(\mathbf{k})$ ,  $\mathcal{E}$ ,  $\mathcal{E}v_i(\mathbf{k})$ . However with this choice additional constitutive functions are introduced due to the terms

$$\int_{\mathcal{B}} f \frac{\partial \psi(\mathbf{k})}{\partial k_j} d^3\mathbf{k}.$$

In the following we will consider only the system (10)–(13), because our main aim is to get explicit closure relations when the Kane dispersion relation is adopted for the energy band of the electrons, and to compare with the results obtained by Tang et al. [16].

#### 4 Maximum entropy principle and closure relations

The set of moment equations (10)–(13) is not closed. If we assume as fundamental variables  $n$ ,  $V^i$ ,  $W$  and  $S^i$ , which have a direct physical interpretation, the closure problem consists in expressing  $U^{ij}$ ,  $R^{ij}$ ,  $P^i$  and  $N^i$  and the moments of the collision term  $C_P^i$ ,  $C_W$  and  $C_N^i$  as functions of  $n$ ,  $V^i$ ,  $W$  and  $S^i$ .

We want to stress that the role of the mean velocity  $V^i$  here is radically different from that played in gas dynamics. In fact, for a simple gas the explicit dependence of fluxes on the velocity can be predicted by requiring Galilean invariance of the constitutive functions. Instead (10)–(13) 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 may be considered as inertial and it is thus 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 [5, 6, 7, 20] 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 extremum of the entropy functional under the constraints that it yields exactly the known moments  $M_A$

$$\int_{\mathcal{B}} \psi_A f_{ME} d^3 \mathbf{k} = M_A. \quad (14)$$

If we assume that the electron gas is sufficiently dilute the entropy functional can be taken as the classical limit of the expression arising in the Fermi statistics

$$s = -k_B \int_{\mathcal{B}} (f \log f - f) d^3 \mathbf{k}. \quad (15)$$

In order to employ the entropy principle for closing the balance equations (10)–(13), if we introduce the Lagrangian multipliers  $\Lambda_A$ , the problem to maximize  $s$  under the constraints (14) is equivalent to maximize

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

the Legendre transform of  $s$ , without constraints,

$$\delta s' = 0.$$

This gives

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

Since the latter relation must hold for arbitrary  $\delta f$ , it follows

$$f_{ME} = \exp \left[ -\frac{1}{k_B} \Lambda_A \psi^A \right]. \quad (16)$$

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

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

and

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

with the components of  $\Lambda$  Lagrangian multipliers relative to the density  $n$ , to the velocity  $V^j$ , to the energy  $W$  and to the energy flux  $S^j$  respectively.

Then the maximum entropy distribution function reads

$$f_{ME} = \exp \left[ -\left( \frac{1}{k_B} \lambda + \lambda^W \mathcal{E} + \lambda_i v^i + \lambda_i^W v^i \mathcal{E} \right) \right], \quad (17)$$

with  $\Lambda$  function of the moments  $M_A$ .

In order to get the dependence of the Lagrangian multipliers from the  $M_A$ , one has to invert the constraints (14). Then by taking the moments of  $f_{ME}$  and  $\mathcal{E}[f_{ME}]$  one finds the closure relations for the fluxes and the production terms. However on account of the technical difficulties we will get only an approximate explicit expression for the Lagrangian multipliers under a reasonable physical assumption on the distribution function.

At equilibrium the distribution function is isotropic

$$f_{EQ} = \exp \left[ - \left( \frac{1}{k_B} \lambda_E + \frac{\mathcal{E}}{k_B T_0} \right) \right], \quad (18)$$

that is at equilibrium

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

Monte Carlo simulations for electron transport in Si show that the anisotropy of  $f$  is small [12, 16, 21] even far from equilibrium. The physical reason is that in Si the main scattering mechanisms, the interaction of electrons with acoustic and non-polar optical phonons, are both isotropic.

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

$$\lambda = \lambda^{(0)} + \delta^2 \lambda^{(2)}, \quad (19)$$

$$\lambda^W = \lambda^{W(0)} + \delta^2 \lambda^{W(2)}, \quad (20)$$

$$\lambda_i = \delta \lambda_i^{(1)}, \quad (21)$$

$$\lambda_i^W = \delta \lambda_i^{W(1)}. \quad (22)$$

Therefore  $f_{ME}$  can be written as

$$f_{ME} = \exp \left( - \frac{\lambda^{(0)}}{k_B} - \lambda^{W(0)} \mathcal{E} \right) \left[ 1 - \delta x + \delta^2 \left( \frac{x^2}{2} - \frac{\lambda^{(2)}}{k_B} - \lambda^{W(2)} \mathcal{E} \right) \right], \quad (23)$$

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  $\lambda$  and  $\lambda^W$ , but the part arising in case  $f_{ME}$  is isotropic.

