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Original Article

Hydrodynamical model of charge transport in GaAs based on the maximum entropy principle

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A hydrodynamical model based on the maximum entropy principle is formulated for GaAs semiconductors. Explicit closure relations for the moment equations of the electron density, energy, velocity and energy-flux are obtained by using the Kane dispersion approximation for the description of the conduction bands. All the relevant scattering mechanisms are included: interaction of electrons with acoustic, polar and non-polar optical phonons, impurities. Application to the bulk case reveals that the model describes with accuracy the effect of negative differential conductivity, typical of GaAs, as well as the velocity overshoot and saturation.

1 Introduction

The semiclassical Boltzmann transport equation accurately describes the transport properties of electrons in semiconductors. However simulating submicron electron devices by a direct integration of the Boltzmann equation is a daunting computational task and it is not practical for computer aided design purposes. This has led to the development of macroscopic models whose main problem is the closure of the evolution equations. This arises because the number of unknown functions exceeds that of the balance equations. In the past, several hydrodynamical models, with *ad hoc* closure relations containing free adjustable parameters, have been introduced (e.g. see [1, 2]) without any thermodynamically consistent justification.

Recently a systematic approach to the question, based on the maximum entropy principle, has been followed for silicon semiconductors [3, 4, 5, 6] in the framework of extended thermodynamics [7, 8], in the case of parabolic and Kane's dispersion relations for the description of the electron energy bands. Previous attempts in the same direction can also be found in [9, 10, 11]. These models may also be arranged in the context of the moment theory of Levermore [12].

Here we consider the case of Gallium Arsenide (GaAs), which is a compound semiconductor currently used as a generator of microwave radiation. Its main peculiarity is the negative differential conductivity. While in silicon the velocity is an increasing function of the electric field, in GaAs beyond a certain threshold value of the electric field the velocity decreases with the increasing of the field. This non-monotone behaviour of the velocity-field relation generates instabilities that give rise to electromagnetic emissions.

A further difference of GaAs compared to silicon is the presence of the polar optical phonon scattering mechanism, typical of polar semiconductors. Being anisotropic, this process introduces considerable difficulties in the hydrodynamical modeling.

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We also remark that the treatment of the scattering with impurities, which we propose, is different from that in [5]. Here the Grinberg-Luryi approximation is not used, but the general form of the collision operator is retained.

The plan of the paper is as follows. In Sect. 2 a brief account of the electron transport and scattering mechanisms in GaAs is given. In Sect. 3 the balance equations are deduced as moment equations of the Boltzmann equation and the maximum entropy principle is employed for getting approximate forms of the electron distribution functions. These functions are used in Sect. 4 to obtain the necessary closure relations. In Sect. 5 applications to bulk GaAs are presented, with particular attention to velocity overshoot and saturation and to negative differential conductivity.

2 Main transport properties in GaAs

In this section we present a brief account of the main transport properties of electrons in GaAs. For more details the interested reader is referred to [13].

2.1 Energy bands and transport equations

The solution of the single-electron stationary Schrödinger equation, with the periodic potential generated by the ions of the crystal lattice, gives the relation between the electron energy $\mathscr{E}$ in each conduction band and the wave vector $\mathbf{k}$ varying in the first Brillouin zone.

At normal operating conditions of electron devices, it is sufficient to take into account only the lowest conduction band, because the others are scarcely populated. Moreover, the electrons in this band are essentially located in the neighborhoods of the lowest energy local minima, the so-called *valleys*.

In the case of GaAs the lowest conduction band has an absolute minimum at the center of the Brillouin zone, the Γ-point, and local minima at the 4 L-points along the Λ crystallographic orientations, see Fig. 1 and [13]. There are also other secondary minima which become relevant only at very high electric fields and will be neglected in the following.

In the deduction of hydrodynamical models, the energy in each valley is represented by analytical approximations. Among these the most common are the parabolic one and the Kane dispersion relation.

In the isotropic parabolic band approximation, the energy $\mathscr{E}_A$ of the A-valley, measured from the bottom of the valley $\overline{\mathscr{E}_A}$, $A = \Gamma, L$, has an expression similar to that of a classical free particle

$$\mathscr{E}_A = \frac{\hbar^2 |\mathbf{k}_A|^2}{2m_A^*}, \quad \mathbf{k}_A \in \Re^3, \tag{1}$$

where m_A^* is the effective mass of electrons in the A-valley, see Table 1. $\hbar\mathbf{k}_A$ is the crystal momentum with respect to the bottom of the valley and $\mathbf{k}_A$ is assumed to vary in all $\Re^3$.

In the case of Kane's dispersion relation which, at higher energies, furnishes a better approximation than the parabolic one, $\mathscr{E}_A$ still depends only on k_A, the magnitude of $\mathbf{k}_A$, but the dependence is given by the more complex expression

$$\mathscr{E}_A(k_A)\left[1 + \alpha_A \mathscr{E}_A(k_A)\right] = \frac{\hbar^2 |\mathbf{k}_A|^2}{2m_A^*}, \quad \mathbf{k}_A \in \Re^3, \quad A = \Gamma, L, \tag{2}$$

involving a parameter α_A, called the non-parabolicity factor, see Table 1.

