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2008 J. Phys. A: Math. Theor. 41 215103

(http://iopscience.iop.org/1751-8121/41/21/215103)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **41** (2008) 215103 (30pp) doi:10.1088/1751-8113/41/21/215103

The maximum entropy principle hydrodynamical model for holes in silicon semiconductors: the case of the warped bands

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Received 31 October 2007, in final form 2 April 2008
Published 9 May 2008
Online at stacks.iop.org/JPhysA/41/215103

Abstract
The maximum entropy principle is used to get a consistent hydrodynamical model for the transport of holes in semiconductors. Heavy, light and split-off valence bands are considered. The first two are described by the warped functions while for the split-off band a parabolic approximation is used. Intra- and inter-band scatterings of holes with non-polar optical phonons, acoustic phonons and impurities are taken into account along with the generation-recombination mechanism. Limiting energy-transport and drift-diffusion models are deduced and simulations in bulk silicon are performed.

PACS number: 72.20.−i

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Holes give a relevant contribution to the charge transport properties in a great variety of different semiconductor materials and devices: silicon p-channel field-effect transistors, bipolar transistors, heterostructures bipolar transistors, compound semiconductor p-channel field-effect transistors and optoelectronic devices as lasers and light emitting diodes.

Although modern computers operate at continuously increasing CPU speed, the direct integration of the system of semiclassical Boltzmann transport equations for electrons and holes is a daunting computational task. For this reason, many authors have developed macroscopic models, for example, see [1–12] and references therein. The main problem related to these models is that of the closure since the number of unknown functions exceeds that of the balance equations. The hydrodynamical models, usually employed in applications, are based on heuristic arguments and *ad hoc* relations, containing free adjustable parameters, without any mathematical or physical justification in the framework of a consistent non-equilibrium thermodynamical theory.

In industrial applications the simulation of hole transport, in bipolar devices, is usually obtained by integrating the drift-diffusion model [13, 14], which is based on the assumption of isothermal charge flow. This is well justified in devices such as MOSFETs (metal oxide field effect transistors) since the contribution of holes to the total current is marginal. However in devices as bipolar heterojunctions the role of holes in charge transport is of the same order or even greater than that of electrons. In such situations more sophisticated models are needed.

In this paper, we present a hydrodynamical model of hole transport in silicon semiconductors based on the maximum entropy principle (hereafter MEP) following the same approach presented in [6, 15–17] for electrons.

A similar approach has already been used in [18] adopting the simplified model with only a single parabolic band. Here both heavy and light holes are considered along with the split-off band. Intra- and inter-band transitions are considered including scattering with non-polar optical phonons, acoustic phonons and impurities. Also the main generation-recombination mechanisms for silicon are taken into account: the Auger and the Schockley–Read–Hall effects in their relaxation approximations [19, 20].

Due to the anisotropy of the bands the determination of the constitutive equations is rather involved and suitable expansions must be introduced to make the problem analytically tractable as already well known in other previous approaches [21, 22].

The plan of the paper is as follows. First, in section 2 we recall the main concepts regarding the energy band structure and hole transport. Then we present the macroscopic balance equations in section 3 and use the MEP in sections 4 and 5 to obtain the closure relations for fluxes (section 6) and production terms (section 7). In section 8, limiting energy-transport and drift-diffusion models are recovered under suitable scaling assumptions. In the last section simulations in homogenous silicon are presented.

2. The kinetic semiclassical model

The hole energy spectrum in Si is represented by three bands [23]. A schematic representation is given in figure 1. The first two bands are the heavy and light valence bands which are degenerate at $\mathbf{k} = 0$, where they reach their maximum. The third one is the so-called split-off band which is separated from the first two by the spin–orbit energy $\Delta = 0.0443$ eV at $\mathbf{k} = 0$. Because of its low density of states and its energy separation the split-off valence band is usually neglected.

In [18] a simplified model has been used: a single spherical parabolic band, that of the heavy holes, with an effective mass related to some plausible average in the $\mathbf{k}$ space. Here a more refined approach is followed: all the three valence bands are included.

The energy bands of heavy and light holes are analytically approximated with *warped bands*

$$\mathcal{E}_H(\mathbf{k}) = \frac{\hbar^2}{2m_e}\left\{Ak^2 \mp \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2}\right\}, \qquad H = +, -, \tag{1}$$

where $+$ and $-$ stand for the light and heavy hole bands respectively. k_x, k_y, k_z are the component of $\mathbf{k}$ with respect to the principal crystallographic axes. $\mathbf{k}$ varies over $\mathbb{R}^3$. The parameters A, B and C depend on the specific material. The constant energy surfaces have a warped form (see figure 2).

The (microscopic) hole velocity $\mathbf{v}$ in the heavy and light warped bands is obtained with the quantum mechanics formula $v^i = \frac{1}{\hbar}\nabla\mathcal{E}$ and reads

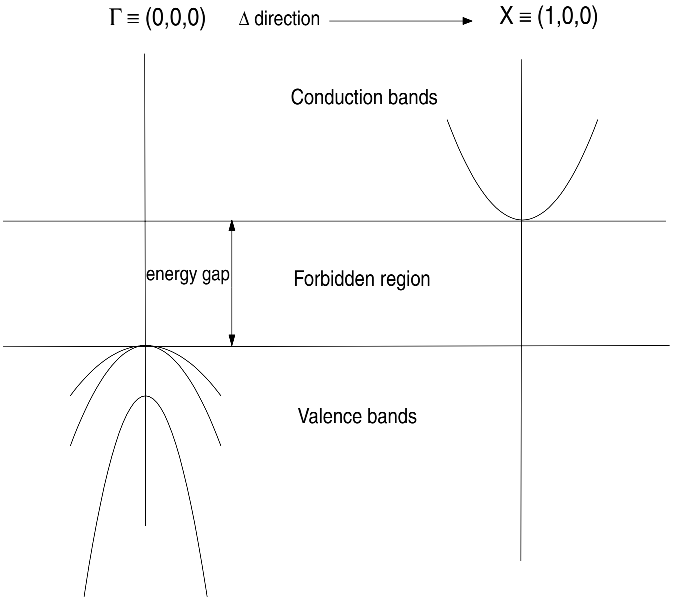

Figure 1. A schematic representation of the energy conduction and valence bands ($\mathcal{E}(\mathbf{k})$ versus $\mathbf{k}$ in arbitrary units) in Si. The conduction bands for holes are obtained from those of valence by reversing the sign.

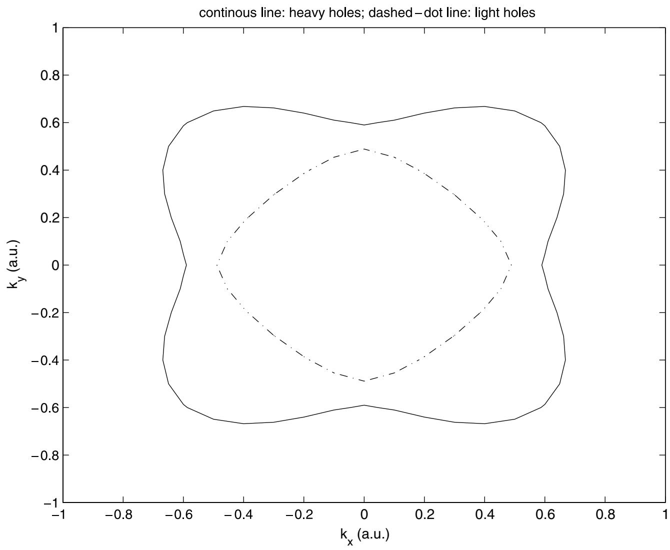

Figure 2. Constant energy surface of the warped bands at $k_z = 0$.

$$v_i = \frac{\hbar}{2m_e} k_i \left\{ 2A \mp \frac{2k^2 B^2 + C^2 k_\perp^2}{\sqrt{B^2 k^4 + C^2 \left(k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2 \right)}} \right\},$$

where $\mathbf{k}_\perp$ is the component of $\mathbf{k}$ orthogonal to the ith crystallographic axis.

The split-off hole band is described by the parabolic approximation

$$\mathcal{E} = \hbar^2 \frac{|\mathbf{k}|^2}{2m_H^*}, \qquad v^i = \frac{1}{\hbar}\nabla\mathcal{E} = \frac{\hbar k^i}{m_H^*}$$

with m_H^* being the effective mass.

From a formal point of view the parabolic band is recovered from the warped one by setting $A = 1$, $B = C = 0$ and replacing m_e with m_H^*.

Simple properties, useful in the sequel, are the following.

Proposition 1. *The warped energy bands have the same (discrete) symmetries of the cube, in particular the permutation of axes.*

The semiclassical description of hole transport in semiconductors consists of a transport equation for each band coupled to the Poisson equation for the electric potential

$$\frac{\partial f_H}{\partial t} + v^i(\mathbf{k})\frac{\partial f_H}{\partial x^i} + \frac{eE^i}{\hbar}\frac{\partial f_H}{\partial k^i} = \mathcal{C}[f_H, f_G] + \mathcal{I}[f_H, f_{\overline{A}}], \tag{2}$$

$$E_i = -\frac{\partial \phi}{\partial x_i}, \tag{3}$$

$$\epsilon\Delta\phi = -e(N_D - N_A - n + p), \tag{4}$$

where ϵ is the dielectric constant, n, p, N_D, N_A are the electron, hole, acceptor and donor densities respectively. e is the absolute value of the elementary charge. The indexes H and G can be + (light holes), − (heavy holes) or SO (split-off band). The model is completed by adding the transport equations for electrons in the conduction bands which are coupled to those for holes through the recombination-generation terms $\mathcal{I}[f_H, f_{\overline{A}}]$, where the index $\overline{A}$ runs over the considered electron bands or valleys.

$\mathcal{C}[f_H, f_G]$ comprises intra- and inter-band acoustic, non-polar optical and impurity scatterings in an additive way. In the linear approximation each of them is written as

$$\mathcal{C}[f_H, f_G] = \int \mathrm{d}\mathbf{k}'_{\mathbf{G}}[P(\mathbf{k}'_{\mathbf{G}}, \mathbf{k}_{\mathbf{H}})f'_G - P(\mathbf{k}_{\mathbf{H}}, \mathbf{k}'_{\mathbf{G}})f_H]$$

with $P(\mathbf{k}_{\mathbf{H}}, \mathbf{k}'_{\mathbf{G}})$ being the transition rate from the state with wave vector $\mathbf{k}_{\mathbf{H}}$ to the state with wave vector $\mathbf{k}'_{\mathbf{G}}$. This latter belongs to another band in the case of inter-band collision.

In the sequel we will make use of the detailed balance principle which both for intra-band and inter-band transition reads

$$P(\mathbf{k}'_{\mathbf{G}}, \mathbf{k}_{\mathbf{H}}) = \exp\left[-\frac{(\mathcal{E}_H - \mathcal{E}'_G) + \Delta_{HG}}{k_B T_L}\right] P(\mathbf{k}_{\mathbf{H}}, \mathbf{k}'_{\mathbf{G}}), \tag{5}$$

where Δ_{HG} is the difference between the bottom of the energy bands. Δ_{HG} is zero for intra-band transition and for inter-band transition between light and heavy holes.

In detail the scattering mechanisms are taken to have the following scattering rates [24, 25]. All the physical parameters are summarized in table 1.

- *intra-band non-polar optical phonon scattering*

$$P(\mathbf{k}, \mathbf{k}') = \mathcal{K}_{op}\begin{bmatrix} N_{op} \\ N_{op}+1 \end{bmatrix}\delta[\mathcal{E}_c(\mathbf{k}') - \mathcal{E}_c(\mathbf{k}) \mp \hbar\omega_{op}],$$

where δ is Dirac's delta, $\mathcal{K}_{op} = \frac{(D_t K)^2}{8\pi^2\rho\omega_{op}}$ is a coupling constant and N_{op} is the optical phonon distribution at equilibrium

$$N_{op} = \frac{1}{\exp(\hbar\omega_{op}/k_B T_L) - 1}, \tag{6}$$

Table 1. Values of the physical parameters used for silicon. The values have been taken according to [26].

m_e	Electron rest mass	9.1095×10^{-28} g
q	Absolute electric charge	$1.602\,177\,33^{-19}$ C
m_H^*	Split-off band mass	$0.57\ m_e$
T_L	Lattice temperature	$300°$ K
ρ	Silicon density	2.33 g cm $^{-3}$
v_s	Longitudinal sound speed	9.18×10^5 cm s $^{-1}$
$\hbar\omega_{op}$	Non-polar optical phonon energy	0.0612 eV
ϵ_r	Relative dielectric constant	11.7
ϵ_0	Vacuum dieletric constant	8.85×10^{-18} C V $^{-1}\mu$ m $^{-1}$
ϵ	Absolute dielectric constant	$\epsilon_r\epsilon_0$
A	Band parameter	4.22
B	Band parameter	0.78
C	Band parameter	4.8

- *intra-band acoustic phonon scattering*

$$P(\mathbf{k}, \mathbf{k}') = \mathcal{K}_{ac} q \begin{bmatrix} N_q \\ N_q + 1 \end{bmatrix} \frac{1}{4}(1 + 3(\mathbf{n} \cdot \mathbf{n}')^2)\delta(\mathcal{E}_c(\mathbf{k}') - \mathcal{E}_c(\mathbf{k}) \mp \hbar q v_s),$$

where the acoustic phonon wave vector is approximated by [25]

$$q = \sqrt{2}k\sqrt{1 - \mathbf{n} \cdot \mathbf{n}'},$$

$\mathcal{K}_{ac} = \frac{\Xi_d^2}{8\pi^2 \rho v_s}$, with $\mathbf{n} = \mathbf{k}/k$, $\mathbf{n}' = \mathbf{k}'/k'$, v_s is the longitudinal component of the sound speed.