## 5 Closure relations for Kane's dispersion relation

Now we shall look for explicit constitutive equations starting from the distribution function obtained with the MEP when the dispersion relation is given by (2). To begin with we will give a first guess of the constitutive relations just on the basis of general considerations then the distribution (23) will be employed to get the specific results.

From the definition we have

$$P^i = \frac{1}{n} \int_{\mathcal{B}} k^i f d^3 \mathbf{k} = \frac{1}{n} \int_{\mathcal{B}} f v^i m^* [1 + 2\alpha \mathcal{E}(k)] d^3 \mathbf{k} = m^* (V^i + 2\alpha S^i) \quad (24)$$

and

$$N^i = m^* (S^i + 2\alpha H^i), \quad (25)$$

where

$$H^i = \frac{1}{n} \int_{\mathcal{B}} v^i \mathcal{E}^2(k) f d^3 \mathbf{k}. \quad (26)$$

Moreover, if we decompose the electron velocity into the mean and random part,



$$v^i = V^i + c^i, \quad \text{with} \quad \int_{\mathcal{B}} c^i f d^3\mathbf{k} = 0,$$

and introduce a similar decomposition for  $k^i$ ,

$$k^i = P^i + \kappa^i \quad \text{with} \quad \int_{\mathcal{B}} \kappa^i f d^3\mathbf{k} = 0,$$

we have

$$U^{ij} = m^* V^i V^j + 2\alpha m^* V^i S^j + u^{ij},$$

where

$$u^{ij} = \frac{1}{n} \int_{\mathcal{B}} c_i \kappa_j f d^3\mathbf{k}.$$

Likewise for  $R^{ij}$  one finds

$$nR^{ij} = nV^i P^j W + V^i \int_{\mathcal{B}} \kappa^j \mathcal{E} f d^3\mathbf{k} + P^j \int_{\mathcal{B}} c_i \mathcal{E} f d^3\mathbf{k} + r^{ij},$$

with

$$r^{ij} = \int_{\mathcal{B}} c^i \kappa^j \mathcal{E} f d^3\mathbf{k}.$$

Therefore to find constitutive equations for  $N^i$ ,  $U^{ij}$  and  $R^{ij}$  is equivalent to finding constitutive equations for  $H^i$ ,  $u^{ij}$  and  $r^{ij}$ .

### 5.1 Lagrangian multipliers

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

$$n = \int_{\mathcal{B}} f_{ME} d^3\mathbf{k}, \quad (27)$$

$$nW = \int_{\mathcal{B}} \mathcal{E} f_{ME} d^3\mathbf{k}, \quad (28)$$

$$nV^i = \int_{\mathcal{B}} v^i f_{ME} d^3\mathbf{k}, \quad (29)$$

$$nS^i = \int_{\mathcal{B}} v^i \mathcal{E} f_{ME} d^3\mathbf{k}. \quad (30)$$

By retaining only the terms up to second order in  $\delta$ , from the constraints (27)–(30), we get the following algebraic system ( $V_i$  and  $S_i$  are consistently considered as terms of order  $\delta$ )

$$n = \exp \left[ - \left( \frac{1}{k_B} \lambda^{(0)} \right) \right] \int_{\mathcal{B}} \exp [ - (\lambda^{W(0)} \mathcal{E}) ] d^3\mathbf{k}, \quad (31)$$

$$W = \exp \left[ - \left( \frac{1}{k_B} \lambda^{(0)} \right) \right] \int_{\mathcal{B}} \mathcal{E} \exp [ - (\lambda^{W(0)} \mathcal{E}) ] d^3\mathbf{k}, \quad (32)$$

$$0 = \int_{\mathcal{B}} \exp (\lambda^{W(0)} \mathcal{E}) \left[ \frac{1}{k_B} \lambda^{(2)} + \lambda^{W(2)} \mathcal{E} - \frac{x^2}{2} \right], \quad (33)$$

$$0 = \int_{\mathcal{B}} \mathcal{E} \exp (\lambda^{W(0)} \mathcal{E}) \left[ \frac{1}{k_B} \lambda^{(2)} + \lambda^{W(2)} \mathcal{E} - \frac{x^2}{2} \right], \quad (34)$$

$$nV^i = - \int_{\mathcal{B}} v^i \exp (\lambda^{W(0)} \mathcal{E}) x d^3\mathbf{k}, \quad (35)$$

$$nS^i = - \int_{\mathcal{B}} v^i \mathcal{E} \exp (\lambda^{W(0)} \mathcal{E}) x d^3\mathbf{k}. \quad (36)$$