The electrons in each valley are treated as different populations and described by distinct distribution functions. Due to the symmetries of the Brillouin zone, which are inferred by the symmetries of the crystal, the evolution of the L-valley distribution functions is the same. Therefore, at a kinetic level, a semi-classic description is based on two Boltzmann equations, one for the Γ-valley and the other for one L-valley. These equations, which are coupled through the Poisson equation and the collision terms, read

$$\begin{aligned} &\frac{\partial f_A}{\partial t} + \mathbf{v}_A(\mathbf{k}_A) \cdot \frac{\partial f_A}{\partial \mathbf{x}} - \frac{q\mathbf{E}}{\hbar} \cdot \frac{\partial f_A}{\partial \mathbf{k}_A} = \mathscr{C}_A[f], \quad A = \Gamma, L, \\ &\nabla_{\mathbf{x}} \cdot (\epsilon \mathbf{E}) = q\left[N_+(\mathbf{x}) - N_-(\mathbf{x}) - n(\mathbf{x})\right], \end{aligned} \tag{3}$$

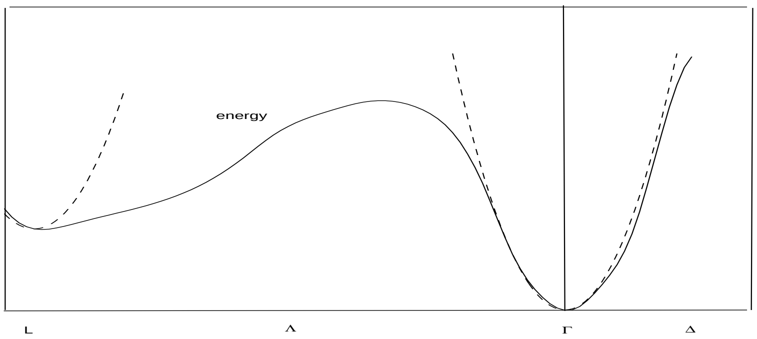

Fig. 1. A schematic representation of the lowest energy electron conduction band along the Λ direction ($\mathscr{E}(k)$ versus k in arbitrary units). Note the presence of two minima at the Γ and L points. The dashed lines represent the Kane approximation

where $f_A(\mathbf{x}, t, \mathbf{k}_A)$ is the one-particle distribution function relative to the electrons in the A-valley and $\mathbf{k}_A$ the correspondent wave vector, q represents the absolute value of the electron charge, $\mathbf{E}$ the electric field, $\hbar$ the reduced Planck constant, ϵ the dielectric constant, N_+ and N_- the donor and acceptor concentrations respectively, and n the total electron number density. $\mathbf{v}_A$, the electron group velocity in the A-valley, depends on the correspondent energy $\mathscr{E}_A$ through the relation

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

$\mathscr{C}_A[f]$ is the collision term, which we proceed to discuss.

2.2 The collision operator

The expression for the collision term is obtained by means of the *Fermi's golden rule* [15, 16]. It reflects the various scattering mechanisms the electrons undergo in a semiconductor. Some of them leave the electrons in the same valley as they are before the collision (intravalley transitions), while other scatterings can drive the electrons into a different valley (intervalley transitions) according to suitable selection rules. Therefore, in general, the collision term may be split according to

$$\mathscr{C}_A[f] = \mathscr{C}_A[f_A, f_A] + \sum_B \mathscr{C}_A[f_A, f_B].$$

The first term represents the intravalley scatterings, the second one takes into account the intervalley scatterings. The main scattering mechanisms, to which electrons are subjected in semiconductors, are the ones with phonons, impurities, other electrons and stationary imperfections of the crystal such as vacancies and external and internal crystal boundaries. In the present paper the electron-electron scattering will not be considered, because it is relevant only for very high doping, which usually occurs at ohmic contacts where electrons are in thermal equilibrium. We also neglect the stationary imperfections.

GaAs is a compound semiconductor, therefore the electrons interact with the phonons not only because of the deformation of the crystal but also through the polarization waves, see [17]. The deformation of the lattice, due to vibrations of the ions about their equilibrium positions, is described by deformation potentials. Either the acoustic or the optical modes can be excited. The scattering arising from the excitation of the acoustic mode is typically called acoustic scattering, while the one arising from the excitation of the optical mode is called non-polar optical scattering.

The coupling through the polarization waves is due to the permanent electric dipole moment of the constituent ions in a compound material. This coupling can be mediated through both the optical and the acoustic branches, but the latter contribution is marginal at room temperature in very pure semiconductors.

In the present paper we consider the following scattering mechanisms:

- the acoustic phonon scattering,
- the non-polar optical phonon scattering,
- the polar optical phonon scattering,

- the impurity scattering.

All these scattering mechanisms are intravalley, except the non-polar optical phonon scattering. Their contributions to the collision operator, in the non-degenerate approximation, [1] may schematically be written, respectively for the intravalley and intervalley scatterings, as

$$\begin{aligned} \mathscr{C}_A^{(\eta)}[f_A, f_A] &= \int_{\Re^3} \left[P^{(\eta)}(\mathbf{k}'_A, \mathbf{k}_A) f_A(\mathbf{k}'_A) - P^{(\eta)}(\mathbf{k}_A, \mathbf{k}'_A) f_A(\mathbf{k}_A) \right] \, d\mathbf{k}'_A, \\ \mathscr{C}_A^{(\eta)}[f_A, f_B] &= \int_{\Re^3} \left[P^{(\eta)}(\mathbf{k}'_B, \mathbf{k}_A) f_B(\mathbf{k}'_B) - P^{(\eta)}(\mathbf{k}_A, \mathbf{k}'_B) f_A(\mathbf{k}_A) \right] \, d\mathbf{k}'_B, \end{aligned} \tag{4}$$

where $P^{(\eta)}(\mathbf{k}, \mathbf{k}')$ is the electron transition probability per unit time from a state $\mathbf{k}$ to a state $\mathbf{k}'$ and η labels the different types of scattering. The first terms in (4) represent the gains and the second ones the losses. From the principle of detailed balance we have

$$P^{(\eta)}(\mathbf{k}'_B, \mathbf{k}_A) = P^{(\eta)}(\mathbf{k}_A, \mathbf{k}'_B) \exp\left(- \frac{\mathscr{E}_A - \mathscr{E}_B + \Delta_{AB}}{k_B T_L} \right),$$

where k_B is the Boltzmann constant, T_L the lattice temperature, which will be taken as constant, and $\Delta_{AB} = \overline{\mathscr{E}}_A - \overline{\mathscr{E}}_B$.

In the case of acoustic phonon scattering in its elastic approximation, valid when the thermal energy is much greater than that of the phonon involved in the scattering, we have

$$P^{(ac)}(\mathbf{k}_A, \mathbf{k}'_A) = K_{ac} \delta(\mathscr{E}_A - \mathscr{E}'_A), \tag{5}$$

where δ is the Dirac delta function and K_{ac} a physical parameter.