- *intra-band impurity scattering*

$$P(\mathbf{k}, \mathbf{k}') = \mathcal{K}_{\text{imp}} \frac{1 + 3(\mathbf{n} \cdot \mathbf{n}')^2}{(\beta^2 + q^2)^2} \delta(\mathcal{E}_c' - \mathcal{E}_c),$$

where, with the same approximation as for the acoustic phonon,

$$K_{\text{imp}} = \frac{Z^2 n_I e^4}{4\hbar\pi^2\epsilon^2}, \qquad q = \sqrt{2}k\sqrt{1 - \mathbf{n} \cdot \mathbf{n}'},$$

with Z being the impurity atomic number, n_I the impurity concentration and β is inverse Debye length

$$\beta = \sqrt{\frac{n_I e^2}{\epsilon k_B T_L}}.$$

- *inter-band non-polar optical phonon scattering*. We will adopt the approximation of writing this scattering as the intra-band case
- *inter-band acoustic phonon scattering*. The only difference with respect to the intra-bands case is the change of the overlap factor

$$P(\mathbf{k}_H, \mathbf{k}'_G) = \mathcal{K}_{ac} q \begin{bmatrix} N_q \\ N_q + 1 \end{bmatrix} \frac{3(1 - (\mathbf{n} \cdot \mathbf{n}')^2)}{4} \delta(\mathcal{E}_c(\mathbf{k}'_G) - \mathcal{E}_c(\mathbf{k}_H) \mp \hbar q v_s),$$

with $\mathbf{k}_H$ and $\mathbf{k}'_G$ belonging to the H-band and the G-band respectively.

- *inter-band impurity scattering.* Also in this case the difference with respect to the intra-band scatterings is the change of the overlap factor

$$P(\mathbf{k}, \mathbf{k}') = 3\mathcal{K}_{\text{imp}} \frac{(1 - (\mathbf{n} \cdot \mathbf{n}')^2)}{(\beta^2 + q^2)^2} \delta(\mathcal{E}_c' - \mathcal{E}_c),$$

- *electron–hole generation recombination*. It includes several mechanisms. We will consider the most important ones for Si that is the Auger and the Schockley–Read–Hall processes in their relaxation approximations [19]

$$\mathcal{I}[f_A, f_{\overline{A}}] = -\Gamma_A[n_A n_{\overline{A}} f_A - n_A {n_i}^2 \mathcal{M}_A] - \Gamma_{\overline{A}}[n_A n_{\overline{A}} f_{\overline{A}} - n_{\overline{A}} {n_i}^2 \mathcal{M}_{\overline{A}}] + \frac{n_{\overline{A}} f_A - {n_i}^2 \mathcal{M}_A}{\tau_h(n+n_i) + \tau_e(p+n_i)},$$

where Γ_A are constants, $\mathcal{M}_A$ the Maxwellians normalized to unit density, τ_A the carrier life time and n_i the intrinsic concentration. The τ_A's will be assumed constant.

Remark. The direct integration of the transport equations requires a huge amount of CPU time and it is not practical for CAD purposes. Our aim is to develop a macroscopic model more suited for engineering applications starting form the kinetic approach.

The simple *drift-diffusion model* is affected by serious drawbacks at submicron scale and does not contain the energy as dynamical variable. Therefore one looks for hydrodynamical models. A consistent hydrodynamical model on MEP has been formulated in [18] assuming a single parabolic band. Here we extend such a model by including the warped effects and all the three valence bands.

3. Macroscopic balance equations

Starting from the Boltzmann equation (2), it is possible to obtain the macroscopic equations for the holes multiplying equation (2) by a weight function $\psi = \psi(\mathbf{k})$ and integrating with respect to $\mathbf{k}$ over $\mathbb{R}^3$. If one indicates with f_H the hole distribution in one of the bands and sets

$$M_\psi = \int_{\mathbb{R}^3} \psi(\mathbf{k}) f_H(\mathbf{x}, \mathbf{k}, t)\, \mathrm{d}\mathbf{k},$$

which is the moment of f_H relative to the weight function $\psi(\mathbf{k})$, the following equation:

$$\frac{\partial M_\psi}{\partial t} + \int_{\mathbb{R}^3} \psi(\mathbf{k}) \mathbf{v} \cdot \nabla_{\mathbf{x}} f_H \,\mathrm{d}\mathbf{k} + \frac{e\mathbf{E}}{\hbar} \cdot \int_{\mathbb{R}^3} \psi(\mathbf{k}) \nabla_{\mathbf{k}} f_H \,\mathrm{d}\mathbf{k} = \int_{\mathbb{R}^3} \psi(\mathbf{k}) \mathcal{C}[f_H]\,\mathrm{d}\mathbf{k} \tag{7}$$

is obtained. Noting that both ψ and $\mathbf{v}$ do not depend on the variable $\mathbf{x}$ we can write

$$\int_{\mathbb{R}^3} \psi(\mathbf{k}) \mathbf{v} \cdot \nabla_{\mathbf{x}} f_H \,\mathrm{d}\mathbf{k} = \nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}^3} \psi(\mathbf{x}) \mathbf{v} f_H \,\mathrm{d}\mathbf{k}.$$

Moreover, applying the Gauss theorem and noting that f_H has to rapidly tend to 0 as $\mathbf{k}$ tends to ∞ in order to guarantee the existence of the integrals, we get[1]

$$\frac{\partial M_\psi}{\partial t} + \frac{\partial}{\partial x^i} \int_{\mathbb{R}^3} \psi(\mathbf{k}) v^i f_H \,\mathrm{d}\mathbf{k} - \frac{eE^i}{\hbar} \int_{\mathbb{R}^3} \frac{\partial \psi}{\partial k^i} f_H \,\mathrm{d}\mathbf{k} = \int_{\mathbb{R}^3} \psi(\mathbf{k}) \mathcal{C}[f_H]\,\mathrm{d}\mathbf{k}. \tag{8}$$

First, we set $\psi(\mathbf{k}) = 1$ and get the balance equation for the hole density

$$\frac{\partial p_H}{\partial t} + \frac{\partial \left(p_H V_H^i\right)}{\partial x^i} = p_H C_p, \tag{9}$$

where

$$p_H = \int_{\mathbb{R}^3} f_H \,\mathrm{d}\mathbf{k} \qquad \text{is the hole density,}$$

$$V_H^i = \frac{1}{p_H} \int_{\mathbb{R}^3} v^i f_H \,\mathrm{d}\mathbf{k} \qquad \text{is the average hole velocity,}$$

$$C_p = \frac{1}{p_H} \int_{\mathbb{R}^3} \mathcal{C}[f_H]\,\mathrm{d}\mathbf{k} \qquad \text{is the density production.}$$

[1] Einstein summation over repeated letters is understood.

As the second weight function we take $\psi(\mathbf{k}) = \hbar k^i$, $i = 1, 2, 3$ and after some simple algebra, we get the average crystal momentum balance equation

$$\frac{\partial\left(p_H P_H^j\right)}{\partial t} + \frac{\partial\left(p_H U_H^{ij}\right)}{\partial x^i} - p_H e E^j = p_H C_{P_H}^j, \qquad j = 1, 2, 3, \tag{10}$$

where

$$P_H^j = \frac{1}{p_H}\int_{\mathbb{R}^3} \hbar k^j f_H \,\mathrm{d}\mathbf{k} \qquad j = 1, 2, 3 \qquad \text{is the average crystal momentum,}$$

$$U_H^{ij} = \frac{1}{p_H}\int_{\mathbb{R}^3} f_H v^i \hbar k^j \,\mathrm{d}\mathbf{k} \qquad \text{is the crystal momentum flux,}$$

$$C_{P_H}^j = \frac{1}{p_H}\int_{\mathbb{R}^3} \hbar k^j \mathcal{C}[f_H](\mathbf{x}, \mathbf{k}, t) \,\mathrm{d}\mathbf{k} \qquad \text{is the average crystal momentum production.}$$

Now if we assume that $\psi(\mathbf{k}) = \mathcal{E}(\mathbf{k})$, we get the balance equation for the average hole energy

$$\frac{\partial(p_H W_H)}{\partial t} + \frac{\partial(p_H S_H^i)}{\partial x^i} - p_H e E_i V_H^i = p_H C_{W_H}, \tag{11}$$

where

$$W_H = \frac{1}{p_H}\int_{\mathbb{R}^3} \mathcal{E}(\mathbf{k}) f_H \,\mathrm{d}\mathbf{k} \qquad \text{is the average hole energy,}$$

$$S_H^i = \frac{1}{p_H}\int_{\mathbb{R}^3} \mathcal{E}(\mathbf{k}) f_H v^i d\mathbf{k} \qquad \text{is the energy flux,}$$

$$C_{W_H} = \frac{1}{p_H}\int_{\mathbb{R}^3} \mathcal{E}(\mathbf{k})\mathcal{C}[f_H](\mathbf{x}, \mathbf{k}, t) \,\mathrm{d}\mathbf{k} \qquad \text{is the energy production.}$$

Finally, let us set $\psi(\mathbf{k}) = \mathcal{E}(\mathbf{k})v^j$, $j = 1, 2, 3$, obtaining the balance equation for the energy-flux

$$\frac{\partial\left(p_H S_H^j\right)}{\partial t} + \frac{\partial\left(p_H F_H^{ij}\right)}{\partial x^i} - p_H e E_i G_H^{ji} = p_H C_{S_H}^j, \tag{12}$$

where

$$F_H^{ij} = \frac{1}{p_H}\int_{\mathbb{R}^3} \mathcal{E}(\mathbf{k}) v^i v^j f \,\mathrm{d}\mathbf{k} \qquad \text{is the flux of energy flux,}$$

$$G_H^{ij} = \frac{1}{p_H}\int_{\mathbb{R}^3} \frac{1}{\hbar} f_H \frac{\partial(\mathcal{E} v^i)}{\partial k^j} \,\mathrm{d}\mathbf{k},$$

$$C_{S_H}^j = \frac{1}{p_H}\int_{\mathbb{R}^3} \mathcal{E}(\mathbf{k}) v^j \mathcal{C}[f_H] \,\mathrm{d}\mathbf{k} \qquad \text{is the flux energy production.}$$

With this choice of the functions $\psi(\mathbf{k})$, our model is given by the following system of balance equations for each population of holes:

$$\frac{\partial p_H}{\partial t} + \frac{\partial\left(p_H V_H^i\right)}{\partial x^i} = p_H C_p, \tag{13}$$

$$\frac{\partial\left(p_H P_H^j\right)}{\partial t} + \frac{\partial\left(p_H U_H^{ij}\right)}{\partial x^j} - p_H e E^j = p_H C_{P_H}^j, \qquad j = 1, 2, 3, \tag{14}$$

$$\frac{\partial p_H W_H}{\partial t} + \frac{\partial\left(p_H S_H^i\right)}{\partial x^i} - p_H e E_i V_H^i = p_H C_{W_H}, \tag{15}$$

$$\frac{\partial\left(p_H S_H^j\right)}{\partial t} + \frac{\partial\left(p_H F_H^{ij}\right)}{\partial x^i} - p_H e E_i G_H^{ji} = p_H C_{S_H}^j \qquad j = 1, 2, 3, \tag{16}$$

where p_H, $\mathbf{V}_H$, W_H and $\mathbf{S}_H$ are assumed as fundamental variables since they have a direct physical meaning. Therefore there is the problem of closing the system (13)–(16) by expressing the fluxes U_H^{ij}, F_H^{ij}, G_H^{ij} and the production term C_p, $C_{P_H}^j$, C_{W_H}, $C_{S_H}^j$ as functions of p_H, V_H^i, W_H and S_H^i.

4. Maximum entropy principle and closure relations

In order to get the closure relations for semiconductor hydrodynamical models, many strategies have been proposed, often without any consistent mathematical or physical rationale [27]. In [15–17], the MEP [28–31] has been used to solve the problem of finding self-consistent closure relations for electron macroscopic balance equations, both for Si and GaAs. Here we employ MEP to get the required closure relations for the system (13)–(16).

According to this principle, if we have a finite number of known moments for each band H

$$M_{H,\alpha} = \int_{\mathbb{R}^3} \psi_\alpha f_H \, \mathrm{d}\mathbf{k}, \qquad H = -, +, SO,$$

then the distribution function f_H^{ME}, which can be used for an evaluation of the unknown moments, corresponds to the extremum of the entropy functional, under the restrictions

$$M_{H,\alpha} = \int_{\mathbb{R}^3} \psi_\alpha f_H^{ME} \, \mathrm{d}\mathbf{k}. \tag{17}$$

The formal setting of the MEP has been developed in the framework of the information theory by Shannon and applied for the first time to statistical mechanics by Jaynes [28]. He showed that many questions of classical and quantum mechanics can be reformulated as statistical inference problems where the MEP distribution represents the least biased distribution with respect to the only knowledge of a finite number of moments.