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

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

(31), (32) decouple from the other equations and explicitly read

$$n = 4\pi \exp\left(-\frac{\lambda^{(0)}}{k_B}\right) \int_0^\infty \exp(-\lambda^{W(0)} \mathcal{E}) m^* \sqrt{2m^* \mathcal{E} (1 + \alpha \mathcal{E})} \times (1 + 2\alpha \mathcal{E}) d\mathcal{E}, \quad (37)$$

$$W = \frac{\int_0^\infty \mathcal{E} \sqrt{\mathcal{E} (1 + \alpha \mathcal{E})} (1 + 2\alpha \mathcal{E}) \exp(-\lambda^{W(0)} \mathcal{E}) d\mathcal{E}}{\int_0^\infty \sqrt{\mathcal{E} (1 + \alpha \mathcal{E})} (1 + 2\alpha \mathcal{E}) \exp(-\lambda^{W(0)} \mathcal{E}) d\mathcal{E}}. \quad (38)$$

Relation (38) shows that  $\lambda^{W(0)}$  depends only on  $W$ . The analytical inversion of (38) is rather involved and we have resorted to a numerical inversion. The results are shown in Fig. 1. Near global thermal equilibrium the value of  $\lambda^{W(0)}$  is the same for both the parabolic and Kane dispersion relation. When  $W$  increases, the value of  $\lambda^{W(0)}$  in the Kane case is greater.

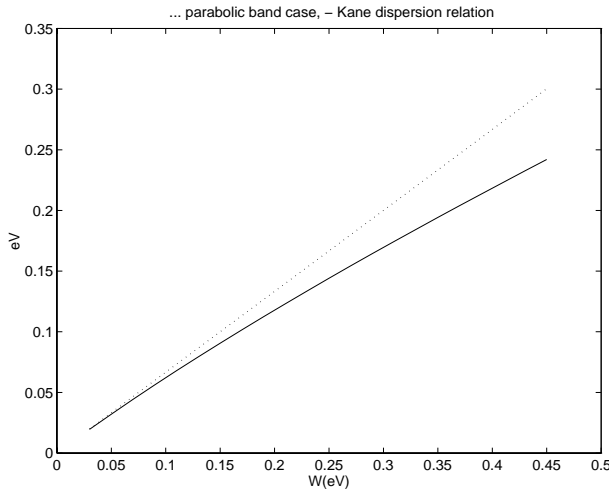


Fig. 1. Inverse of the Lagrangian multipliers  $\lambda^{W(0)}$  vs. the energy  $W$

The knowledge of  $\lambda^{W(0)}$  allows us to get the constitutive functions for the other Lagrangian multipliers. Relation (37) gives  $\lambda^{(0)}$ , which essentially plays the role of a normalization factor

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

with

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

The Lagrangian multipliers  $\lambda_i$  and  $\lambda_i^W$  can be obtained by inverting the linear system represented by (35)–(36).

By taking into account the following formula<sup>2</sup> valid for  $\mathbf{l}$  belonging to  $S^2$ , the unit sphere of  $\mathbf{R}^3$ ,

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

one finds

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

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

The coefficients  $b_{ij}$  are given by

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

with

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

and

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

$d_k$  and  $p_k$  being

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

Finally, the second order corrections to  $\lambda$  and  $\lambda^W$ , are obtained by solving the linear system (33)–(34). The following expressions are found

$$\frac{\lambda^{(2)}}{k_B} = \alpha_1 \mathbf{V} \cdot \mathbf{V} + 2\alpha_2 \mathbf{S} \cdot \mathbf{V} + \alpha_3 \mathbf{S} \cdot \mathbf{S}, \quad (39)$$

$$\lambda^{W(2)} = \alpha_4 \mathbf{V} \cdot \mathbf{V} + 2\alpha_5 \mathbf{S} \cdot \mathbf{V} + \alpha_6 \mathbf{S} \cdot \mathbf{S}, \quad (40)$$

where

$$\alpha_1 = \frac{3m^*d_0^2 [d_1p_1(p_2^2 - p_3p_1) - d_2p_2(p_1^2 - p_0p_2)]}{4\hat{D}}, \quad (41)$$

$$\alpha_2 = \frac{3m^*d_0^2 [d_2p_1(p_1^2 - p_0p_2) - d_1p_0(p_2^2 - p_1p_3)]}{4\hat{D}}, \quad (42)$$