For the non-polar optical phonon interaction, the transition rate is given by the sum of an absorption and an emission term

$$P^{(np)}(\mathbf{k}_A, \mathbf{k}'_B) = Z_{AB} \, K_{np} \, \left[N^{(np)} \delta(\mathscr{E}'_B - \mathscr{E}_A - \hbar\omega^+_{np}) + (N^{(np)} + 1) \delta(\mathscr{E}'_B - \mathscr{E}_A + \hbar\omega^-_{np}) \right], \tag{6}$$

where K_{np} is a physical parameter, $\hbar\omega^{\pm}_{np} = \hbar\omega_{np} \pm \Delta_{AB}$, $\hbar\omega_{np}$ is the longitudinal optical phonon energy, $N^{(np)}$ is the equilibrium non-polar optical phonon Bose-Einstein distribution given by

$$N^{(np)} = \frac{1}{\exp(\hbar\omega_{np}/k_B T_L) - 1},$$

and Z_{AB}, see Table 1, is the degeneracy of the final valley, that is the valley the electron reachs after the scattering, with respect to the initial one. In GaAs, non-polar optical phonons contribute to the electron intervalley transfer between two L-valleys and between Γ-valley and L-valleys.

As said, the polar optical phonon scattering is a very important scattering mechanism in compound semiconductors. It is an intravalley inelastic process whose transition rate is given by

$$\begin{aligned} P^{(p)}(\mathbf{k}_A, \mathbf{k}'_A) &= \frac{K_p}{8\pi^2 \hbar |\mathbf{k}_A - \mathbf{k}'_A|^2} \mathscr{G}(\mathbf{k}_A, \mathbf{k}'_A) \left[N^{(p)} \delta(\mathscr{E}'_A - \mathscr{E}_A - \hbar\omega_p) + \right. \\ &\quad \left. + (N^{(p)} + 1) \delta(\mathscr{E}'_A - \mathscr{E}_A + \hbar\omega_p) \right], \end{aligned} \tag{7}$$

where K_p is a physical parameter, $\hbar\omega_p$ is the polar optical phonon energy, $N^{(p)}$ the thermal equilibrium polar optical phonon number and $\mathscr{G}(\mathbf{k}_A, \mathbf{k}'_A)$ the so-called overlap factor given by [15]

$$\mathscr{G}(\mathbf{k}_A, \mathbf{k}'_A) = (a_A a'_A + c_A c'_A \, \mathbf{e}_A \cdot \mathbf{e}'_A)^2, \tag{8}$$

where $\mathbf{e}_A$ and $\mathbf{e}'_A$ are unit vectors pointing in the directions of $\mathbf{k}_A$ and $\mathbf{k}'_A$ and

$$a_A = \sqrt{\frac{1 + \alpha_A \mathscr{E}_A}{1 + 2\alpha_A \mathscr{E}_A}}, \quad a'_A = \sqrt{\frac{1 + \alpha_A \mathscr{E}'_A}{1 + 2\alpha_A \mathscr{E}'_A}}, \quad c_A = \sqrt{\frac{\alpha_A \mathscr{E}_A}{1 + 2\alpha_A \mathscr{E}_A}}, \quad c'_A = \sqrt{\frac{\alpha_A \mathscr{E}'_A}{1 + 2\alpha_A \mathscr{E}'_A}}.$$

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[1] That is by linearizing the operator with respect to the distribution functions.

At last, the transition rate for the scattering with impurities, which is an elastic mechanism of interaction, reads

$$P^{(imp)}(\mathbf{k}_A, \mathbf{k}'_A) = \frac{K_{imp}}{\left[|\mathbf{k}_A - \mathbf{k}'_A|^2 + \beta^2\right]^2}\, \delta(\mathscr{E}'_A - \mathscr{E}_A),$$

where K_{imp} is a physical parameter, and β is the inverse Debye length.

The values of K_{ac}, K_{np}, K_p, K_{imp} and β are indicated in Sect. 7.

3 Moment equations and maximum entropy principle

Starting from the transport equations (3), one can get balance equations for macroscopic quantities associated with the electron flow. For simplicity we drop the valley label.

Multiplying eqs (3) by a regular generic function $\psi(\mathbf{k})$ and integrating over the wave vector space, one finds

$$\frac{\partial M_\psi}{\partial t} + \int_{\Re^3} \psi(\mathbf{k}) v^i(\mathbf{k}) \frac{\partial f}{\partial x^i} d^3\mathbf{k} - \frac{qE^j}{\hbar} \int_{\Re^3} \psi(\mathbf{k}) \frac{\partial f}{\partial k^j} d^3\mathbf{k} = \int_{\Re^3} \psi(\mathbf{k}) \mathscr{C}[f] d^3\mathbf{k}, \tag{9}$$

with

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

as the moment corresponding to ψ.

By taking ψ as 1, $\hbar\mathbf{k}_A$, $\mathscr{E}_A$ and $\mathscr{E}_A\, \mathbf{v}_A$, with $A = \Gamma$, L, one has the following set of balance equations, [4, 5],

$$\frac{\partial n_A}{\partial t} + \frac{\partial (n_A V_A^i)}{\partial x^i} = n_A\, C_{n_A}, \tag{10}$$

$$\frac{\partial (n_A P_A^i)}{\partial t} + \frac{\partial (n_A U_A^{ij})}{\partial x^j} + n_A q E^i = n_A C_{P_A^i}, \tag{11}$$

$$\frac{\partial (n_A W_A)}{\partial t} + \frac{\partial (n_A S_A^j)}{\partial x^j} + n_A q V_A^j E_j = n_A C_{W_A}, \tag{12}$$

$$\frac{\partial (n_A S_A^i)}{\partial t} + \frac{\partial (n_A F_A^{ij})}{\partial x^j} + n_A q E_j G_A^{ij} = n_A C_{S_A^i}, \tag{13}$$