In the case of a sufficiently dilute hole gas the entropy functional, according to the classical limit of the expression arising in the Fermi statistics, is for each population

$$-k_B \int_{\mathbb{R}^3} (f_H \log f_H - f_H) \, \mathrm{d}\mathbf{k}, \tag{18}$$

while the total entropy reads

$$s = -k_B \sum_H \int_{\mathbb{R}^3} (f_H \log f_H - f_H) \, \mathrm{d}\mathbf{k}_H. \tag{19}$$

By introducing the Lagrangian multipliers $\Lambda_{H,\alpha}$, looking for the extremals of the entropy is equivalent to looking for the extremals without constraints of the following functional:

$$s' = \sum_{H,\alpha} \Lambda_{H,\alpha} \left(\int_{\mathbb{R}^3} \psi_{H,\alpha} f_H \, \mathrm{d}\mathbf{k} - M_{H,\alpha} \right) - s \tag{20}$$

which is the Legendre transform of the entropy functional s. From variational calculus,

$$\delta s' = k_B \sum_H \int_{\mathbb{R}^3} \delta f_H \log f_H \, \mathrm{d}\mathbf{k} + \sum_{H,\alpha} \Lambda_{H,\alpha} \int_{\mathbb{R}^3} \psi_{H,\alpha} \delta f_H \, \mathrm{d}\mathbf{k} = 0$$

for arbitrary δf_H. Therefore for each band H,

$$\log f_H + \frac{\Lambda_{H,\alpha}\psi_{H,\alpha}}{k_B} = 0$$

from which we get the maximum entropy distribution function as

$$f_H^{ME} = \exp\left(-\sum_\alpha \frac{\Lambda_{H,\alpha}\psi_{H,\alpha}}{k_B}\right). \tag{21}$$

If we make the choice of the weight functions $\psi_{H,\alpha} = (1, \mathbf{v}, \mathcal{E}, \mathcal{E}\mathbf{v})$ for each band $H = +, -,$ SO, one has to introduce the Lagrangian multipliers $\Lambda_H = \left(\lambda_H, \boldsymbol{\lambda}_H^P, \lambda_H^W, \boldsymbol{\lambda}_H^S\right)$ and the maximum entropy distribution function reads

$$f_H^{ME} = \exp\left[-\left(\frac{1}{k_B}\lambda_H + \boldsymbol{\lambda}_H^P\cdot\mathbf{v} + \lambda_H^W\mathcal{E} + \boldsymbol{\lambda}_H^S\cdot\mathbf{v}\mathcal{E}\right)\right]. \tag{22}$$

In order to complete the program, it is necessary to express the Lagrangian multipliers in terms of the fundamental variables by evaluating the constraints (17). On account of the high nonlinearities, we were not able to find out an analytical explicit form of the multipliers, but, by proceeding as in [15], we expand f_H^{ME} with respect to a parameter of anisotropy δ and solve the resulting equations at several orders in such a parameter. In particular with the previous choice of the weights in the moments, one expand f_H^{ME} as

$$\begin{aligned} f_H^{ME} &= \exp\left[-\left(\frac{1}{k_B}\lambda_H + \lambda_H^W\mathcal{E} + \delta\boldsymbol{\lambda}_H^P\cdot\mathbf{v} + \delta\boldsymbol{\lambda}_H^S\cdot\mathbf{v}\mathcal{E}\right)\right] \\ &= \exp\left(-\frac{1}{k_B}\lambda_H - \lambda^W\mathcal{E}\right)\left[1 - \delta\left(\boldsymbol{\lambda}_H^P\cdot\mathbf{v} + \boldsymbol{\lambda}_H^S\cdot\mathbf{v}\mathcal{E}\right)\right] + o(\delta). \end{aligned} \tag{23}$$

For the split-off valence band, since a parabolic approximation is used, we are in the same case considered in [18]. For the other two valence bands, the situation is much more involved. In the following sections by using the distribution in (23) we will able to obtain up to first order in δ closure relations for the system (13)–(16) also for light and heavy holes.

5. Determination of the Lagrangian multipliers

The first step in order to get the required closure relations consists of expressing the Lagrangian multipliers as a function of the moments, that is, with the previous choice of the weights, as functions of $p_H, \mathbf{V}_H, W_H, \mathbf{S}_H$. To this aim, one has to solve the following nonlinear algebraic system (in this and the following section we will drop the band index for simplifying the notation):

$$p = \int_{\mathbb{R}^3} f^{ME}\,\mathrm{d}\mathbf{k}, \tag{24}$$

$$V_i = \frac{1}{p}\int_{\mathbb{R}^3} v_i f^{ME}\,\mathrm{d}\mathbf{k}, \tag{25}$$

$$W = \frac{1}{p}\int_{\mathbb{R}^3} \mathcal{E} f^{ME}\,\mathrm{d}\mathbf{k}, \tag{26}$$

$$S_i = \frac{1}{p}\int_{\mathbb{R}^3} v_i\mathcal{E} f^{ME}\,\mathrm{d}\mathbf{k}, \tag{27}$$

where f_{ME} is approximated from now on with (23). By introducing the polar and azimuthal angles ϑ and φ with respect to the main crystallographic axes, the expression of the energy valence bands can be rewritten as

$$\mathcal{E}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_e}[A \mp g(\vartheta, \varphi)], \tag{28}$$

where

$$g(\vartheta, \varphi) = \sqrt{B^2 + C^2(\sin^2\vartheta\cos^2\vartheta + \sin^4\vartheta\cos^2\varphi\sin^2\varphi)}$$

and the element of volume $\mathrm{d}\mathbf{k}$ can be written as

$$\mathrm{d}\mathbf{k} = \frac{\sqrt{2}m_e^{3/2}}{\hbar^3}\sqrt{\mathcal{E}}\,[A \mp g(\vartheta, \varphi)]^{-3/2}\,\mathrm{d}\mathcal{E}\,\mathrm{d}\Omega,$$

with $\mathrm{d}\Omega = \sin\vartheta\,\mathrm{d}\vartheta\,\mathrm{d}\varphi$ being the element of solid angle. Moreover the unit vector $\mathbf{n}$ has components $(\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$

In the following we will make also use of the fact that for integral over S^2, the unit sphere of $\mathbb{R}^3$, one has[2]

$$\int_{S^2} l^{i_1}\cdots l^{i_k}\,\mathrm{d}\Omega = \begin{cases} 0 & \text{if } k \text{ is odd} \\ \dfrac{4\pi}{k+1}\delta^{(i_1 i_2}\cdots\delta^{i_{k-1}i_k)} & \text{if } k \text{ is even.}\end{cases} \tag{29}$$

The starting point is the following crucial relation:

Proposition 2. *The Lagrangian multiplier relative to the energy up to first order in δ has the same expression as the parabolic case*

$$\lambda^W = \frac{3}{2W}.$$

Proof. According to the representation theorem for tensor-valued isotropic functions, W must depend on $\boldsymbol{\lambda}^P$ and $\boldsymbol{\lambda}^S$ only through their modulus. Since the integrals

$$\int_{\mathbb{R}^3}\exp\left(-\frac{1}{k_B}\lambda - \lambda^W\mathcal{E}\right)(\boldsymbol{\lambda}^P\cdot\mathbf{v} + \boldsymbol{\lambda}^S\cdot\mathbf{v}\mathcal{E})\,\mathrm{d}\mathbf{k},$$
$$\int_{\mathbb{R}^3}\mathcal{E}\exp\left(-\frac{1}{k_B}\lambda - \lambda^W\mathcal{E}\right)(\boldsymbol{\lambda}^P\cdot\mathbf{v} + \boldsymbol{\lambda}^S\cdot\mathbf{v}\mathcal{E})\,\mathrm{d}\mathbf{k}$$

are linear in $\boldsymbol{\lambda}^P$ and $\boldsymbol{\lambda}^S$ they must vanishes. Therefore the constraint (26) gives

$$W = \frac{\int_{\mathbb{R}^3}\mathcal{E}\exp\left(-\frac{1}{k_B}\lambda - \lambda^W\mathcal{E}\right)\mathrm{d}\mathbf{k}}{\int_{\mathbb{R}^3}\exp\left(-\frac{1}{k_B}\lambda - \lambda^W\mathcal{E}\right)\mathrm{d}\mathbf{k}} = \frac{\int_0^{+\infty}\mathcal{E}^{3/2}\exp(-\lambda^W\mathcal{E})\,\mathrm{d}\mathcal{E}}{\int_0^{+\infty}\mathcal{E}^{1/2}\exp(-\lambda^W\mathcal{E})\,\mathrm{d}\mathcal{E}} = \frac{3}{2\lambda^W},$$

after we have used the relation valid for any $a, \nu > 0$

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

with $\Gamma(\nu)$ being the special Gamma function, which satisfies for positive integer p,

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

□

Once λ^W has been explicitly determined, we can evaluate the other constraints. For the Lagrangian multipliers relative to the density, with consideration similar to that for λ^W, one finds

$$\lambda = -k_B\log\frac{\hbar^3 p}{2J_1\pi^{1/2}(m_e W/3)^{3/2}} \qquad \text{with} \qquad J_1 = \int_{S^2} D^{-3/2}\,\mathrm{d}\Omega,$$

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

Table 2. Values of the parameters entering in the constitutive relations.

Parameter	Heavy holes	Light holes
J_1	4.945 21	0.777 36
J_2	15.3740	6.859 86
J_3	6.593 62	1.036 48
J_4	38.4350	23.3588
J_5	27.7599	0.190 82
J_6	9.253 29	0.063 61
J_7	−4.380 55	−0.029 78
J_8	16.3034	0.402 86
J_9	20.3154	0.418 760
J_{10}	−7.710 68	−0.188 442
J_{11}	38.0139	2.666 28

where

$$D = A \mp \sqrt{B^2 + C^2 \sin^2\vartheta(\sin^2\vartheta \sin^2\varphi\cos^2\varphi + \cos^2\vartheta)}.$$

Concerning $\boldsymbol{\lambda}^P$ and $\boldsymbol{\lambda}^S$ from the representation formulae we have

$$\boldsymbol{\lambda}^V = b_{11}(W)\mathbf{V} + b_{12}(W)\mathbf{S} \tag{30}$$

$$\boldsymbol{\lambda}^S = b_{21}(W)\mathbf{V} + b_{22}(W)\mathbf{S} \tag{31}$$

Evaluating the constraints (14) and (16) one gets

$$b_{11} = -\frac{7m_e}{W}\frac{J_1}{J_2}, \qquad b_{12} = b_{21} = \frac{3m_e}{W^2}\frac{J_1}{J_2}, \qquad b_{22} = -\frac{9m_e}{5W^3}\frac{J_1}{J_2}, \tag{32}$$

where

$$J_2 = \int_{S^2}\frac{T^2}{D^{3/2}}\cos^2\vartheta\,\mathrm{d}\Omega \qquad \text{with}$$

$$T = \left(2A \mp \frac{2B^2 + C^2\sin^2\vartheta}{\sqrt{B^2 + C^2\sin^2\vartheta(\sin^2\vartheta\sin^2\varphi\cos^2\varphi + \cos^2\vartheta)}}\right)\frac{1}{\sqrt{D}}.$$

The integrals J_1 and J_2 do not depend on W. They have been evaluated with standard numerical methods and their numerical values are reported in table 2. In the parabolic band case we have evaluated J_1 and J_2 analytically, obtaining

$$\begin{aligned} &\frac{\lambda}{k_B} = -\log\frac{\hbar^3 p}{\left(\frac{4}{3}\pi m_H^* W\right)^{3/2}}, \qquad \lambda^W = \frac{3}{2W}, \\ &\boldsymbol{\lambda}^P = -\frac{21m_H^*}{4W}\mathbf{V} + \frac{9m_H^*}{4W^2}\mathbf{S}, \qquad \boldsymbol{\lambda}^S = \frac{9m_H^*}{4W^2}\mathbf{V} - \frac{27m_H^*}{20W^3}\mathbf{S} \end{aligned} \tag{33}$$

and the distribution function given by the maximum entropy principle becomes

$$f^{ME} = \frac{\exp\left(-\frac{3}{2W}\mathcal{E}\right)}{\left(\frac{4}{3}\pi m_H^* W\right)^{3/2}}p\left[1 - \left(-\frac{21m_H^*}{4W}\mathbf{V} + \frac{9m_H^*}{4W^2}\mathbf{S}\right)\cdot\mathbf{v} - \mathcal{E}\left(\frac{9m_H^*}{4W^2}\mathbf{V} - \frac{27m_H^*}{20W^3}\mathbf{S}\right)\cdot\mathbf{v}\right]. \tag{34}$$

6. Closure relations: fluxes

Since f^{ME} is now explicitly expressed in terms of the moments p, $\mathbf{V}$, W, $\mathbf{S}$, we can evaluated all the unknown moments present in the system (13)–(16). In this section we will consider P_H^j and the fluxes U^{ij}, F^{ij}, G^{ij}. First we observe that, as in the parabolic case,

$$P_H^j = m^* V_H^j, \tag{35}$$

where m^* is the holes effective mass whose explicit expression is given by

$$m^* = \frac{J_3}{J_2} m_e \tag{36}$$

with

$$J_3 = 2\int_{S^2} \frac{T}{D^2}\cos^2\vartheta \,\mathrm{d}\Omega.$$

Although the anisotropy of the energy bands, on account of their symmetry, the tensors U^{ij}, F^{ij}, G^{ij} are isotropic as stated by the following proposition:

Proposition 3. *Up to first order in δ one has*

$$U^{ij} = U(W)\delta^{ij}, \qquad F^{ij} = F(W)\delta^{ij}, \qquad G^{ij} = G(W)\delta^{ij},$$

where

$$U(W) = \frac{2}{3} W \,(\text{as in the parabolic case}), \tag{37a}$$

$$F(W) = \frac{5}{6m_e}\frac{J_2}{J_1} W^2, \tag{37b}$$

$$G(W) = \frac{1}{2m_e}\frac{J_4}{J_1} W \tag{37c}$$

with

$$J_4 = \int_{S^2}\left[\frac{\cos^2\vartheta}{D^{3/2}}\frac{(2A - T\sqrt{D})^2 \mp 4B^2}{\sqrt{B^2 + C^2\sin^2\vartheta(\sin^2\vartheta\sin^2\varphi\cos^2\varphi + \cos^2\vartheta)}} + \frac{T}{D} + \frac{T^2}{D^{3/2}}\cos^2\vartheta\right]\mathrm{d}\Omega.$$

Proof. From the definition

$$U^{ij} = \frac{1}{p}\int_{\mathbb{R}^3} f^{ME} v^i \hbar k^j \,\mathrm{d}\mathbf{k}.$$

Up to first order in δ, by using the ϑ, ϕ, $\mathcal{E}$ coordinates, it is simple matter to show that the off-diagonal components vanishes while the diagonal terms are given by

$$U_{11} = \frac{1}{m_e p}\int_{\mathbb{R}^3}\exp\left(-\frac{1}{k_B}\lambda - \lambda^W\mathcal{E}\right)k_x^2\left[A \mp \frac{2k^2B^2 + C^2\left(k_y^2 + k_z^2\right)}{2\sqrt{B^2k^4 + C^2\left(k_x^2k_y^2 + k_xk_z^2 + k_y^2k_z^2\right)}}\right]\mathrm{d}k_x\,\mathrm{d}k_y\,\mathrm{d}k_z$$

$$U_{22} = \frac{1}{m_e p}\int_{\mathbb{R}^3}\exp\left(-\frac{1}{k_B}\lambda - \lambda^W\mathcal{E}\right)k_y^2\left[A \mp \frac{2k^2B^2 + C^2\left(k_x^2 + k_z^2\right)}{2\sqrt{B^2k^4 + C^2\left(k_x^2k_y^2 + k_xk_z^2 + k_y^2k_z^2\right)}}\right]\mathrm{d}k_x\,\mathrm{d}k_y\,\mathrm{d}k_z$$

$$U_{33} = \frac{1}{m_e p}\int_{\mathbb{R}^3}\exp\left(-\frac{1}{k_B}\lambda - \lambda^W\mathcal{E}\right)k_z^2\left[A \mp \frac{2k^2B^2 + C^2\left(k_x^2 + k_y^2\right)}{2\sqrt{B^2k^4 + C^2\left(k_x^2k_y^2 + k_xk_z^2 + k_y^2k_z^2\right)}}\right]\mathrm{d}k_x\,\mathrm{d}k_y\,\mathrm{d}k_z,$$

where k is the modulus of $\mathbf{k}$. Since $\mathcal{E}$ is invariant with respect to any permutation of the axes (proposition 1), it follows that $U_{11} = U_{22} = U_{33}$, that is the tensor U_{ij} is isotropic. By evaluating U_{33} in the $\vartheta, \varphi, \mathcal{E}$ coordinates, one has (37*a*).