$$\alpha_3 = \frac{3m^*d_0^2 [(d_1p_1 + d_2p_0)(p_0p_2 - p_1^2) + d_1p_0(p_1p_2 - p_3p_0)]}{4\hat{D}}, \quad (43)$$

$$\alpha_4 = -\frac{3m^*d_0^2 [d_1p_2(p_2p_0 - p_1^2) + d_0p_1(p_2^2 - p_1p_3)]}{4\hat{D}}, \quad (44)$$

$$\alpha_5 = \frac{3m^*d_0^2 [d_1p_1(p_2p_0 - p_1^2) + d_0p_0(p_2^2 - p_1p_3)]}{4\hat{D}}, \quad (45)$$

$$\alpha_6 = -\frac{3m^*d_0^2 [(d_1p_0 + p_1d_0)(p_2p_0 - p_1^2) + d_0p_0(p_1p_2 - p_0p_3)]}{4\hat{D}}. \quad (46)$$

with

$$\hat{D} = (d_0d_2 - d_1^2)(p_0p_2 - p_1^2)^2. \quad (47)$$

## 5.2 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.

Up to second order terms the constitutive equations for the fluxes are of the form

$$H^i = \delta H^{i(1)}, \quad (48)$$

$$U_{ij} = U_{ij}^{(0)} + \delta^2 U_{ij}^{(2)}, \quad (49)$$

$$R_{ij} = R_{ij}^{(0)} + \delta^2 R_{ij}^{(2)}. \quad (50)$$

From the definition

$$H^{i(1)} = -\frac{1}{n} \int_{\mathcal{B}} v^i x \mathcal{E}^2 \exp\left(-\frac{\lambda^{(0)}}{k_B} - \lambda^{W(0)}\right) d^3\mathbf{k},$$

Therefore

$$H^i = \beta_1 V^i + \beta_2 S^i, \quad (51)$$

where

$$\beta_1 = h_1 b_{11} + h_2 b_{12}, \quad \beta_2 = h_1 b_{12} + h_2 b_{22}.$$

with

$$h_1 = \frac{2p_2}{3m^*d_0}, \quad (52)$$

$$h_2 = \frac{2p_3}{3m^*d_0}. \quad (53)$$

Concerning the tensor  $U^{ij}$  and  $R^{ij}$ , at the zero order we have

$$U^{ij(0)} = U^{(0)} \delta^{ij}, \quad (54)$$

$$R^{ij(0)} = R^{(0)} \delta^{ij}, \quad (55)$$

with

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

$$R^{(0)} = \frac{2}{3d_0} \int_0^\infty \mathcal{E}^{5/2} (1 + \alpha \mathcal{E})^{3/2} \exp(-\lambda^{W(0)} \mathcal{E}) d\mathcal{E},$$

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

$$U^{ij(2)} = (\delta_1 \mathbf{V} \cdot \mathbf{V} + 2\delta_2 \mathbf{S} \cdot \mathbf{V} + \delta_3 \mathbf{S} \cdot \mathbf{S}) \delta^{ij} + \delta_4 V^i V^j + 2\delta_5 V^{(i} S^{j)} + \delta_6 S^i S^j. \quad (56)$$

The coefficients  $\delta_k$  are given by

$$\delta_1 = \frac{3m^*d_0}{20\hat{D}} \{2(d_0d_2 - d_1^2)(b_0p_2^2 - 2b_1p_1p_2 + b_2p_1^2) +$$

$$5U^{(0)} [d_0d_2(p_2p_1^2 - p_0p_2^2) - d_0d_1(p_1p_2^2 - p_3p_1^2)]$$

$$+ 5R^{(0)} [d_0d_1(p_0p_2^2 - p_2p_1^2) - d_0^2(p_3p_1^2 - p_1p_2^2)]\}, \quad (57)$$

$$\delta_2 = -\frac{3m^*d_0}{20\hat{D}} \{2(d_0d_2 - d_1^2) [b_0p_1p_2 - b_1(p_0p_2 + p_1^2) + b_2p_0p_1] +$$

$$5U^{(0)} [d_0d_2(p_1^3 - p_0p_1p_2) - d_0d_1(p_0p_2^2 - p_0p_1p_3)]$$

$$+ 5R^{(0)} [d_0d_1(p_0p_1p_2 - p_1^3) - d_0^2(p_0p_1p_3 - p_0p_2^2)]\}, \quad (58)$$