where

$$\begin{aligned}
n_A &= \int_{\Re^3} f_A d\mathbf{k}_A \quad \text{is the electron density,} \\
V_A^i &= \frac{1}{n_A} \int_{\Re^3} v_A^i f_A d\mathbf{k}_A \quad \text{the average electron velocity,} \\
W_A &= \frac{1}{n_A} \int_{\Re^3} \mathscr{E}_A(k_A) f_A d\mathbf{k}_A \quad \text{the average electron energy,} \\
S_A^i &= \frac{1}{n_A} \int_{\Re^3} v_A^i \mathscr{E}_A(k_A) f_A d\mathbf{k}_A \quad \text{the average energy flux,} \\
P_A^i &= \frac{1}{n_A} \int_{\Re^3} \hbar k_A^i f_A d\mathbf{k}_A = m_A^* \left(V_A^i + 2\alpha_A S_A^i\right) \quad \text{the average crystal momentum,} \\
U_A^{ij} &= \frac{1}{n_A} \int_{\Re^3} v_A^i \hbar k_A^j f_A d\mathbf{k}_A \quad \text{the average crystal momentum flux,} \\
G_A^{ij} &= \frac{1}{n_A} \int_{\Re^3} \left[\frac{\partial}{\partial k_A^j} \left(\frac{1}{\hbar} v_A^i\, \mathscr{E}_A(\mathbf{k})\right)\right] f_A d\mathbf{k}_A, \\
F_A^{ij} &= \frac{1}{n_A} \int_{\Re^3} v_A^i v_A^j \mathscr{E}_A(k_A) f_A d\mathbf{k}_A \quad \text{the average flux of energy flux,}
\end{aligned} \tag{14}$$

$$\begin{aligned}
C_{n_A} &= \frac{1}{n_A}\int_{\Re^3} \mathscr{C}_A[f]\,d\mathbf{k}_A \quad \text{the density production,}\\
C_{P_A^i} &= \frac{1}{n_A}\int_{\Re^3} \hbar k_A^i \mathscr{C}_A[f]\,d\mathbf{k}_A \quad \text{the crystal momentum production,}\\
C_{W_A} &= \frac{1}{n_A}\int_{\Re^3} \mathscr{E}_A(k_A)\mathscr{C}_A[f]\,d\mathbf{k}_A \quad \text{the energy production,}\\
C_{S_A^i} &= \frac{1}{n_A}\int_{\Re^3} v_A^i \mathscr{E}_A(k_A)\mathscr{C}_A[f]\,d\mathbf{k}_A \quad \text{the energy flux production.}
\end{aligned}$$

All these quantities refer to electrons in the A-valley, $A = \Gamma,\ L$.

The moment equations (10)-(13) do not form a set of closed relations because the number of the unknowns is greater than that of the equations. Therefore it is necessary to choose a set of fundamental variables and try to express the others in terms of these. A way to get constitutive relations, which lies on sound physical bases, is to use the maximum entropy principle [7, 8, 12, 18]. This principle furnishes the form of the distribution functions that makes the best use of the knowledge of a finite number of moments.

In particular, if we assume as fundamental variables n_A,$\mathbf{V}_A$, W_A and $\mathbf{S}_A$ the maximum entropy distributions f_A are those which make the electron entropy extremal under the constraints of fixed values of the fundamental variables.

The entropy of the electrons in the Γ-valley and the 4 L-valleys read

$$s\left[f_\Gamma, f_L\right] = -k_B\left[\int_{\Re^3}\left(f_\Gamma \log f_\Gamma - f_\Gamma\right)d\mathbf{k}_\Gamma + 4\int_{\Re^3}\left(f_L \log f_L - f_L\right)d\mathbf{k}_L\right].$$

and the distribution functions f_A ($A = \Gamma, L$) that maximize it under the constraints n_A,$\mathbf{V}_A$, W_A and $\mathbf{S}_A$ are given by [2] (see [4])

$$f_A^{ME} = \exp\left[-\left(\frac{1}{k_B}\lambda_A + \lambda_A^W\,\mathscr{E}_A + \lambda_A^{V^i}\,v_A^i + \lambda_A^{S^i}\,v_A^i\,\mathscr{E}_A\right)\right], \quad A = \Gamma\,, L,$$

where the λ's are Lagrange multipliers that take care of the constraints.

In order to determine the Lagrange multipliers in terms of n_A, $\mathbf{V}_A$, W_A, $\mathbf{S}_A$, $A = \Gamma,\ L$, one has to insert the expressions of the maximum-entropy-distribution functions into $(14)_{1-4}$ and solve the resulting system. Then the closure relations can be obtained by evaluating the appropriate moments of f_A, and $\mathscr{C}_A[f]$, with f_A, $A = \Gamma\,, L$, replaced by the corresponding maximum entropy functions. However, on account of the algebraic difficulties, we get only approximate explicit expressions for the Lagrange multipliers under reasonable physical assumptions on the distribution functions.

At equilibrium the distribution functions are isotropic

$$f_A^{(eq)} = \exp\left[-\left(\frac{1}{k_B}\lambda_A^{(eq)} + \frac{\mathscr{E}_A}{k_B\,T_L}\right)\right],$$

that is at equilibrium

$$\lambda_A^{W\,(eq)} = \frac{1}{k_B\,T_L}, \qquad \lambda_A^{V_i\,(eq)} = 0, \qquad \lambda_A^{S_i\,(eq)} = 0, \qquad A = \Gamma\,, L\,.$$

We assume that the anisotropy of the f_A^{ME}, $A = \Gamma\,, L$ remains small even out of equilibrium. We formally introduce a *small* anisotropy parameter δ, assume that the Lagrange multipliers are analytic in δ and expand them around $\delta = 0$ up to the first order. By taking into account the representation theorems for isotropic functions, one has that λ_A and λ_A^W are of order zero in δ, while $\lambda_A^{V^i}$ and $\lambda_A^{S^i}$ are of the first order in δ

$$\begin{aligned}
\lambda_A &= \lambda_A, & \lambda_A^W &= \lambda_A^W\,,\\
\lambda_A^{V_i} &= \delta\,\lambda_A^{V_i}\,, & \lambda_A^{S_i} &= \delta\,\lambda_A^{S_i}\,,
\end{aligned}$$