With similar argumentations the isotropy of F_{ij} and G_{ij} is obtained along with relations (37*b*) and (37*c*). □

The values of J_3 and J_4 are reported in table 2. In the parabolic band limit one has

$$U^{ij} = \frac{2}{3} W \delta^{ij}, \qquad m_H^* F^{ij} = \frac{10}{9} W^2 \delta^{ij}, \qquad G^{ij} = \frac{5}{3m_H^*} W \delta^{ij}. \tag{38}$$

7. Closure relations: production terms

Now we turn our attention to the closure relations of the production terms. Since the various scattering mechanisms contribute in an additive way, we consider them separately.

7.1. Intra-band non-polar optical phonon–hole scattering

By using the chain of equalities

$$\begin{aligned}\int_{\mathbb{R}^3} \psi(\mathbf{k}) \mathcal{C}[f_h](\mathbf{x}, \mathbf{k}, t)\, \mathrm{d}\mathbf{k} &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \psi(\mathbf{k}) [P(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') - P(\mathbf{k}, \mathbf{k}') f(\mathbf{k})]\, \mathrm{d}\mathbf{k}'\, \mathrm{d}\mathbf{k} \\ &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} [\psi(\mathbf{k}') - \psi(\mathbf{k})] P(\mathbf{k}, \mathbf{k}') f(\mathbf{k})\, \mathrm{d}\mathbf{k}'\, \mathrm{d}\mathbf{k},\end{aligned}$$

we get the following expressions for the production terms:

$$C_p^{(op)} = 0 \tag{39}$$

$$C_P^{i(op)} = c_{11}^{(op)} V^i + c_{12}^{(op)} S^i \tag{40}$$

$$C_W^{(op)} = \tilde{\mathcal{K}}_{op} W^{-3/2} J_1 [N_{op} B_1 - (N_{op} + 1) B_2] \tag{41}$$

$$C_S^{i(op)} = c_{21}^{(op)} V^i + c_{22}^{(op)} S^i, \tag{42}$$

where

$$c_{11}^{(op)} = \frac{J_3 \tilde{\mathcal{K}}_{op}}{2\hbar\omega_{op}} W^{-3/2} [N_{op}(-b_{11} B_1' + b_{12} B_1'') + (N_{op} + 1)(-b_{11} B_2' + b_{12} B_2'')],$$

$$c_{12}^{(op)} = \frac{J_3 \tilde{\mathcal{K}}_{op}}{2\hbar\omega_{op}} W^{-3/2} [N_{op}(-b_{12} B_1' + b_{22} B_1'') + (N_{op} + 1)(-b_{12} B_2' + b_{22} B_2'')]$$

$$c_{21}^{(op)} = \frac{J_2 \tilde{\mathcal{K}}_{op}}{2m_e\hbar\omega_{op}} W^{-3/2} [N_{op}(b_{11} B_1'' - b_{12} B_1''') + (N_{op} + 1)(b_{11} B_2'' - b_{12} B_2''')],$$

$$c_{22}^{(op)} = \frac{J_2 \tilde{\mathcal{K}}_{op}}{2m_e\hbar\omega_{op}} W^{-3/2} [N_{op}(b_{12} B_1'' - b_{22} B_1''') + (N_{op} + 1)(b_{12} B_2'' - b_{22} B_2''')].$$

The coefficients b_{ij} are given by (32) for light and heavy holes and by (33) for the holes in the split-off band. The prime refers to the derivative with respect to λ^W while

$$B_1(\lambda^W) = \exp\left(\hbar\omega_{op} \frac{\lambda^W}{2}\right) \frac{\hbar\omega_{op}}{2\lambda^W} K_1 \left(\hbar\omega_{op} \frac{\lambda^W}{2}\right), \tag{43}$$

$$B_2(\lambda^W) = \exp(-\hbar\omega_{op}\lambda^W) B_1(\lambda^W), \tag{44}$$

with Γ being the Gamma function, K_1 the modified Bessel function of second kind of index 1 and

$$\tilde{\mathcal{K}}_{op} = \frac{3(m_e)^{3/2}\omega_{op}\sqrt{3/\pi}}{\hbar^2}\mathcal{K}_{op}.$$

We recall that for the computation of the derivatives of B_1 and B_2 the recurrence formulae

$$K_n'(z) = \frac{n}{z}K_n(z) - K_{n+1}(z), \qquad K_n'(z) = -\frac{n}{z}K_n - K_{n-1}(z)$$

can be used.

In the parabolic case one has

$$C_p^{(op)} = 0, \tag{45}$$

$$C_P^{i(op)} = c_{11}^{(op)}V^i + c_{12}^{(op)}S^i, \tag{46}$$

$$C_W^{(op)} = \tfrac{3}{2}\hbar\omega_{op}\hat{\mathcal{K}}_{op}W^{-3/2}[N_{op}B_1 - (N_{op}+1)B_2] \tag{47}$$

$$C_S^{i(op)} = c_{21}^{(op)}V^i + c_{22}^{(op)}S^i, \tag{48}$$

where

$$\begin{aligned}
c_{11}^{(op)} &= \hat{\mathcal{K}}_{op}W^{-3/2}[N_{op}(-b_{11}B_1' + b_{12}B_1'') + (N_{op}+1)(-b_{11}B_2' + b_{12}B_2'')],\\
c_{12}^{(op)} &= \hat{\mathcal{K}}_{op}W^{-3/2}[N_{op}(-b_{12}B_1' + b_{22}B_1'') + (N_{op}+1)(-b_{12}B_2' + b_{22}B_2'')]\\
c_{21}^{(op)} &= \frac{\hat{\mathcal{K}}_{op}}{m_H^*}W^{-3/2}[N_{op}(b_{11}B_1'' - b_{12}B_1''') + (N_{op}+1)(b_{11}B_2'' - b_{12}B_2''')],\\
c_{22}^{(op)} &= \frac{\hat{\mathcal{K}}_{op}}{m_H^*}W^{-3/2}[N_{op}(b_{12}B_1'' - b_{22}B_1''') + (N_{op}+1)(b_{12}B_2'' - b_{22}B_2''')].
\end{aligned}$$

with $\hat{\mathcal{K}}_{op} = \frac{8(m_H^*)^{3/2}\sqrt{3\pi}}{\hbar^3}\mathcal{K}_{op}$.

7.2. Intra-band acoustic phonon–hole scattering

First of all we observe that by using the principle of detailed balance (5), the moment of the collision term with respect to the weight function $\psi(\mathbf{k})$ can be written as

$$\begin{aligned}
M_\psi &= \int_{\mathbb{R}^3\times\mathbb{R}^3}\psi(\mathbf{k})[P(\mathbf{k}',\mathbf{k})f(\mathbf{k}') - P(\mathbf{k},\mathbf{k}')f(\mathbf{k})]\,\mathrm{d}\mathbf{k}'\,\mathrm{d}\mathbf{k}\\
&= \int_{\mathbb{R}^3\times\mathbb{R}^3}\psi(\mathbf{k})P(\mathbf{k},\mathbf{k}')[f(\mathbf{k}')e^{\frac{\mathcal{E}'-\mathcal{E}}{k_BT_L}} - f(\mathbf{k})]\,\mathrm{d}\mathbf{k}'\,\mathrm{d}\mathbf{k}\\
&= \frac{1}{4}\mathcal{K}_{ac}q\left\{\int_{\mathbb{R}^3\times\mathbb{R}^3}N_q(1+3\cos^2\vartheta)\delta(\mathcal{E}'-\mathcal{E}-\hbar\omega_q)\big[f(\mathbf{k}')\,\mathrm{e}^{\frac{\mathcal{E}'-\mathcal{E}}{k_BT_L}} - f(\mathbf{k})\big]\psi(\mathbf{k})\,\mathrm{d}\mathbf{k}'\,\mathrm{d}\mathbf{k}\right.\\
&\quad\left.+\int_{\mathbb{R}^3\times\mathbb{R}^3}(N_q+1)(1+3\cos^2\vartheta)\delta(\mathcal{E}'-\mathcal{E}+\hbar\omega_q)\big[f(\mathbf{k}')\,\mathrm{e}^{\frac{\mathcal{E}'-\mathcal{E}}{k_BT_L}} - f(\mathbf{k})\big]\psi(\mathbf{k})\,\mathrm{d}\mathbf{k}'\,\mathrm{d}\mathbf{k}\right\}.
\end{aligned} \tag{49}$$

By expanding N_q in Laurent's series with respect to $\hbar\omega_q/k_BT_L$

$$N_q \simeq \frac{k_BT_L}{\hbar\omega_q} - \frac{1}{2} + \frac{1}{12}\frac{\hbar\omega_q}{k_BT_L} + o\left(\frac{\hbar\omega_q}{k_BT_L}\right),$$

and by taking into account that the phonon energy can be expressed as

$$\hbar\omega_q = 2v_s\sqrt{\frac{m_e\mathcal{E}}{D}(1-\mathbf{n}\cdot\mathbf{n}')},$$

after a lengthy calculation one gets the following contribution to the production terms due to the acoustic phonon scattering up to first order in $\sqrt{m_e v_s^2 / k_B T_L}$:

$$C_p^{(ac)} = 0, \tag{50}$$

$$C_P^{i(ac)} = c_{11}^{(ac)} V^i + c_{12}^{(ac)} S^i, \tag{51}$$

$$C_W^{(ac)} = -8 m_e v_s^2 \frac{J_5}{J_1} \mathcal{K}'_{ac} W^{1/2} \left(W - \frac{3}{2} k_B T_L \right), \tag{52}$$

$$C_S^{i(ac)} = c_{21}^{(ac)} V^i + c_{22}^{(ac)} S^i, \tag{53}$$

where

$$\begin{aligned} c_{11}^{(ac)} = \frac{27}{16 J_2} \mathcal{K}'_{ac} W^{-3/2} \Bigg\{ & \frac{128 m_e^2 v_s^2}{81 k_B T_L} (J_6 - J_7) W^3 \\ & + \left(\frac{64 m_e^2 v_s^2 J_6}{27} - \frac{256 m_e^2 v_s^2 J_7}{27} - \frac{64 m_e k_B T_L J_8}{27} \right) W^2 \\ & + \frac{8 m_e^2 v_s^2 k_B T_L}{3} (8 J_7 + J_6) W \Bigg\}, \\ c_{12}^{(ac)} = \frac{27}{16 J_2} \mathcal{K}'_{ac} W^{-3/2} \Bigg\{ & \frac{128 m_e^2 v_s^2}{45 k_B T_L} (J_7 - J_6) W^2 \\ & - \left(\frac{64 m_e^2 v_s^2 J_6}{45} - \frac{256 m_e^2 v_s^2 J_7}{45} - \frac{64 m_e k_B T_L J_8}{45} \right) W \\ & - \frac{8 m_e^2 v_s^2 k_B T_L}{15} (8 J_7 + J_6) \Bigg\}, \\ c_{21}^{(ac)} = \frac{27}{16 J_2} \mathcal{K}'_{ac} W^{-3/2} \Bigg\{ & \frac{1024 m_e v_s^2}{81 k_B T_L} (J_9 - J_{10}) W^4 \\ & + \left(\frac{256 m_e v_s^2 J_{10}}{9} - \frac{128 m_e v_s^2 J_9}{27} + \frac{128 k_B T_L J_{11}}{27} \right) W^3 \\ & + \frac{32 m_e v_s^2 k_B T_L}{9} \left(8 J_{10} + \frac{J_9}{3} \right) W^2 \Bigg\}, \\ c_{22}^{(ac)} = \frac{27}{16 J_2} \mathcal{K}'_{ac} W^{-3/2} \Bigg\{ & \frac{1024 m_e v_s^2}{81 k_B T_L} (J_{10} - J_9) W^3 \\ & + \left(\frac{-256 m_e v_s^2 J_{10}}{5} + \frac{128 m_e v_s^2 J_9}{15} - \frac{128 k_B T_L J_{11}}{15} \right) W^2 \\ & + \frac{32 m_e v_s^2 k_B T_L}{15} \left(8 J_{10} + \frac{J_9}{3} \right) W \Bigg\}, \end{aligned}$$

with

$$\mathcal{K}'_{ac} = \frac{4\sqrt{3} m_e^{3/2}}{9 \pi^{1/2} \hbar^4 v_s} K_{ac}. \tag{54}$$

J_5, J_6, J_7, J_8, J_9, J_{10}, J_{11} are defined in the appendix. Their numerical values are reported in table 2.