$$\delta_3 = \frac{3m^*d_0}{20\hat{D}} \left\{ 2(d_0d_2 - d_1^2)(b_0p_1^2 - 2b_1p_0p_1 + b_2p_0^2) + 5U^{(0)} [d_0d_1(p_1^3 - 2p_0p_1p_2 + p_0^2p_3) - d_0d_2(p_0^2p_2 - p_0p_1^2)] + 5R^{(0)} [d_0d_1(p_0^2p_2 - p_0p_1^2) - d_0^2(p_0^2p_3 - 2p_0p_1p_2 + p_1^3)] \right\}, \quad (59)$$

$$\delta_4 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2} (b_0p_2^2 - 2b_1p_1p_2 + b_2p_1^2), \quad (60)$$

$$\delta_5 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2} [p_0(b_1p_2 - b_2p_1) + p_1(b_1p_1 - b_0p_2)], \quad (61)$$

$$\delta_6 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2} (b_0p_1^2 - 2b_1p_1p_0 + b_2p_0^2), \quad (62)$$

with

$$b_k = \int_0^\infty \frac{\mathcal{E}^k [\mathcal{E}(1 + \alpha\mathcal{E})]^{5/2}}{(1 + 2\alpha\mathcal{E})^2} \exp(-\lambda^{(0)}\mathcal{E}) d\mathcal{E}. \quad (63)$$

Likewise for  $R^{ij(2)}$ , we find

$$R^{ij(2)} = (\gamma_1 \mathbf{V} \cdot \mathbf{V} + 2\gamma_2 \mathbf{S} \cdot \mathbf{V} + \gamma_3 \mathbf{S} \cdot \mathbf{S}) \delta^{ij} + \gamma_4 V^i V^j + 2\gamma_5 V^i S^j + \gamma_6 S^i S^j. \quad (64)$$

The coefficients  $\gamma_i$  are given by

$$\gamma_1 = -\frac{3m^*d_0}{20\hat{D}} \left\{ 2(d_1^2 - d_0d_2)(b_1p_2^2 - 2b_2p_1p_2 + b_3p_1^2) + 5R^{(0)} [d_0d_1(p_1p_2^2 - p_1^2p_3) + d_0d_2(p_0p_2^2 - p_2p_1^2)] + 5G^{(0)} [d_0^2(p_3p_1^2 - p_1p_2^2) + d_0d_1(p_2p_1^2 - p_0p_2^2)] \right\}, \quad (65)$$

$$\gamma_2 = \frac{3m^*d_0}{20\hat{D}} \left\{ 2(d_1^2 - d_0d_2) [b_1p_1p_2 - b_2(p_0p_2 + p_1^2) + b_3p_0p_1] + 5R^{(0)} [d_0d_1(p_0p_2^2 - p_0p_1p_3) + d_0d_2(p_0p_1p_2 - p_1^3)] + 5G^{(0)} [d_0^2(p_0p_1p_3 - p_0p_2^2) + d_0d_1(p_1^3 - p_0p_1p_2)] \right\}, \quad (66)$$

$$\gamma_3 = \frac{3m^*d_0}{20\hat{D}} \left\{ 2(d_0d_2 - d_1^2)(b_1p_1^2 - 2b_2p_0p_1 + b_3p_0^2) + 5R^{(0)} [d_0d_1(p_1^3 - 2p_0p_1p_2 + p_0^2p_3) + d_0d_2(p_0p_1^2 - p_0^2p_2)] + 5G^{(0)} [d_0d_1(p_0^2p_2 - p_0p_1^2) - d_0^2(p_0^2p_3 - 2p_0p_1p_2 + p_1^3)] \right\}, \quad (67)$$

$$\gamma_4 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2} (b_1p_2^2 - 2b_2p_1p_2 + b_3p_1^2), \quad (68)$$

$$\gamma_5 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2} [p_0(b_2p_2 - b_3p_1) + p_1(b_2p_1 - b_1p_2)], \quad (69)$$

$$\gamma_6 = \frac{3m^*d_0}{5(p_0p_2 - p_1^2)^2} (b_1p_1^2 - 2b_2p_1p_0 + b_3p_0^2), \quad (70)$$

where  $G^{(0)}$  is defined as

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

## 6 Parabolic band approximation

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

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

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

with  $\Gamma(\nu)$  as the special Gamma function, that satisfies for positive integers  $p$