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[2] Summation over repeated lowercase letters is understood.

and the maximum entropy distribution functions can be written as

$$f_A^{ME} = \exp\left(-\frac{\lambda_A}{k_B} - \lambda_A^W \mathscr{E}_A\right)\left[1 - \delta\left(\lambda_A^{V_i}\, v_A^i + \lambda_A^{S_i}\, v_A^i \mathscr{E}_A\right)\right], \quad A = \Gamma\,, L\,. \tag{15}$$

4 Inversion of the constraint relations

In order to express the Lagrange multipliers in terms of the fundamental moments, we have to invert the following system of equations

$$\begin{aligned} n_\Gamma &= \int_{\Re^3} f_\Gamma^{ME}\, d\mathbf{k}_\Gamma, & n_L &= \int_{\Re^3} f_L^{ME}\, d\mathbf{k}_L, \\ n_\Gamma\, W_\Gamma &= \int_{\Re^3} \mathscr{E}_\Gamma f_\Gamma^{ME}\, d\mathbf{k}_\Gamma, & n_L\, W_L &= \int_{\Re^3} \mathscr{E}_L f_L^{ME}\, d\mathbf{k}_L, \\ n_\Gamma\, V_\Gamma^i &= \int_{\Re^3} v_\Gamma^i f_\Gamma^{ME}\, d\mathbf{k}_\Gamma, & n_L\, V_L^i &= \int_{\Re^3} v_L^i f_L^{ME}\, d\mathbf{k}_L, \\ n_\Gamma\, S_\Gamma^i &= \int_{\Re^3} v_\Gamma^i \mathscr{E}_\Gamma f_\Gamma^{ME}\, d\mathbf{k}_\Gamma, & n_L\, S_L^i &= \int_{\Re^3} v_L^i \mathscr{E}_L f_L^{ME}\, d\mathbf{k}_L\,. \end{aligned} \tag{16}$$

where f_Γ^{ME} and f_L^{ME} are given by (15).

For computational reasons, it is better to express the volume element $d\mathbf{k}_A$, $A = \Gamma$, L, in terms of energy $\mathscr{E}_A$ and the elementary solid angle $d\,\Omega_A$

$$d\mathbf{k}_A = k_A^2\, dk_A\, d\,\Omega_A = \frac{m_A^*}{\hbar^3}\sqrt{2m_A^* \mathscr{E}_A\left(1 + \alpha_A \mathscr{E}_A\right)}\left(1 + 2\alpha_A \mathscr{E}_A\right) d\,\mathscr{E}_A\, d\,\Omega_A.$$

By retaining only the terms up to the first order in δ, from the constraints [3] (16), we get the following results

$$\begin{aligned} \lambda_\Gamma &= -k_B \log\left(\frac{\hbar^3 n_\Gamma}{4\,\pi\, m_\Gamma^*\,\sqrt{2\,m_\Gamma^*}\, d_0^\Gamma}\right), & \lambda_L &= -k_B \log\left(\frac{\hbar^3 n_L}{4\,\pi\, m_L^*\,\sqrt{2\,m_L^*}\, d_0^L}\right), \\ \lambda_\Gamma^W &= g_\Gamma^{-1}(W_\Gamma), & \lambda_L^W &= g_L^{-1}(W_L), \\ \lambda_\Gamma^{V_i} &= b_{11}^\Gamma\, V_\Gamma^i + b_{12}^\Gamma\, S_\Gamma^i, & \lambda_L^{V_i} &= b_{11}^L\, V_L^i + b_{12}^L\, S_L^i, \\ \lambda_\Gamma^{S_i} &= b_{12}^\Gamma\, V_\Gamma^i + b_{22}^\Gamma\, S_\Gamma^i, & \lambda_L^{S_i} &= b_{12}^L\, V_L^i + b_{22}^L\, S_L^i, \end{aligned} \tag{17}$$

where

$$d_k^A\left(\lambda_A^W\right) = \int_0^\infty \mathscr{E}_A^k\,\sqrt{\mathscr{E}_A\left(1 + \alpha_A\,\mathscr{E}_A\right)}\left(1 + 2\,\alpha_A\,\mathscr{E}_A\right)\exp(-\lambda_A^W\,\mathscr{E}_A)\, d\,\mathscr{E}_A,$$

g_A^{-1} are the inverse functions of

$$g_A\left(\lambda_A^W\right) = \frac{d_1^A\left(\lambda_A^W\right)}{d_0^A\left(\lambda_A^W\right)}, \quad A = \Gamma, L, \tag{18}$$

and the coefficients b_{ij}^A, $A = \Gamma\,, L$, are given by

$$b_{11}^A = \frac{a_{22}^A}{\Delta^A}, \qquad b_{12}^A = -\frac{a_{12}^A}{\Delta^A}, \qquad b_{22}^A = \frac{a_{11}^A}{\Delta^A}, \tag{19}$$

with

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

and

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[3] V_A^i and S_A^i, $A = \Gamma\,, L$, are consistently considered as terms of order δ.