In the parabolic case one finds

$$C_p^{(ac)} = 0 \tag{55}$$

$$C_P^{i(ac)} = c_{11}^{(ac)} V^i + c_{12}^{(ac)} S^i \tag{56}$$

$$C_W^{(ac)} = -64 m_H^* v_s^2 \mathcal{K}'_{ac} W^{1/2} \left(W - \frac{3}{2} k_B T_L \right) \tag{57}$$

$$C_S^{i(ac)} = c_{21}^{(ac)} V^i + c_{22}^{(ac)} S^i, \tag{58}$$

where

$$c_{11}^{(ac)} = \hat{\mathcal{K}}_{ac} W^{1/2} \left\{ b_{11} \left[16 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{164}{15} k_B T_L - \frac{688}{15} \lambda_W^{-1} + \frac{352}{15} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right.$$
$$\left. + b_{12} \lambda_W^{-1} \left[48 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{328}{15} k_B T_L - \frac{688}{5} \lambda_W^{-1} + \frac{1408}{15} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right\},$$

$$c_{12}^{(ac)} = \hat{\mathcal{K}}_{ac} W^{1/2} \left\{ b_{12} \left[16 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{164}{15} k_B T_L - \frac{688}{15} \lambda_W^{-1} + \frac{352}{15} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right.$$
$$\left. + b_{22} \lambda_W^{-1} \left[48 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{328}{15} k_B T_L - \frac{688}{5} \lambda_W^{-1} + \frac{1408}{15} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right\},$$

$$c_{21}^{(ac)} = \frac{2}{3 m_H^*} \hat{\mathcal{K}}_{ac} W^{3/2} \left\{ b_{11} \left[48 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{408}{5} k_B T_L - \frac{912}{5} \lambda_W^{-1} + \frac{1408}{15} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right.$$
$$\left. + b_{12} \lambda_W^{-1} \left[192 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{1224}{5} k_B T_L - \frac{3648}{5} \lambda_W^{-1} + \frac{1408}{3} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right\},$$

$$c_{22}^{(ac)} = \frac{2}{3 m_H^*} \hat{\mathcal{K}}_{ac} W^{3/2} \left\{ b_{12} \left[48 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{408}{5} k_B T_L - \frac{912}{5} \lambda_W^{-1} + \frac{1408}{15} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right.$$
$$\left. + b_{22} \lambda_W^{-1} \left[192 k_B T_L/\lambda_W + m_H^* v_s^2 \left(\frac{1224}{5} k_B T_L - \frac{3648}{5} \lambda_W^{-1} + \frac{1408}{3} \lambda_W^{-2} \Big/ k_B T_L \right) \right] \right\}.$$

with

$$\hat{\mathcal{K}}_{ac} = \frac{4\sqrt{3\pi} m_H^{*3/2}}{9\hbar^4 v_s} \mathcal{K}_{ac}.$$

In figures 3 and 4 the coefficients c_{ij}'s and the energy relaxation time are plotted.

7.3. Intraband scattering with impurities

In the case of heavy and light holes the contribution to the production term due to the impurities is given by

$$C_p^{(\text{imp})} = 0 \tag{59}$$

$$C_P^{i(\text{imp})} = c_{11}^{(\text{imp})} V^i + c_{12}^{(\text{imp})} S^i \tag{60}$$

$$C_W^{(\text{imp})} = 0 \tag{61}$$

$$C_S^{i(\text{imp})} = c_{21}^{(\text{imp})} V^i + c_{22}^{(\text{imp})} S^i, \tag{62}$$

where

$$\begin{pmatrix} c_{11}^{(\text{imp})} & c_{12}^{(\text{imp})} \\ c_{21}^{(\text{imp})} & c_{22}^{(\text{imp})} \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix}$$

with

$$q_{11} = \frac{2m_e\tilde{\mathcal{K}}_{\text{imp}}}{J_1} W^{-3/2} \int_{[0,\infty]\times S^2\times S'^2} \alpha_1(\mathcal{E},\mathbf{n},\mathbf{n}')\,\mathrm{e}^{-\lambda_W\mathcal{E}}\,\mathrm{d}\mathcal{E}\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$q_{12} = \frac{2m_e\tilde{\mathcal{K}}_{\text{imp}}}{J_1} W^{-3/2} \int_{[0,\infty]\times S^2\times S'^2} \alpha_1(\mathcal{E},\mathbf{n},\mathbf{n}')\mathcal{E}\,\mathrm{e}^{-\lambda_W\mathcal{E}}\,\mathrm{d}\mathcal{E},$$

$$q_{21} = \frac{\tilde{\mathcal{K}}_{\text{imp}}}{J_1} W^{-3/2} \int_{[0,\infty]\times S^2\times S'^2} \alpha_2(\mathcal{E},\mathbf{n},\mathbf{n}')\,\mathrm{e}^{-\lambda_W\mathcal{E}}\,\mathrm{d}\mathcal{E}\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$q_{22} = \frac{\tilde{\mathcal{K}}_{\text{imp}}}{J_1} W^{-3/2} \int_{[0,\infty]\times S^2\times S'^2} \alpha_2(\mathcal{E},\mathbf{n},\mathbf{n}')\mathcal{E}\,\mathrm{e}^{-\lambda_W\mathcal{E}}\,\mathrm{d}\mathcal{E}\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$\alpha_1(\mathcal{E},\mathbf{n},\mathbf{n}') = \mathcal{E}^2 \frac{1+3(\mathbf{n}\cdot\mathbf{n}')^2}{\left(\beta^2 + \frac{4m_e\mathcal{E}(1-\mathbf{n}\cdot\mathbf{n}')}{\hbar^2 D(\vartheta,\varphi)}\right)^2}[T(\vartheta,\varphi)\cos\vartheta - T(\vartheta',\varphi')\cos\vartheta']$$
$$\times D^{-5/2}(\vartheta,\varphi)D^{-3/2}(\vartheta',\varphi')\cos\vartheta,$$

$$\alpha_2(\mathcal{E},\mathbf{n},\mathbf{n}') = \mathcal{E}^3 \frac{1+3(\mathbf{n}\cdot\mathbf{n}')^2}{\left(\beta^2 + \frac{4m_e\mathcal{E}(1-\mathbf{n}\cdot\mathbf{n}')}{\hbar^2 D(\vartheta,\varphi)}\right)^2}[T(\vartheta,\varphi)\cos\vartheta - T(\vartheta',\varphi')\cos\vartheta']$$
$$\times D^{-3/2}(\vartheta,\varphi)D^{-3/2}(\vartheta',\varphi')T(\vartheta,\varphi)\cos\vartheta,$$

$$\tilde{\mathcal{K}}_{\text{imp}} = \frac{3}{2\hbar^3}\sqrt{\frac{3m_e}{\pi}}K_{\text{imp}}. \tag{63}$$

The integrals appearing in the coefficients q_{ij} can be evaluated by using Gaussian quadrature formulae with respect to energy and iterated standard formulae for simple integral, e.g. Simpson rule.

In the parabolic case one has

$$C_p^{(\text{imp})} = 0 \tag{64}$$

$$C_P^{i(\text{imp})} = c_{11}^{(\text{imp})}V^i + c_{12}^{(\text{imp})}S^i \tag{65}$$

$$C_W^{(\text{imp})} = 0 \tag{66}$$

$$C_S^{i(\text{imp})} = c_{21}^{(\text{imp})}V^i + c_{22}^{(\text{imp})}S^i, \tag{67}$$

where

$$\begin{pmatrix} c_{11}^{(\text{imp})} & c_{12}^{(\text{imp})} \\ c_{21}^{(\text{imp})} & c_{22}^{(\text{imp})} \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{pmatrix}\begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix}$$

with

$$q_{11} = \hat{\mathcal{K}}_{\text{imp}} W^{-3/2}\int_0^\infty \Phi(\mathcal{E})\,\mathrm{e}^{-\lambda_W\mathcal{E}}\,\mathrm{d}\mathcal{E},$$

$$q_{12} = \hat{\mathcal{K}}_{\text{imp}} W^{-3/2}\int_0^\infty \Phi(\mathcal{E})\mathcal{E}\,\mathrm{e}^{-\lambda_W\mathcal{E}}\,\mathrm{d}\mathcal{E},$$

$$q_{21} = q_{12}/m_H^*,$$

$$q_{22} = \hat{\mathcal{K}}_{\text{imp}} W^{-3/2}\int_0^\infty \Phi(\mathcal{E})\mathcal{E}^2\,\mathrm{e}^{-\lambda_W\mathcal{E}}\,\mathrm{d}\mathcal{E},$$

$$\Phi(\mathcal{E}) = \log(1+8a\mathcal{E})\frac{64a^2\mathcal{E}^2+48a\mathcal{E}+9}{256a^2\mathcal{E}^2} - \frac{160a^2\mathcal{E}^2+84a\mathcal{E}+9}{32a\mathcal{E}(1+8a\mathcal{E})}$$

$$\hat{\mathcal{K}}_{\text{imp}} = \frac{\sqrt{3} n_I Z^2 e^4}{\pi^{3/2}\sqrt{m_H^*}\epsilon^2}, \qquad a = \frac{m_H^*}{\hbar^2 \beta^2}.$$

7.4. Inter-band non-polar optical phonon–hole scattering

For the holes in the A-band (A = +, −) we get the following expressions for the production terms by taking into account the inter-band scatterings with the holes in the B-band (B = −, +),

$$C_p^{(op)} = \frac{\tilde{\mathcal{K}}_{op}}{\hbar\omega_{op}}(\gamma_{1B} + \gamma_{1A}) \tag{68}$$

$$C_P^{i(op)} = c_{11}^{(op)} V_A^i + c_{12}^{(op)} S_A^i \tag{69}$$

$$C_W^{(op)} = \frac{\tilde{\mathcal{K}}_{op}}{\hbar\omega_{op}}(\gamma_{2B} + \gamma_{2A}) \tag{70}$$

$$C_S^{i(op)} = c_{21}^{(op)} V_A^i + c_{22}^{(op)} S_A^i, \tag{71}$$

where

$$\gamma_{1B} = J_1^A W_B^{-3/2} \frac{p_B}{p_A} B_1^B \left\{ N_{op} \exp\left[-\hbar\omega_{op}\left(\lambda_B^W - \frac{1}{k_B T_L}\right)\right] + (N_{op}+1)\exp\left(-\frac{\hbar\omega_{op}}{k_B T_L}\right)\right\},$$

$$\gamma_{1A} = -J_1^B W_A^{-3/2} B_1^A \left[N_{op} + (N_{op}+1)\exp\left(-\hbar\omega_{op}\lambda_A^W\right)\right],$$

$$\begin{aligned}\gamma_{2B} = -J_1^A W_B^{-3/2} \frac{p_B}{p_A} \bigg\{ & N_{op} \exp\left[-\hbar\omega_{op}\left(\lambda_B^W - \frac{1}{k_B T_L}\right)\right]\left(B_1^B\right)' \\ & + (N_{op}+1)\exp\left[\hbar\omega_{op}\left(\lambda_B^W - \frac{1}{k_B T_L}\right)\right]\left(B_2^B\right)'\bigg\}\end{aligned}$$

$$\gamma_{2A} = J_1^B W_A^{-3/2}\left[N_{op}\left(B_1^A\right)' + (N_{op}+1)\left(B_2^A\right)'\right],$$

$$c_{11}^{(op)} = \frac{J_3^A J_1^B \tilde{\mathcal{K}}_{op}}{2J_1^A \hbar\omega_{op}} W_A^{-3/2}\left[N_{op}\left(-b_{11}^A\left(B_1^A\right)' + b_{12}^A\left(B_1^A\right)''\right) + (N_{op}+1)\left(-b_{11}^A\left(B_2^A\right)' + b_{12}^A\left(B_2^A\right)''\right)\right],$$

$$c_{12}^{(op)} = \frac{J_3^A J_1^B \tilde{\mathcal{K}}_{op}}{2J_1^A \hbar\omega_{op}} W_A^{-3/2}\left[N_{op}\left(-b_{12}^A\left(B_1^A\right)' + b_{22}^A\left(B_1^A\right)''\right) + (N_{op}+1)\left(-b_{12}^A\left(B_2^A\right)' + b_{22}^A\left(B_2^A\right)''\right)\right],$$

$$c_{21}^{(op)} = \frac{J_2^A J_1^B \tilde{\mathcal{K}}_{op}}{2J_1^A m_e \hbar\omega_{op}} W_A^{-3/2}\left[N_{op}\left(b_{11}^A\left(B_1^A\right)'' - b_{12}^A\left(B_1^A\right)'''\right) + (N_{op}+1)\left(b_{11}^A\left(B_2^A\right)'' - b_{12}^A\left(B_2^A\right)'''\right)\right],$$

$$c_{22}^{(op)} = \frac{J_2^A J_1^B \tilde{\mathcal{K}}_{op}}{2J_1^A m_e \hbar\omega_{op}} W_A^{-3/2}\left[N_{op}\left(b_{12}^A\left(B_1^A\right)'' - b_{22}^A\left(B_1^A\right)'''\right) + (N_{op}+1)\left(b_{12}^A\left(B_2^A\right)'' - b_{22}^A\left(B_2^A\right)'''\right)\right].$$

Here B_i^A and B_i^B are the functions appearing in (43), (44) with the energy Lagrangian multiplier λ^W equals to $\lambda_A^W = \frac{3}{2W_A}$ and $\lambda_B^W = \frac{3}{2W_B}$ respectively. Moreover b_{ij}^A are the functions b_{ij} appearing in (30), (31) relative to the A-band.