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

Concerning the Lagrangian multipliers one has

$$\frac{\lambda}{k_B} = -\log \frac{n}{\left(\frac{4}{3}\pi m^* W\right)^{3/2}} + \frac{9m^*}{4W^2} \mathbf{V} \cdot \mathbf{S} - \frac{27m^*}{20W^3} \mathbf{S} \cdot \mathbf{S}, \quad (71)$$

$$\lambda^W = \frac{3}{2W} + \frac{21m^*}{8W^2} \mathbf{V} \cdot \mathbf{V} - \frac{9m^*}{2W^3} \mathbf{V} \cdot \mathbf{S} + \frac{81m^*}{40W^4} \mathbf{S} \cdot \mathbf{S}, \quad (72)$$

$$\lambda_i = -\frac{21m^*}{4W} V_i + \frac{9m^*}{4W^2} S_i, \quad (73)$$

$$\lambda_i^W = \frac{9m^*}{4W^2} V_i - \frac{27m^*}{20W^3} S_i. \quad (74)$$

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

$$\begin{aligned} f_{ME}^{(P)} &= \frac{n \exp(-\lambda^{W(0)} \mathcal{E})}{\left(\frac{4}{3}\pi m^* W\right)^{3/2}} \times \\ &\left\{ 1 - \left( -\frac{21m^*}{4W} V_i + \frac{9m^*}{4W^2} S_i \right) v^i - \left( \frac{9m^*}{4W^2} V_i - \frac{27m^*}{20W^3} S_i \right) \mathcal{E} v^i \right. \\ &+ \frac{1}{2} \left[ \left( -\frac{21m^*}{4W} V_i + \frac{9m^*}{4W^2} S_i \right) v^i + \left( \frac{9m^*}{4W^2} V_i - \frac{27m^*}{20W^3} S_i \right) \mathcal{E} v^i \right]^2 \\ &- \left( \frac{9m^*}{4W^2} \mathbf{V} \cdot \mathbf{S} - \frac{27m^*}{20W^3} \mathbf{S} \cdot \mathbf{S} \right) \\ &\left. - \left( \frac{21m^*}{8W^2} \mathbf{V} \cdot \mathbf{V} - \frac{9m^*}{2W^3} \mathbf{V} \cdot \mathbf{S} + \frac{81m^*}{40W^4} \mathbf{S} \cdot \mathbf{S} \right) \mathcal{E} \right\} \end{aligned} \quad (75)$$

and the constitutive equations become

$$H_i^{(P)} = -\frac{35}{9} W^2 V_i + \frac{14}{3} W S_i, \quad (76)$$

$$\begin{aligned} U_{ij}^{(P)} &= \frac{2}{3} W \delta_{ij} + \left( -\frac{7}{6} m^* \mathbf{V} \cdot \mathbf{V} + \frac{7m^*}{5W} \mathbf{S} \cdot \mathbf{V} - \frac{27m^*}{50W^2} \mathbf{S} \cdot \mathbf{S} \right) \delta^{ij} + \\ &\frac{7}{2} m^* V^i V^j - \frac{21m^*}{5W} V^{(i} S^{j)} + \frac{81m^*}{50W^2} S^i S^j, \end{aligned} \quad (77)$$

$$\begin{aligned} R_{ij}^{(P)} &= \frac{10}{9} W^2 \delta_{ij} + \left( -\frac{7}{18} m^* W \mathbf{V} \cdot \mathbf{V} + \frac{m^*}{15} \mathbf{S} \cdot \mathbf{V} - \frac{9m^*}{50W} \mathbf{S} \cdot \mathbf{S} \right) \delta^{ij} + \\ &\frac{77}{6} m^* W V^i V^j - \frac{91m^*}{5} V^{(i} S^{j)} + \frac{357m^*}{50W} S^i S^j. \end{aligned} \quad (78)$$

In order to compare the results with those obtained for the monatomic gas and the hydrodynamical models of semiconductors presented in [8, 9, 10, 11], we observe that

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

Therefore, by defining the electron temperature through

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

and introducing the heat flux

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

and the shear tensor<sup>3</sup>

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

we have up to second order terms

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

Then the Lagrangian multipliers read

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

which are the same as those obtained for a monatomic gas in the inviscid case. This shows that according to the results presented in [10], the explicit dependence of the multipliers on the velocity is the same as that found for a monatomic gas by operating the decomposition of the Lagrangian multipliers into convective and non convective parts (compare the previous expressions for the  $\lambda$ 's with those reported in [22, 23]).