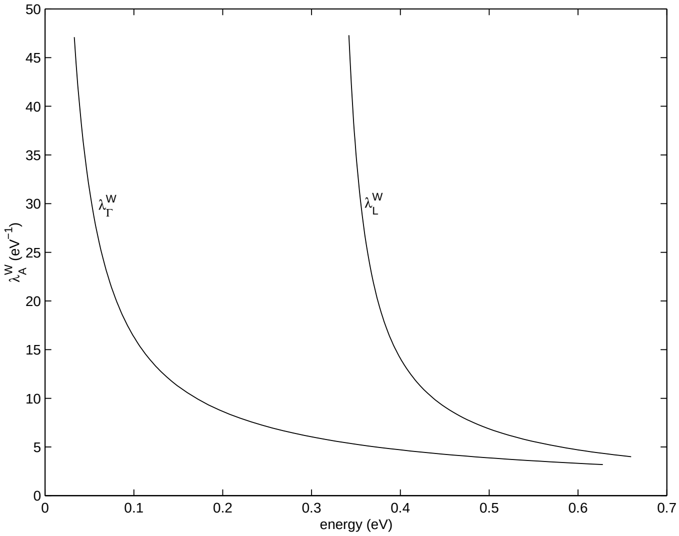

Fig. 2. λ_Γ^W and λ_L^W vs. the electron average energy. Note the difference in the energy range of the two valleys

$$\varDelta^A = a_{11}^A\, a_{22}^A - \left(a_{12}^A\right)^2 , \qquad A = \varGamma\, , L\, ,$$

p_k^A being

$$p_k^A = \int_0^\infty \frac{\mathscr{E}_A^k\, \left[\mathscr{E}_A \left(1 + \alpha_A\, \mathscr{E}_A\right)\right]^{3/2}}{1 + 2\, \alpha_A\, \mathscr{E}_A} \exp(-\lambda_A^W\, \mathscr{E}_A)\, d\, \mathscr{E}_A\, , \quad A = \varGamma\, , L\, .$$

For the inversion of the functions (18) we have resorted to a numerical approach. The results are shown in Fig. 2.

5 Fluxes

Once the Lagrangian multipliers are expressed as functions of the fundamental variables, the constitutive equations for the fluxes can be obtained. Up to the first order terms, one has

$$U_A^{ij} = U_A\, \delta^{ij}\, , \quad F_A^{ij} = F_A\, \delta^{ij}\, , \quad G_A^{ij} = G_A\, \delta^{ij}\, , \qquad A = \varGamma,\, L\, ,$$

with

$$\begin{aligned}
U_A &= \frac{2}{3\, d_0^A} \int_0^\infty \left[\mathscr{E}_A \left(1 + \alpha_A\, \mathscr{E}_A\right)\right]^{3/2} \exp(-\lambda_A^W\, \mathscr{E}_A)\, d\, \mathscr{E}_A,\\
F_A &= \frac{2}{3\, m_A^*}\, \frac{p_1^A}{d_0^A},\\
G_A &= \frac{1}{m_A^*\, d_0^A} \int_0^\infty \left[1 + \frac{2}{3}\, \frac{1 + \alpha_A\, \mathscr{E}_A}{\left(1 + 2\, \alpha_A\, \mathscr{E}_A\right)^2}\right] \mathscr{E}_A^{3/2} \sqrt{1 + \alpha_A\, \mathscr{E}_A}\, \exp(-\lambda_A^W\, \mathscr{E}_A)\, d\, \mathscr{E}_A\, .
\end{aligned}$$

In Fig. 3 we represent these tensors as functions of the electron average energy.

6 Production terms

By using the same procedure as before, also the expressions of the moments of the collision term can be found.

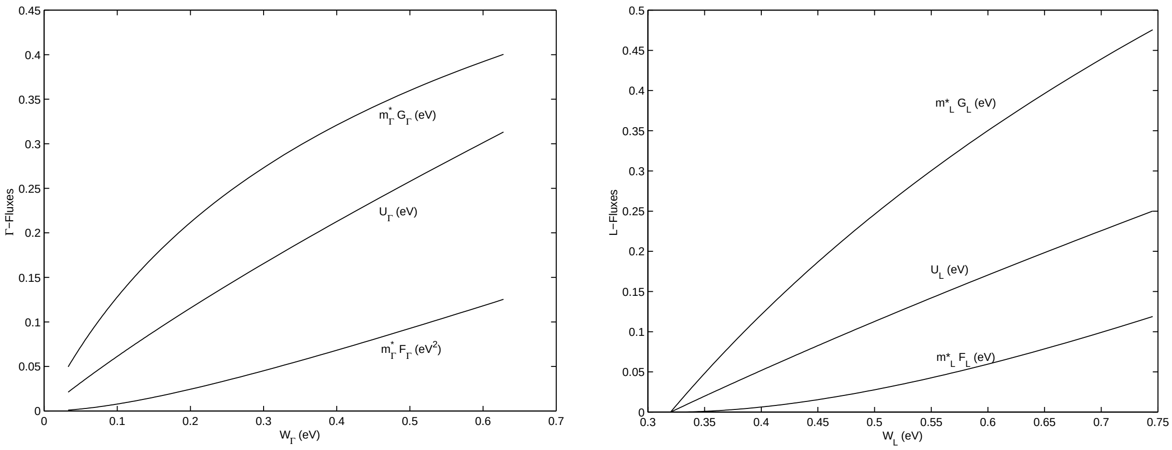

Fig. 3. The fluxes U_A, $m^*_A F_A$ and $m^*_A G_A$, $A = \Gamma, L$

6.1 Acoustic phonon scattering

The collision term for acoustic phonon scattering reads

$$\begin{aligned}\mathscr{C}_A^{(ac)}[f_A, f_A] &\approx \mathscr{C}_A^{(ac)}[f_A^{ME}, f_A^{ME}]\\ &= \frac{\sqrt{2}\, n_A K_{ac}}{\sqrt{m_A^*}\, d_0^A} \left\{ \mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right) \left(\lambda_A^{V_i} + \mathscr{E}_A\, \lambda_A^{S_i}\right) \exp(-\lambda_A^W\, \mathscr{E}_A)\, e_A^i \right\} .\end{aligned}$$