7.5. Inter-band acoustic phonon–hole scattering

One gets the following contribution to the production terms due to the acoustic phonon scattering up to first order in $\sqrt{m_e v_s^2 / k_B T_L}$ with a meaning of the symbols similar to that of the previous subsection:

$$C_p^{(ac)} = \tfrac{3}{2}\mathcal{K}'_{ac}(\zeta_{1A} + \zeta_{1B}) \tag{72}$$

$$C_P^{i(ac)} = c_{11A}^{(ac)} V_A^i + c_{12A}^{(ac)} S_A^i + c_{11B}^{(ac)} V_B^i + c_{12B}^{(ac)} S_B^i \tag{73}$$

$$C_W^{(ac)} = \tfrac{3}{2} \mathcal{K}'_{ac} (\zeta_{2A} + \zeta_{2B}) \tag{74}$$

$$C_S^{i(ac)} = c_{21A}^{(ac)} V_A^i + c_{22A}^{(ac)} S_A^i + c_{21B}^{(ac)} V_B^i + c_{22B}^{(ac)} S_B^i, \tag{75}$$

where

$$\zeta_{1B} = \frac{p_B}{p_A J_1^B} k_B T_L I_1 W_B^{1/2},$$

$$\zeta_{1A} = -\frac{1}{J_1^A} k_B T_L I_1 W_A^{1/2},$$

$$\zeta_{2B} = \frac{p_B}{p_A J_1^B} \left[\frac{64 m_e v_s^2 I_3}{81 k_B T_L} W_B^{5/2} - \left(\frac{160}{27} m_e v_s^2 I_3 - \frac{32}{27} k_B T_L I_1 \right) W_B^{3/2} + \frac{20}{3} m_e v_s^2 I_3 k_B T_L W_B^{1/2} \right],$$

$$\zeta_{2A} = \frac{1}{J_1^A} \left[-\frac{64 m_e v_s^2 I_3}{81 k_B T_L} W_A^{5/2} + \left(\frac{32}{27} m_e v_s^2 I_3 - \frac{32}{27} k_B T_L I_1 \right) W_A^{3/2} + \frac{4}{9} m_e v_s^2 I_3 k_B T_L W_A^{1/2} \right],$$

$$c_{11A}^{(ac)} = \frac{27}{16 J_2^A} \mathcal{K}'_{ac} W_A^{-3/2} \left\{ \frac{128 m_e^2 v_s^2}{81 k_B T_L} I_4 W_A^3 + \left(\frac{64 m_e^2 v_s^2 I_4}{27} - \frac{64 m_e k_B T_L I_5}{27} \right) W_A^2 \right.$$
$$\left. + \frac{8 m_e^2 v_s^2 k_B T_L}{3} I_4 W_A \right\},$$

$$c_{11B}^{(ac)} = \frac{27 p_B}{16 p_A J_2^B} \mathcal{K}'_{ac} W_B^{-3/2} \left\{ -\frac{128 m_e^2 v_s^2}{81 k_B T_L} I_6 W_B^3 - \frac{256 m_e^2 v_s^2}{27} I_6 W_B^2 + \frac{64 m_e^2 v_s^2 k_B T_L}{3} I_6 \Big) W_B \right\},$$

$$c_{12A}^{(ac)} = \frac{27}{16 J_2^A} \mathcal{K}'_{ac} W_A^{-3/2} \left\{ -\frac{128 m_e^2 v_s^2}{45 k_B T_L} I_4 W_A^2 + \left(\frac{64 m_e^2 v_s^2 I_4}{45} - \frac{64 m_e k_B T_L I_5}{45} \right) W_A \right.$$
$$\left. - \frac{8 m_e^2 v_s^2 k_B T_L}{15} I_4 \right\},$$

$$c_{12B}^{(ac)} = \frac{27 p_B}{16 p_A J_2^B} \mathcal{K}'_{ac} W_B^{-3/2} \left\{ \frac{128 m_e^2 v_s^2}{45 k_B T_L} I_6 W_B^2 - \frac{256 m_e^2 v_s^2}{45} I_6 W_B - \frac{64 m_e^2 v_s^2 k_B T_L}{15} I_6 \right\},$$

$$c_{21A}^{(ac)} = \frac{27}{16 J_2^A} \mathcal{K}'_{ac} W_A^{-3/2} \left\{ \frac{1024 m_e v_s^2}{81 k_B T_L} I_7 W_A^4 + \left(-\frac{128 m_e v_s^2 I_7}{27} + \frac{128 k_B T_L I_8}{27} \right) W_A^3 \right.$$
$$\left. + \frac{32 m_e v_s^2 k_B T_L}{27} I_7 W_A^2 \right\},$$

$$c_{21B}^{(ac)} = \frac{27 p_B}{16 p_A J_2^B} \mathcal{K}'_{ac} W_B^{-3/2} \left\{ -\frac{1024 m_e v_s^2}{81 k_B T_L} I_2 W_B^4 + \frac{256 m_e v_s^2}{9} I_2 W_B^3 + \frac{256 m_e v_s^2 k_B T_L}{9} I_2 W_B^2 \right\},$$

$$c_{22A}^{(ac)} = \frac{27}{16 J_2^A} \mathcal{K}'_{ac} W_A^{-3/2} \left\{ -\frac{1024 m_e v_s^2}{81 k_B T_L} I_7 W_A^3 + \left(\frac{128 m_e v_s^2}{15} I_7 - \frac{128 k_B T_L}{15} I_8 \right) W_A^2 \right.$$
$$\left. + \frac{32 m_e v_s^2 k_B T_L}{45} I_7 W_A \right\},$$

$$c_{22B}^{(ac)} = \frac{27 p_B}{16 p_A J_2^B} \mathcal{K}'_{ac} W_B^{-3/2} \left\{ \frac{1024 m_e v_s^2}{81 k_B T_L} I_2 W_B^3 - \frac{256 m_e v_s^2}{5} I_2 W_B^2 + \frac{256 m_e v_s^2 k_B T_L}{15} I_2 W_B \right\}.$$

The integrals I_j are defined in the appendix where their numerical values are also reported.

7.6. Inter-band scattering with impurities

The contribution to the production terms due to the inter-band scattering with impurities is given by

$$C_p^{(\mathrm{imp})} = 2m_e\tilde{K}_{\mathrm{imp}}\big(r_{1B}W_B^{-3/2} + r_{1A}W_A^{-3/2}\big) \tag{76}$$

$$C_P^{i(\mathrm{imp})} = \big(c_{11A}^{(\mathrm{imp})}V_A^i + c_{12A}^{(\mathrm{imp})}S_A^i\big)W_A^{-3/2} + \big(c_{11B}^{(\mathrm{imp})}V_B^i + c_{12B}^{(\mathrm{imp})}S_B^i\big)W_B^{-3/2} \tag{77}$$

$$C_W^{(\mathrm{imp})} = 2m_e\tilde{K}_{\mathrm{imp}}(r_{2B}W_B^{-3/2} + r_{2A}W_A^{-3/2}) \tag{78}$$

$$C_S^{i(\mathrm{imp})} = \big(c_{21A}^{(\mathrm{imp})}V_A^i + c_{22A}^{(\mathrm{imp})}S_A^i\big)W_A^{-3/2} + \big(c_{21B}^{(\mathrm{imp})}V_B^i + c_{22B}^{(\mathrm{imp})}S_B^i\big)W_B^{-3/2}, \tag{79}$$

where for $X = A, B$

$$\begin{pmatrix} c_{11X}^{(\mathrm{imp})} & c_{12X}^{(\mathrm{imp})} \\ c_{21X}^{(\mathrm{imp})} & c_{22X}^{(\mathrm{imp})} \end{pmatrix} = \begin{pmatrix} q_{11X} & q_{12X} \\ q_{21X} & q_{22X} \end{pmatrix}\begin{pmatrix} b_{11X} & b_{12X} \\ b_{12X} & b_{22X} \end{pmatrix}$$

$$r_{1B} = \frac{p_B}{p_A J_1^B}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}\alpha_3(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^B\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$r_{1A} = -\frac{1}{J_1^A}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}\alpha_3(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^A\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$r_{2B} = \frac{p_B}{p_A J_1^B}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}{}^2\alpha_3(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^B\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$r_{2A} = -\frac{1}{J_1^A}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}{}^2\alpha_3(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^A\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{11A} = \frac{2m_e\tilde{K}_{\mathrm{imp}}}{J_1^A}\int_{[0,\infty]\times S^2\times S'^2} \alpha_{1A}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^A\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{11B} = \frac{2m_e\tilde{K}_{\mathrm{imp}}}{J_1^B}\frac{p_B}{p_A}\int_{[0,\infty]\times S^2\times S'^2} \alpha_{1B}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^B\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{12A} = \frac{2m_e\tilde{K}_{\mathrm{imp}}}{J_1^A}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}\alpha_{1A}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^A\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{12B} = \frac{2m_e\tilde{K}_{\mathrm{imp}}}{J_1^B}\frac{p_A}{p_B}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}\alpha_{1B}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^A\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{21A} = \frac{\tilde{K}_{\mathrm{imp}}}{J_1^A}\int_{[0,\infty]\times S^2\times S'^2} \alpha_{2A}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^A\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{21B} = \frac{\tilde{K}_{\mathrm{imp}}}{J_1^B}\frac{p_B}{p_A}\int_{[0,\infty]\times S^2\times S'^2} \alpha_{2B}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^B\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{22A} = \frac{\tilde{K}_{\mathrm{imp}}}{J_1^A}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}\alpha_{2A}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^A\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B',$$

$$q_{22B} = \frac{\tilde{K}_{\mathrm{imp}}}{J_1^B}\frac{p_B}{p_A}\int_{[0,\infty]\times S^2\times S'^2} \mathcal{E}_{\mathcal{A}}\alpha_{2B}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}')\,\mathrm{e}^{-\lambda_W^B\mathcal{E}_A}\,\mathrm{d}\mathcal{E}_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega_B'.$$

$$\alpha_{1A}(\mathcal{E}_{\mathcal{A}},\mathbf{n_A},\mathbf{n_B}') = \mathcal{E}_{\mathcal{A}}{}^2\frac{3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2}{\left(\beta^2 + \frac{4m_e\mathcal{E}_{\mathcal{A}}(1-\mathbf{n_A}\cdot\mathbf{n_B}')}{\hbar^2 D_A(\vartheta_A,\varphi_A)}\right)^2}T_A(\vartheta_A,\varphi_A)D_A^{-5/2}(\vartheta_A,\varphi_A)$$
$$\times\, D_B^{-3/2}(\vartheta_B',\varphi_B')\cos^2\vartheta_A,$$

$$\alpha_{1B}(\mathcal{E}_A, \mathbf{n_A}, \mathbf{n_B}') = -\mathcal{E}_A{}^2 \frac{3 - 3(\mathbf{n_A} \cdot \mathbf{n_B}')^2}{\left(\beta^2 + \frac{4m_e \mathcal{E}_A(1-\mathbf{n_A}\cdot\mathbf{n_B}')}{\hbar^2 D_A(\vartheta_A,\varphi_A)}\right)^2} T_B(\vartheta_B', \varphi_B') D_A^{-5/2}(\vartheta_A, \varphi_A)$$
$$\times D_B^{-3/2}(\vartheta_B', \varphi_B') \cos\vartheta_A \cos\vartheta_B',$$

$$\alpha_{2A}(\mathcal{E}_A, \mathbf{n_A}, \mathbf{n_B}') = \mathcal{E}_A{}^3 \frac{3 - 3(\mathbf{n_A} \cdot \mathbf{n_B}')^2}{\left(\beta^2 + \frac{4m_e \mathcal{E}_A(1-\mathbf{n_A}\cdot\mathbf{n_B}')}{\hbar^2 D_A(\vartheta_A,\varphi_A)}\right)^2} T_A^2(\vartheta_A, \varphi_A) D_A^{-3/2}(\vartheta_A, \varphi_A)$$
$$\times D_B^{-3/2}(\vartheta_B', \varphi_B') \cos^2\vartheta_A,$$

$$\alpha_{2B}(\mathcal{E}_A, \mathbf{n_A}, \mathbf{n_B}') = -\mathcal{E}_A{}^3 \frac{3 - 3(\mathbf{n_A} \cdot \mathbf{n_B}')^2}{\left(\beta^2 + \frac{4m_e \mathcal{E}_A(1-\mathbf{n_A}\cdot\mathbf{n_B}')}{\hbar^2 D_A(\vartheta_A,\varphi_A)}\right)^2} T_A(\vartheta_A, \varphi_A) T_B(\vartheta_B', \varphi_B')$$
$$\times D_A^{-3/2}(\vartheta_A, \varphi_A) D_B^{-3/2}(\vartheta_B', \varphi_B') \cos\vartheta_A \cos\vartheta_B',$$

$$\alpha_3(\mathcal{E}_A, \mathbf{n_A}, \mathbf{n_B}') = \frac{3 - 3(\mathbf{n_A} \cdot \mathbf{n_B}')^2}{\left(\beta^2 + \frac{4m_e \mathcal{E}_A(1-\mathbf{n_A}\cdot\mathbf{n_B}')}{\hbar^2 D_A(\vartheta_A,\varphi_A)}\right)^2} D_A^{-3/2}(\vartheta_A, \varphi_A) D_B^{-3/2}(\vartheta_B', \varphi_B').$$

7.7. Generation-recombination terms

Here only the productions for holes are written. Of course similar terms must be also considered for electrons. However the latter ones can be easily obtained with a similar procedure.