The constitutive equations (77), (78) become

$$U_{ij}^{(P)} = m^* V_i V_j + k_B T \delta_{ij} + \frac{4m^*}{5k_B T} V_{\langle i} q_{j \rangle} + \frac{18m^*}{25(k_B T)^2} q_{\langle i} q_{j \rangle}, \quad (79)$$

$$\begin{aligned} R_{ij}^{(P)} &= \left( \frac{1}{2} m^* V^2 k_B T + \frac{5}{2} (k_B T)^2 - \frac{8}{15} m^* \mathbf{V} \cdot \mathbf{q} - \frac{3}{25} \frac{m^* q^2}{k_B T} \right) \delta_{ij} + \\ &\quad \frac{7}{2} m^* k_B T V_i V_j + \frac{28}{5} m^* V_{(i} q_{j)} + \frac{119}{25} \frac{m^* q_i q_j}{k_B T}. \end{aligned} \quad (80)$$

By comparing the relation (79) with the analogous expression  $U_{ij}^{(MG)}$  in the case of a monoatomic gas [22]

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

we may make the identification

$$\sigma_{ij} = \frac{4m^*}{5k_B T} V_{\langle i} q_{j \rangle} + \frac{18m^*}{25(k_B T)^2} q_{\langle i} q_{j \rangle}. \quad (81)$$

<sup>3</sup>  $\langle A_{ij} \rangle$  means deviatoric part of  $A_{ij}$ , that is  $\langle A_{ij} \rangle = \frac{1}{2}(A_{ij} + A_{ji}) - 1/3 A_i^l \delta_{lj}$

Now, if such an expression for  $\sigma_{ij}$  is inserted into the expression for  $R_{ij}$  for the monatomic gas [22],  $R_{ij}^{(MG)}$ , with quadratic correction we obtain (we neglect the term of higher order than the second in  $V_k$  and the second order terms involving the shear because they are of the third order in  $V_i$  and  $q_j$ )

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

This is the same expression (80).

## 7 Comparison with previous models

Other hydrodynamical models for carrier transport in semiconductors have been proposed in the case of Kane's dispersion relation. In particular Tang et al. [16] proposed a model by considering the same moment equations (10)–(13) in the stationary case. The constitutive equations have been derived from the analysis of the Monte Carlo (MC) simulations of silicon devices in the stationary regime by considering the Kane dispersion relation for the energy bands.

In [16] the authors have simulated three  $n^+ - n - n^+$  silicon diodes with different doping profile and applied voltage of 2 Volt. The physical situation is schematically represented in Fig. 2 and can be tackled as a one dimensional problem. The semiconductor device is constituted by two regions of high doping density, the  $n^+$  regions (with typical values of the concentration of the order of  $10^{18} \text{ cm}^{-3}$ ), with inside the  $n$  region, a region of low doping density, (with a typical value of the concentration of the order of  $10^{16} \text{ cm}^{-3}$ ).

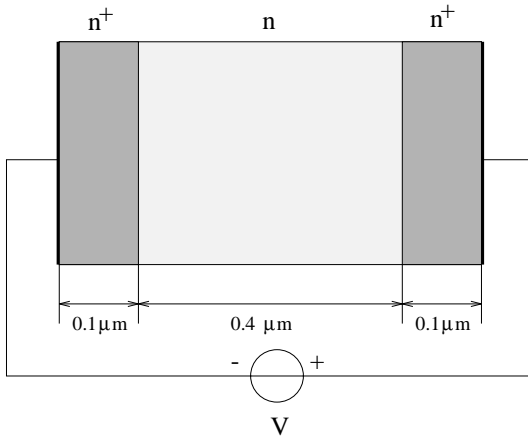


Fig. 2. Schematic representation of a  $n^+ - n - n^+$  ballistic diode

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

The tensor  $U_{ij}$  has been modelled as

$$U_{ij} = U \delta_{ij} + m^* V_i V_j + 2 \alpha m^* V_i S_j \quad (82)$$

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

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

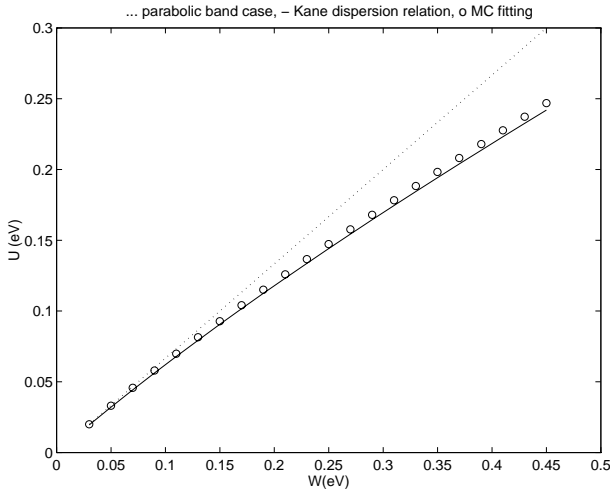


where

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

and

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



**Fig. 3.**  $U^{(0)}$  obtained with the maximum entropy principle in the parabolic case (dotted line), with the Kane dispersion relation (continuous line) and with the MC simulation [16] vs. the energy  $W$

In Fig. 3 we compare the values of the isotropic part of the tensor  $U_{ij}$  obtained in [16], by the fitting of the MC data, and by the fitting of the maximum entropy principle in the case of parabolic band approximation and in the case of the Kane dispersion relation.