Since the scattering is intravalley and elastic, one gets

$$C_{n_A}^{(ac)} = 0, \qquad C_{W_A}^{(ac)} = 0\,, \quad A = \Gamma, L,$$

while for the production terms relative to the crystal momentum and energy flux, we have

$$C_{\mathbf{P}_A}^{(ac)} = c_{A\,11}^{(ac)}(W_A)\mathbf{V}_A + c_{A\,12}^{(ac)}(W_A)\mathbf{S}_A, \tag{20}$$

$$C_{\mathbf{S}_A}^{(ac)} = c_{A\,21}^{(ac)}(W_A)\mathbf{V}_A + c_{A\,22}^{(ac)}(W_A)\mathbf{S}_A. \tag{21}$$

The production matrix

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

is given by

$$\hat{C}_A^{(ac)} = \hat{Q}_A^{(ac)} \hat{B}_A,$$

where the coefficients of the symmetric matrices $\hat{B}_A$ are given in (19) and those of $\hat{Q}_A^{(ac)}$ are

$$q_{A\,11}^{(ac)} = \frac{\overline{K}_{ac}^A}{d_0^A} \int_0^\infty \mathscr{E}_A^2 \left(1 + \alpha_A \mathscr{E}_A\right)^2 \left(1 + 2\alpha_A \mathscr{E}_A\right) \exp\left(-\lambda_A^W \mathscr{E}_A\right)\, d\mathscr{E}_A, \tag{22}$$

$$q_{A\,12}^{(ac)} = \frac{\overline{K}_{ac}^A}{d_0^A} \int_0^\infty \mathscr{E}_A^3 \left(1 + \alpha_A \mathscr{E}_A\right)^2 \left(1 + 2\alpha_A \mathscr{E}_A\right) \exp\left(-\lambda_A^W \mathscr{E}_A\right)\, d\mathscr{E}_A, \tag{23}$$

$$q_{A\,21}^{(ac)} = \frac{\overline{K}_{ac}^A}{m_A^* d_0^A} \int_0^\infty \mathscr{E}_A^3 \left(1 + \alpha_A \mathscr{E}_A\right)^2 \exp\left(-\lambda_A^W \mathscr{E}_A\right)\, d\mathscr{E}_A, \tag{24}$$

$$q_{A\,22}^{(ac)} = \frac{\overline{K}_{ac}^A}{m_A^* d_0^A} \int_0^\infty \mathscr{E}_A^4 \left(1 + \alpha_A \mathscr{E}_A\right)^2 \exp\left(-\lambda_A^W \mathscr{E}_A\right)\, d\mathscr{E}_A, \tag{25}$$

with

$$\overline{K}_{ac}^A = \frac{8\pi\sqrt{2}(m_A^*)^{3/2} K_{ac}}{3\hbar^3}, \quad A = \Gamma, L.$$

6.2 Non-polar optical phonon scattering

The non-polar optical phonon scattering is an intervalley interaction mechanism whose collision term can be written as the sum of a gain and a loss part

$$\mathscr{C}_A^{(np)}[f] \approx \mathscr{C}_A^{(np)}[f_{ME}] = \sum_B \left\{ \mathscr{C}_+^{(np)}[f_A^{ME}, f_B^{ME}] - \mathscr{C}_-^{(np)}[f_A^{ME}, f_B^{ME}] \right\}.$$

As a consequence of the selection rules [15, 16], in this sum when A is equal to $\varGamma$, B can only be equal to L, while when A is L, B can be either $\varGamma$ or L.

At the first order in δ, we have for the gain part

$$\begin{aligned} \mathscr{C}_+^{(np)}[f_A^{ME}, f_B^{ME}] = \frac{3}{2} N^{(np)} \overline{K}_{np}^{AB} \exp\left(-\frac{\lambda_B}{k_B}\right) \left\{ \exp\left(-\lambda_B^W \mathscr{E}_A^+ + \frac{\hbar\omega_{np}}{K_b T_L}\right) \left[\mathscr{E}_A^+ (1 \right.\right. \\ \left.\left. +\alpha_B \mathscr{E}_A^+)\right]^{\frac{1}{2}} \left(1 + 2\alpha_B \mathscr{E}_A^+\right) + \exp\left(-\lambda_B^W \mathscr{E}_A^-\right) \left[\mathscr{E}_A^- \left(1 + \alpha_B \mathscr{E}_A^-\right)\right]^{\frac{1}{2}} \left(1 + 2\alpha_B \mathscr{E}_A^-\right) \right\}, \end{aligned}$$

where $\mathscr{E}_A^{\pm} = \mathscr{E}_A \pm \hbar\omega_{np}^{\pm}$ and

$$\overline{K}_{np}^{AB} = \frac{8\sqrt{2}\pi}{3\hbar^3} m_B^{*\,3/2} Z_{AB} K_{np} .$$

The loss term can be expressed as

$$\begin{aligned} \mathscr{C}_-^{(np)}[f_A^{ME}, f_B^{ME}] = \frac{3}{2} N^{(np)} \overline{K}_{np}^{AB} f_A^{ME}(\mathbf{k}_A) \left\{ \left[\mathscr{E}_A^+ \left(1 + \alpha_B \mathscr{E}_A^+\right)\right]^{\frac{1}{2}} \right. \\ \left. \times \left(1 + 2\alpha_B \mathscr{E}_A^+\right) + \left[\mathscr{E}_A^- \left(1 + \alpha_B \mathscr{E}_A^-\right)\right]^{\frac{1}{2}} \left(1 + 2\alpha_B \mathscr{E}_A^-\right) \exp\left(\frac{\hbar\omega_{np}}{k_B T_L}\right) \right\}. \end{aligned}$$