At variance with the other scatterings, the density of each population of holes is no longer conserved, but we have

$$C_p^{(GR)} = -\Gamma_H \left(p^2 n - p n_i^2\right) - \Gamma_{\overline{A}} \left(n^2 p - n n_i^2\right) + \frac{np - n_i^2}{\tau_h(n + n_i) + \tau_e(p + n_i)}. \tag{80}$$

For the other production terms, one finds

$$C_P^{i(GR)} = -\Gamma_H p^2 n P_H^i - \Gamma_{\overline{A}} n^2 p P_e^i + \frac{np P_H^i}{\tau_h(n + n_i) + \tau_e(p + n_i)} \tag{81}$$

$$C_W^{(GR)} = -\Gamma_H \left(p^2 n W - p n_i^2 W_0\right) - \Gamma_{\overline{A}} \left(n^2 p W_e - n n_i^2 W_0\right) + \frac{npW - n_i^2 W_0}{\tau_h(n + n_i) + \tau_e(p + n_i)} \tag{82}$$

$$C_S^{i(GR)} = -\Gamma_H p^2 n S_H^i - \Gamma_{\overline{A}} n^2 p S_e^i + \frac{np S_H^i}{\tau_h(n + n_i) + \tau_e(p + n_i)}, \tag{83}$$

where W_e is the electron energy, P_e^i is the electron average crystal momentum, S_e^i is the electron energy flux and $W_0 = \frac{3}{2} k_B T_L$ is the crystal energy.

8. Energy-transport and drift-diffusion limit models

Macroscopic models, simpler than the hydrodynamical ones but widely used in simulations, are represented by the so-called energy transport models, which are constituted by two balance equations: one for the density and the other for the energy. Starting from the energy-transport model in the isothermal limit one recovers the *drift-diffusion* models and an expression of the hole mobility based on MEP.

In principle on account of the coupling between electron and holes by means of the generation-recombination terms, the energy-transport model should comprise also the analogous equations for the electrons. However the typical time for the recombination generation interaction is much longer (about a nanosecond) than those of the hole–phonon

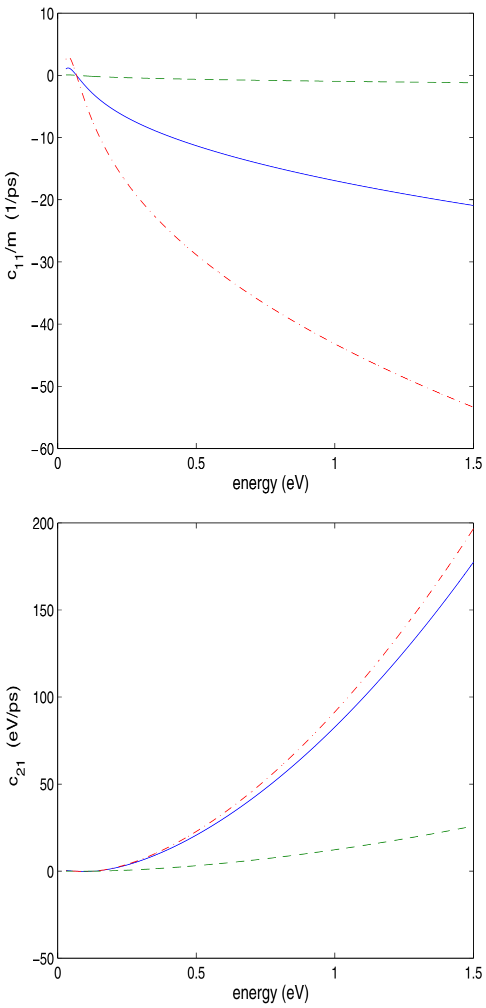

Figure 3. Coefficients c_{ij} versus energy for heavy (continuous line) and light (dashed line) warped bands and for the parabolic band (dashed-dot line) in the intra-band case, neglecting scattering with impurities.

scattering (a fraction of picosecond). Therefore in situation where the characteristic time is of few picoseconds, e.g. simulation of MOSFETs, the generation-recombination terms can be neglected and the constitutive relations for holes and electrons decouple. This approximation will be assumed in the present section. Moreover for the sake of simplicity we consider only intra-band scatterings. Inter-band scatterings can be included in a straightforward way.

First we rewrite the hydrodynamical model for holes in the form

$$\frac{\partial p_H}{\partial t} + \frac{\partial \left(p_H V_H^i\right)}{\partial x^i} = 0, \tag{84}$$

$$\frac{\partial \left(p_H P_H^j\right)}{\partial t} + \frac{\partial \left(p_H U_H^{ij}\right)}{\partial x^j} - e p_H E^j = p_H \left[(c_{11}(W_H) V_H^i + c_{12}(W_H) S_H^i \right], \tag{85}$$

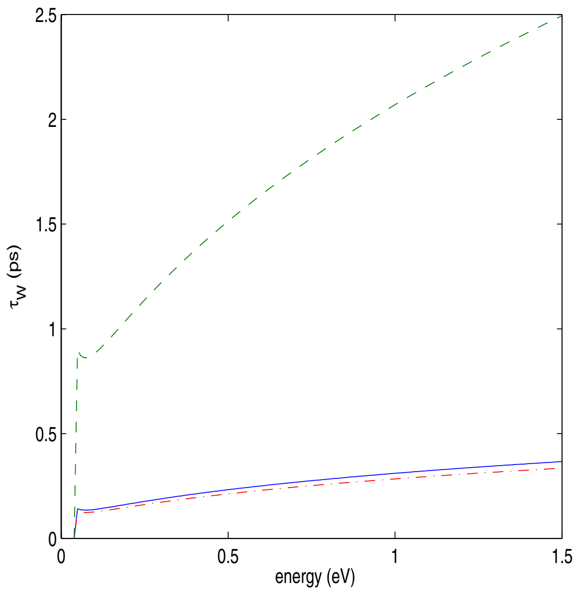

Figure 4. Energy relaxation time as function of the energy W for heavy (continuous line) and light (dashed line) warped bands, and the parabolic band (dashed-dot line) as in figure 3.

$$\frac{\partial p_H W_H}{\partial t} + \frac{\partial\left(p_H S_H^i\right)}{\partial x^i} - e p_H E^i V_H^i = -p_H \frac{W_H - W_0}{\tau_{W_H}}, \tag{86}$$

$$\frac{\partial(p_H S^j)}{\partial t} + \frac{\partial\left(p_H F_H^{ij}\right)}{\partial x^i} - e p_H E^i G_H^{ji} = p_H \left[c_{21}(W_H) V_H^i + c_{22}(W_H) S_H^i\right], \tag{87}$$

with $W_0 = 3/2 k_B T_L$ and with an obvious meaning for τ_{W_H} (the energy relaxation time), $c_{11}(W_H), c_{12}(W_H), c_{21}(W_H), c_{22}(W_H)$.

As in [32] let us assume that the following scaling:

$$t = \mathcal{O}\left(\frac{1}{\delta^2}\right), \tag{88a}$$

$$\tau_W = \mathcal{O}\left(\frac{1}{\delta^2}\right), \tag{88b}$$

$$x^i = \mathcal{O}\left(\frac{1}{\delta}\right), \tag{88c}$$

$$\mathbf{V}_H = \mathcal{O}(\delta), \tag{88d}$$

$$\mathbf{S}_H = \mathcal{O}(\delta) \tag{88e}$$

holds.

The first condition is a long-time scaling that is almost stationary regime. The second one means that the energy relaxation time must be sufficiently long with respect to the typical time of the transient. (88*a*) is the typical diffusion scaling, while (88*d*), (88*e*) are consistent with the expansion made to get the closure relations. Under the conditions (88), equating to zero at the various order in δ the terms appearing in the balance equations one gets the following compatibility conditions:

$$\frac{\partial p_H}{\partial t} + \frac{\partial\left(p_H V_H^i\right)}{\partial x^i} = 0, \tag{89}$$

$$\frac{\partial\left(p_H V_H^i\right)}{\partial t} = 0, \qquad \frac{\partial\left(p_H S_H^i\right)}{\partial t} = 0, \tag{90}$$

$$\frac{\partial\left(p_H U_H^{ij}\right)}{\partial x^j} - e p_H E^i - c_{11} p_H V_H^i - c_{12} p_H S_H^i = 0, \tag{91}$$

$$\frac{\partial\left(p_H W_H\right)}{\partial t} + \frac{\partial\left(p_H S_H^i\right)}{\partial x^i} - e p_H E^i V_H^i + p_H \frac{W_H - W_0}{\tau_{W_H}} = 0, \tag{92}$$

$$\frac{\partial\left(p_H F_H^{ij}\right)}{\partial x^i} - e p_H E^i G_H^{ij} - c_{21} p_H V_H^i - c_{22} p_H S_H^i = 0. \tag{93}$$

Equations (91) and (93) are a linear system for $\mathbf{V}_H$ and $\mathbf{S}_H$ whose solution is

$$\mathbf{V}_H = D_{11}(W_H)\nabla \log p_H + D_{12}(W_H)\nabla W_H + D_{13}(W_H)\nabla\phi, \tag{94}$$

$$\mathbf{S}_H = D_{21}(W_H)\nabla \log p_H + D_{22}(W_H)\nabla W_H + D_{23}(W_H)\nabla\phi. \tag{95}$$

The elements of the diffusion matrix $D = (D_{ij})$ read

$$D_{11} = \frac{\frac{2}{3}c_{22}W_H - \frac{5J_2}{6J_1}c_{12}\frac{W_H^2}{m_e}}{c_{11}c_{22} - c_{12}c_{21}}, \qquad D_{12} = \frac{\frac{2}{3}c_{22} - \frac{10J_2}{6J_1}c_{12}\frac{W_H}{m_e}}{c_{11}c_{22} - c_{12}c_{21}}, \qquad D_{13} = e\frac{c_{22} - \frac{J_4}{2J_1}c_{12}\frac{W_H}{m_e}}{c_{11}c_{22} - c_{12}c_{21}},$$

$$D_{21} = \frac{\frac{5J_2}{6J_1}c_{11}\frac{W_H^2}{m_e} - \frac{2}{3}c_{21}W_H}{c_{11}c_{22} - c_{12}c_{21}}, \qquad D_{22} = \frac{\frac{10J_2}{6J_1}c_{11}\frac{W_H}{m_e} - \frac{2}{3}c_{21}}{c_{11}c_{22} - c_{12}c_{21}}, \qquad D_{23} = -e\frac{c_{21} - \frac{J_4}{2J_1}c_{11}\frac{W_H}{m_e}}{c_{11}c_{22} - c_{12}c_{21}}.$$

The balance equations for density and energy (89) and (93) closed with the relations (94), (95) are the energy-transport model for holes based on MEP. From this latter a drift-diffusion model is obtained as isothermal limit formally setting $\tau_{W_H} \mapsto 0$,

$$\mathbf{J}_H = p_H \mathbf{V}_H = D_{11}(W_0)\nabla p_H + p_H D_{13}(W_0)\nabla\phi, \tag{96}$$

$$\frac{\partial p_H}{\partial t} + \nabla\cdot\mathbf{J}_H = 0. \tag{97}$$

By comparing (96) with the expression of $\mathbf{J}$ in the form

$$\mathbf{J} = -D_p\nabla p_H - \mu_{p0} p_H \nabla\phi,$$

one can identify the diffusivity coefficient D_p and the low field mobility μ_{p0} as

$$D_p = -D_{11}(W_0), \qquad \mu_{p0} = -D_{13}(W_0). \tag{98}$$

One observes that

$$D_p = \mu_{p0}\frac{2W_0}{3e} = \mu_{p0}\frac{k_B T_L}{e}, \tag{99}$$

which is the Einstein relation.

9. Simulations in the bulk case

Here we simulate the case of bulk silicon by taking into account heavy and light holes, which in this section will be denoted by the H and L subscript. The stationary solution is obtained as asymptotic limit of the time-dependent problem. The only non-trivial contribution is along the direction of the electric field which enters into the equation as a parameter. In fact the Poisson equation is solved taking the sum of light and heavy holes equals to the doping concentration and a linear electrostatic potential.

In the homogeneous case, with obvious meaning of the symbols, the hydrodynamical model reads

$$\frac{\mathrm{d}p_H}{\mathrm{d}t} = p_H C_{HH}(W_H) + p_L C_{HL}(W_L) \tag{100}$$

$$\frac{\mathrm{d}(p_H m_H^* V_H)}{\mathrm{d}t} - p_H e E = p_H C_{P_{HH}}(W_H) + p_L C_{P_{HL}}(W_L), \tag{101}$$

$$\frac{\mathrm{d}(p_H W_H)}{\mathrm{d}t} - p_H e E V_H = p_H C_{W_{HH}}(W_H) + p_L C_{W_{HL}}(W_L), \tag{102}$$

$$\frac{\mathrm{d}(p_H S_H)}{\mathrm{d}t} - p_H e E G_H = p_H C_{S_{HH}}(W_H) + p_L C_{S_{HL}}(W_L) \tag{103}$$

$$\frac{\mathrm{d}p_L}{\mathrm{d}t} = p_L C_{LL}(W_L) + p_H C_{LH}(W_H) \tag{104}$$

$$\frac{\mathrm{d}(p_L m_L^* V_L)}{\mathrm{d}t} - p_L e E = p_L C_{P_{LL}}(W_L) + p_H C_{P_{LH}}(W_H), \tag{105}$$

$$\frac{\mathrm{d}(p_L W_L)}{\mathrm{d}t} - p_L e E V_L = p_L C_{W_{LL}}(W_L) + p_H C_{W_{LH}}(W_H), \tag{106}$$

$$\frac{\mathrm{d}(p_L S_L)}{\mathrm{d}t} - p_L e E G_L = p_L C_{S_{LL}}(W_L) + p_H C_{S_{LH}}(W_H) \tag{107}$$

Since the total hole density $p_H + p_L$ is conserved, the following semi-implicit Euler numerical scheme is adopted for the system (100)–(107). We remark that a very stringent stability condition arises if an explicit method is employed, due to the different charge concentration between the heavy and light holes.