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

Concerning the anisotropic part, we observe that although the definition implies that  $U_{ij}$  must be symmetric for Kane's dispersion relation, the expression proposed in [16] is not symmetric. Moreover in the approach of Tang et al. [16] there is the *a priori* assumption that the coefficients of the terms  $S_i V_j$  are zero and the isotropic part does not contain second order corrections.

The tensor  $R_{ij}$  was modelled in [16] as

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

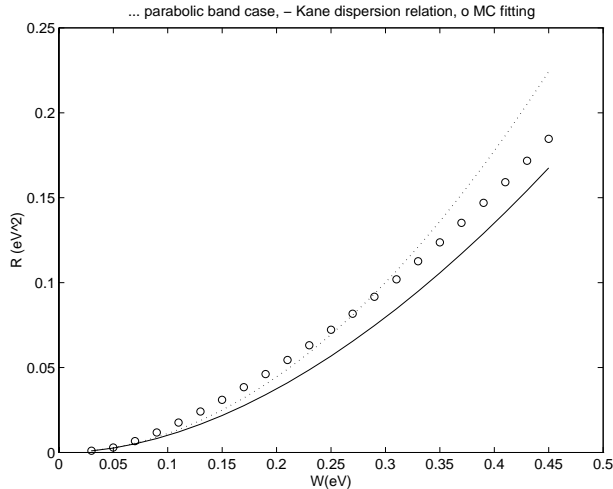
and for  $R$  a fitting formula similar to that for  $U$  was used

$$R = \frac{10}{9} W^2 + g(W) \sum_{k=0}^4 r_k W^k, \quad (83)$$

where

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

Again there is the problem that the last expression for  $R_{ij}$  is not symmetric and the second order terms in the isotropic part are missing. At variance with  $U$  the comparison between  $R$  and  $R^{(0)}$  (Fig. 4) shows that the agreement, although acceptable, does not present the same accuracy. The qualitative behaviour is good in the case of the Kane dispersion relation, but there is a certain quantitative discrepancy. Instead the parabolic approximation presents a little different profile, but the agreement is better. This seems to be a mere coincidence.



**Fig. 4.**  $R^{(0)}$  obtained with the maximum entropy principle in the parabolic case (dotted line), with the Kane dispersion relation (continuous line) and with the MC simulation [16] vs. the energy  $W$

We note that MC closure relations have been determined from one dimensional results and the inferred tridimensional constitutive equations cannot be fully appropriate. Therefore a comparison between the expressions for  $U_{ij}$  and  $R_{ij}$  proposed in [16] and those obtained by using the ME principle cannot be performed by a direct comparison of the coefficients  $\delta_k$  and  $\gamma_k$ . Probably only an analysis of the results of numerical simulations of electron devices in one and two dimensions can assess the validity of the models.

At last the MC constitutive equation for  $H^i$  is not reported in [16] because the stationary case was considered. Since at the present time the relative MC data are not available to us we do not comment on the results obtained for  $H^i$ .

## Conclusions

In this article we have presented a consistent closure for an hydrodynamical model for carrier transport in silicon consisting of the moment equations for electron number density, momentum, energy and energy flux, based on the maximum entropy principle. The explicit form of the maximum entropy distribution function has been obtained by expanding in terms of a small anisotropy parameter up to second order and solving the resulting algebraic equations. In this way we have avoided resorting to the elusive concept of local thermal equilibrium (which, although physically appealing, is difficult to define rigorously in the case of a non parabolic band because of the lack of an unambiguous definition of internal energy) and expansion around it. The nonparabolicity of the energy band has been included by assuming the Kane dispersion relation, improving on other hydrodynamical models based on the approximation of parabolic band which consider the electrons as a gas of classical particles up to a normalization factor in the electron mass.

The closures we have obtained for the fluxes (constitutive functions) have been compared, where meaningful, with the results of Monte Carlo simulations and the agreement is remarkable. What remains to be done in order to build a consistent hydrodynamical model is to evaluate the production terms (which are the moments of the collision operator) with the maximum entropy distribution function. Work along these lines is in progress and will be published elsewhere.

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