By denoting with the superscript n the quantities evaluated at the time t^n and with Δt the time step $t^{n+1} - t^n$, we first advance in time the density, discretizing the balance equation for the densities with all variables but p_H and p_L frozen at the time step t^n,

$$p_H^{n+1} + p_L^{n+1} = p_H^n + p_L^n \tag{108}$$

$$p_H^{n+1} - p_H^n = \Delta t \left[p_H^{n+1} C_{HH}\left(W_H^n\right) - p_L^{n+1} C_{HL}\left(W_L^n\right)\right], \tag{109}$$

and then the energies at the next time are obtained,

$$W_H^{n+1} = \frac{p_H^n}{p_H^{n+1}} W_H^n + \frac{p_L^{n+1}}{p_H^{n+1}} C_{W_{HL}}\left(W_L^n\right)\Delta t + \frac{p_H^n}{p_H^{n+1}} C_{W_{HH}}\left(W_H^n\right)\Delta t + eEV_H^n \Delta t, \tag{110}$$

$$W_L^{n+1} = \frac{p_L^n}{p_L^{n+1}} W_L^n + \frac{p_H^{n+1}}{p_L^{n+1}} C_{W_{LH}}\left(W_H^n\right)\Delta t + \frac{p_L^n}{p_L^{n+1}} C_{W_{LL}}\left(W_L^n\right)\Delta t + eEV_L^n \Delta t. \tag{111}$$

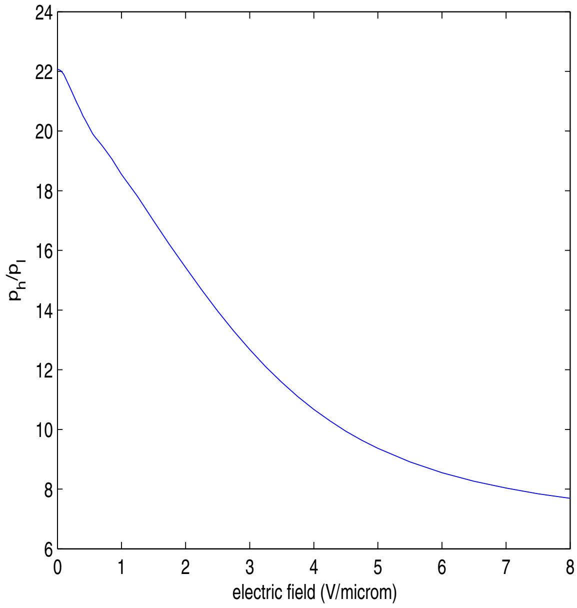

Figure 5. Ratio of the densities versus the electric field.

Once p_H^{n+1}, p_L^{n+1}, W_H^{n+1} and W_L^{n+1} are known, we discretize the equation for the velocity and energy flux getting two uncoupled linear systems wherefrom one finds

$$m_H^* V_H^{n+1} = c_{11_{HH}} V_H^n \Delta t + c_{12_{HH}} S_H^n \Delta t + \frac{p_H^n}{p_H^{n+1}} m_H^* V_H^n + eE\Delta t + \left(c_{11_{HL}} V_L^n + c_{12_{HL}} S_L^n\right) \frac{p_L^{n+1}}{p_H^{n+1}} \Delta t \tag{112}$$

$$S_H^{n+1} = c_{21_{HH}} V_H^n \Delta t + c_{22_{HH}} S_H^n \Delta t + \frac{p_H^n}{p_H^{n+1}} S_H^n + eEG_H^{n+1} \Delta t + \left(c_{21_{HL}} V_L^n + c_{22_{HL}} S_L^n\right) \frac{p_L^{n+1}}{p_H^{n+1}} \Delta t \tag{113}$$

$$m_L^* V_L^{n+1} = c_{11_{LL}} V_L^n \Delta t + c_{12_{LL}} S_L^n \Delta t + \frac{p_L^n}{p_L^{n+1}} m_L^* V_L^n + eE\Delta t + \left(c_{11_{LH}} V_H^n + c_{12_{LH}} S_H^n\right) \frac{p_H^{n+1}}{p_L^{n+1}} \Delta t \tag{114}$$

$$S_L^{n+1} = c_{21_{LL}} V_L^n \Delta t + c_{22_{LL}} S_L^n \Delta t + \frac{p_L^n}{p_L^{n+1}} S_L^n + eEG_L^{n+1} \Delta t + \left(c_{21_{LH}} V_H^n + c_{22_{LH}} S_H^n\right) \frac{p_H^{n+1}}{p_L^{n+1}} \Delta t \tag{115}$$

The band coefficients and the deformation potentials are not given by scattering theory but they are free parameters also for the kinetic models. Their values are usually fitted against the experimental data and there are several sets of values available in the literature.

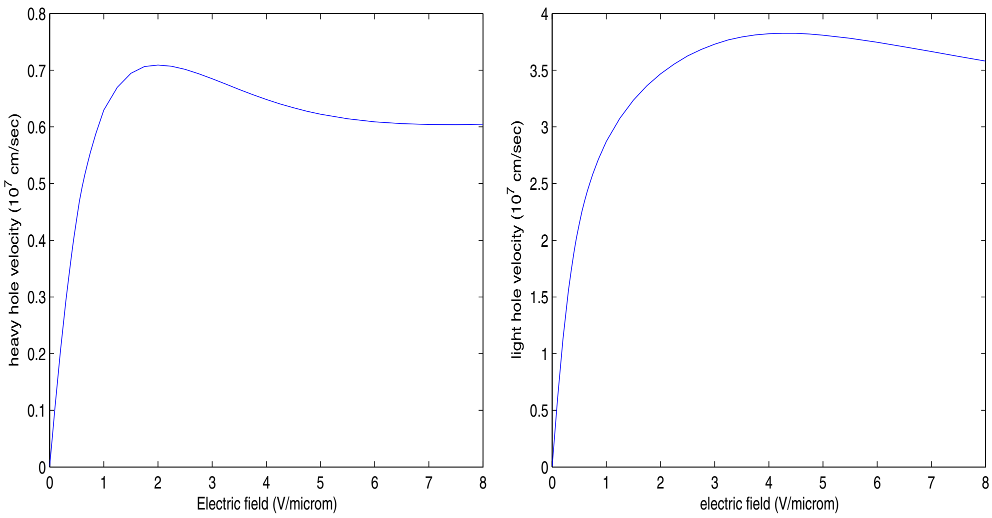

Figure 6. Velocity of the heavy and light holes as function of the electric field.

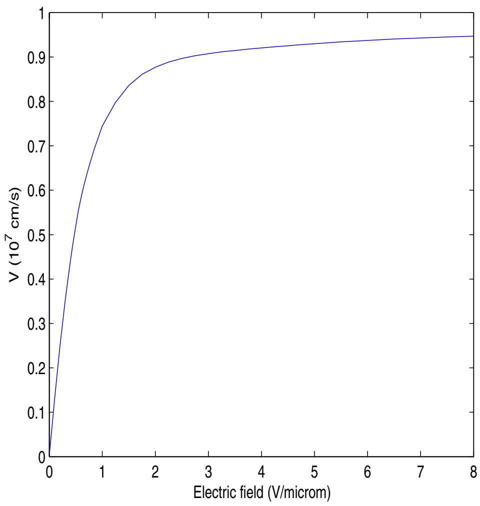

Figure 7. Average velocity as function of the electric field.

We use the physical parameters reported in table 1. Moreover for the heavy holes we take the same values of the scattering coupling constants as in [18], that is $\Xi_d = 5.39$ eV and $D_t K = 13.24 \times 10^8$ eV cm^{-1} according to [26]; instead for the light holes we take $D_t K = 5 \times 10^8$ eV cm^{-1} [24] and $\Xi_d = 3.1$ eV [33].

The stationary solution is reached after about 3 ps. The results are plotted versus the electric field. As expected from a physical point of view, the heavy band is more populated than the light one. The ratio of the concentration between the two bands is reported in figure 5. Similarly, the average velocity of the light holes is much higher than that of the other band (see figure 6) according to the smaller effective mass. The total momentum density is given by

$$J = p_H V_H + p_L V_L$$

and from this an average overall hole velocity can be defined as

$$V = \frac{J}{p_H + p_L}.$$

V is plotted against the field in figure 7 and a good high field velocity is obtained. We note that the V is considerably higher than V_H. This means that calculations with the single heavy band could underestimate the overall hole current.

10. Conclusions

In this paper, we have presented a consistent closure for a hydrodynamical model for the hole transport in silicon by using the maximum entropy principle by describing the band structure with the so-called warped approximation. Both heavy and light bands are taken into account.

Under suitable scaling assumptions, we have obtained an explicit analytical expression for fluxes and production terms. Limiting energy-transport and drift-diffusion models have been deduced.

Simulations in the bulk homogeneous case are performed.

Applications to relevant bipolar devices are under current investigation by the authors.

Acknowledgments

The author acknowledges the financial support by MIUR (PRIN 2004 *Problemi Matematici delle teorie cinetiche*), PRA University of Catania (ex 60 %), CNR (grant no 00.00128.ST74), the EU Marie Curie RTN project COMSON grant no MRTN-CT-2005-019417.

Appendix A. Numerical coefficients

In this appendix, some numerical coefficients present in the constitutive relation are collected.

The definition of the coefficients J_i are given by

$$J_5 = \int_{S^2\times S'^2} D^{-3/2}(\vartheta',\varphi')(1+3(\mathbf{n}\cdot\mathbf{n}')^2)(1-\mathbf{n}\cdot\mathbf{n}')D^{-5/2}(\vartheta,\varphi)\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$J_6 = \int_{S^2\times S'^2} D^{-3/2}(\vartheta',\varphi')(1+3(\mathbf{n}\cdot\mathbf{n}')^2)(1-\mathbf{n}\cdot\mathbf{n}')D^{-3}(\vartheta,\varphi)\frac{T(\vartheta,\varphi)}{2}\cos^2\vartheta\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$J_7 = \int_{S^2\times S'^2} D^{-3/2}(\vartheta',\varphi')(1+3(\mathbf{n}\cdot\mathbf{n}')^2)(1-\mathbf{n}\cdot\mathbf{n}')D^{-3}(\vartheta,\varphi)\frac{T(\vartheta',\varphi')}{2}\cos\vartheta\cos\vartheta'\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$J_8 = \int_{S^2\times S'^2} D^{-3/2}(\vartheta',\varphi')(1+3(\mathbf{n}\cdot\mathbf{n}')^2)D^{-2}(\vartheta,\varphi)\frac{T(\vartheta,\varphi)}{2}\cos^2\vartheta\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$J_9 = \int_{S^2\times S'^2} D^{-3/2}(\vartheta',\varphi')(1+3(\mathbf{n}\cdot\mathbf{n}')^2)(1-\mathbf{n}\cdot\mathbf{n}')D^{-5/2}(\vartheta,\varphi)\frac{T^2(\vartheta,\varphi)}{4}\cos^2\vartheta\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$J_{10} = \int_{S^2\times S'^2} D^{-3/2}(\vartheta',\varphi')(1+3(\mathbf{n}\cdot\mathbf{n}')^2)(1-\mathbf{n}\cdot\mathbf{n}')D^{-5/2}(\vartheta,\varphi)\frac{T(\vartheta',\varphi')}{2} \times \frac{T(\vartheta,\varphi)}{2}\cos\vartheta\cos\vartheta'\,\mathrm{d}\Omega\,\mathrm{d}\Omega',$$

$$J_{11} = \int_{S^2\times S'^2} D^{-3/2}(\vartheta',\varphi')(1+3(\mathbf{n}\cdot\mathbf{n}')^2)D^{-3/2}(\vartheta,\varphi)\frac{T^2(\vartheta,\varphi)}{4}\cos^2\vartheta\,\mathrm{d}\Omega\,\mathrm{d}\Omega'.$$

The numerical values are reported in table 2.

Table 3. Values of the parameters entering in the inter-band acoustic phonon scattering relations.

Parameter	A = − B = +	A = + B = −
I_1	7.688 41	7.688 41
I_2	4.435 48	0.107 800
I_3	4.363 69	1.213 93
I_4	1.454 56	0.404 642
I_5	2.562 74	2.562 74
I_6	−0.553 374	−0.042 758
I_7	3.193 46	2.663 97
I_8	5.975 56	16.9617

The definition of the coefficients I_j are given by

$$I_1 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B) D_A^{-3/2}(\vartheta_A,\varphi_A)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2)\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B,$$

$$I_2 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2)(1-\mathbf{n_A}\cdot\mathbf{n_B}') D_A^{-5/2}(\vartheta_A,\varphi_A)\frac{T_A(\vartheta_A,\varphi_A)}{2}$$
$$\times\frac{T_B(\vartheta'_B,\varphi'_B)}{2}\cos\vartheta_A\cos\vartheta'_B\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B,$$

$$I_3 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2)(1-\mathbf{n_A}\cdot\mathbf{n_B}') D_A^{-5/2}(\vartheta_A,\varphi_A)\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B,$$

$$I_4 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2)(1-\mathbf{n_A}\cdot\mathbf{n_B}') D_A^{-3}(\vartheta_A,\varphi_A)$$
$$\times\frac{T_A(\vartheta_A,\varphi_A)}{2}\cos^2\vartheta_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B,$$

$$I_5 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2) D_A^{-2}(\vartheta_A,\varphi_A)\frac{T_A(\vartheta_A,\varphi_A)}{2}\cos^2\vartheta_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B,$$

$$I_6 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2)(1-\mathbf{n_A}\cdot\mathbf{n_B}') D_A^{-3}(\vartheta_A,\varphi_A)$$
$$\times\frac{T_B(\vartheta'_B,\varphi'_B)}{2}\cos\vartheta_A\cos\vartheta'_B\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B,$$

$$I_7 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2)(1-\mathbf{n_A}\cdot\mathbf{n_B}') D_A^{-5/2}(\vartheta_A,\varphi_A)$$
$$\times\frac{T_A^2(\vartheta_A,\varphi_A)}{4}\cos^2\vartheta_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B,$$

$$I_8 = \int_{S^2\times S'^2} D_B^{-3/2}(\vartheta'_B,\varphi'_B)(3-3(\mathbf{n_A}\cdot\mathbf{n_B}')^2) D_A^{-3/2}(\vartheta_A,\varphi_A)\frac{T_A^2(\vartheta_A,\varphi_A)}{4}\cos^2\vartheta_A\,\mathrm{d}\Omega_A\,\mathrm{d}\Omega'_B.$$

The numerical values are reported in table 3.

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