When acting from $\varGamma$ to L valleys or vice versa, the non-polar optical scattering does not conserve the electron number density and one has

$$n_A\, C_{n\ AB}^{(np)} = n_B\, C_{n\ AB}^{(np)+}(W_B) - n_A\, C_{n\ AB}^{(np)-}(W_A)\,,$$

with

$$\begin{aligned} n_B\, C_{n\ AB}^{(np)+} &= \frac{3}{2} \left(\frac{m_A^*}{m_B^*}\right)^{3/2} \frac{n_B}{d_0^B} N^{(np)} \overline{K}_{np}^{AB} \left[e^{\left(-\lambda_B^W \hbar\omega_{np}^+ + \frac{\hbar\omega_{np}}{K_b T_L}\right)} \eta_0^+ \left(\lambda_B^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,+}\right) \right. \\ &\quad \left. + \exp\left(\lambda_B^W \hbar\omega_{np}^-\right) \eta_0^- \left(\lambda_B^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,-}\right) \right], \\ n_A\, C_{n\ AB}^{(np)-} &= \frac{3}{2} \frac{n_A}{d_0^A} N^{(np)} \overline{K}_{np}^{AB} \left[\eta_0^+ \left(\lambda_A^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,+}\right) \right. \\ &\quad \left. + \exp\left(\frac{\hbar\omega_{np}}{K_b T_L}\right) \eta_0^- \left(\lambda_A^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,-}\right) \right], \quad A \neq B. \end{aligned}$$

The functions $\eta_k^{\pm}$ together with the $\overline{\mathscr{E}}_{AB}^{\,\pm}$ are reported in Appendix A.

Also energy is not conserved and, up to the first order in δ, one finds

$$n_A\, C_{W\ AB}^{(np)} = n_B\, C_{W\ AB}^{(np)+}(W_B) - n_A\, C_{W\ AB}^{(np)-}(W_A),$$

with

$$\begin{aligned} n_B\, C_{W\ AB}^{(np)+} &= \frac{3}{2} \left(\frac{m_A^*}{m_B^*}\right)^{3/2} \frac{n_B}{d_0^B} N^{(np)} \overline{K}_{np}^{AB} \left[e^{\left(-\lambda_B^W \hbar\omega_{np}^+ + \frac{\hbar\omega_{np}}{K_b T_L}\right)} \eta_1^+ \left(\lambda_B^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,+}\right) \right. \\ &\quad \left. + \exp\left(\lambda_B^W \hbar\omega_{np}^-\right) \eta_1^- \left(\lambda_B^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,-}\right) \right], \\ n_A\, C_{W\ AB}^{(np)-} &= \frac{3}{2} \frac{n_A}{d_0^A} N^{(np)} \overline{K}_{np}^{AB} \left[\eta_1^+ \left(\lambda_A^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,+}\right) \right. \\ &\quad \left. + \exp\left(\frac{\hbar\omega_{np}}{K_b T_L}\right) \eta_1^- \left(\lambda_A^W, \alpha_A, \alpha_B, \overline{\mathscr{E}}_{AB}^{\,-}\right) \right], \quad A \neq B \text{ or } A = B = L\,. \end{aligned}$$

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

$$C^{(np)}_{\mathbf{P}_{AB}} = c^{(np)}_{AB\,11}(W_A)\mathbf{V}_A + c^{(np)}_{AB\,12}(W_A)\mathbf{S}_A, \tag{26}$$

$$C^{(np)}_{\mathbf{S}_{AB}} = c^{(np)}_{AB\,21}(W_A)\mathbf{V}_A + c^{(np)}_{AB\,22}(W_A)\mathbf{S}_A. \tag{27}$$

The production matrix

$$\hat{C}^{(np)}_{AB} = \begin{pmatrix} c^{(np)}_{AB\,11} & c^{(np)}_{AB\,12} \\ c^{(np)}_{AB\,21} & c^{(np)}_{AB\,22} \end{pmatrix}$$

is given by

$$\hat{C}^{(np)}_{AB} = \hat{Q}^{(np)}_{AB}\hat{B}_A,$$

and the components of the matrix $\hat{Q}^{(np)}_{AB}$ read

$$q^{(np)}_{AB\,11} = \frac{N^{(np)}\overline{K}^{AB}_{np}}{d^A_0}\left\{\zeta^V_0\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,+}_{AB}\right) + e^{\left(\frac{\hbar\omega_{np}}{K_b T_L}\right)}\zeta^V_0\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,-}_{AB}\right)\right\}, \tag{28}$$

$$q^{(np)}_{AB\,12} = \frac{N^{(np)}\overline{K}^{AB}_{np}}{d^A_0}\left\{\zeta^V_1\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,+}_{AB}\right) + e^{\left(\frac{\hbar\omega_{np}}{K_b T_L}\right)}\zeta^V_1\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,-}_{AB}\right)\right\}, \tag{29}$$

$$q^{(np)}_{AB\,21} = \frac{N^{(np)}\overline{K}^{AB}_{np}}{m^*_A d^A_0}\left\{\zeta^S_1\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,+}_{AB}\right) + e^{\left(\frac{\hbar\omega_{np}}{K_b T_L}\right)}\zeta^S_1\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,-}_{AB}\right)\right\}, \tag{30}$$

$$q^{(np)}_{AB\,22} = \frac{N^{(np)}\overline{K}^{AB}_{np}}{m^*_A d^A_0}\left\{\zeta^S_2\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,+}_{AB}\right) + e^{\left(\frac{\hbar\omega_{np}}{K_b T_L}\right)}\zeta^S_2\left(\lambda^W_A, \alpha_A, \alpha_B, \overline{\mathscr{E}}^{\,-}_{AB}\right)\right\}, \tag{31}$$

$$A \neq B \quad \text{or} \quad A = B = L.$$

The functions ζ^V_k and ζ^S_k are also reported in Appendix A.

6.3 Polar optical phonon scattering

The polar optical phonon collision term reads

$$\mathscr{C}^{(p)}_A[f_A, f_A] \approx \mathscr{C}^{(p)}_A[f^{ME}_A, f^{ME}_A] =$$
$$= \overline{K}^p_A N^{(p)}\left\{R(\mathscr{E}_A, \mathscr{E}_A^{+p}) + S(\mathscr{E}_A, \mathscr{E}_A^{-p}) + \sqrt{\frac{2}{m^*_A}}\, e^i_A\left[R_i(\mathscr{E}_A, \mathscr{E}_A^{+p}) + S_i(\mathscr{E}_A, \mathscr{E}_A^{-p})\right]\right\},$$

where $\overline{K}^p_A = \frac{\sqrt{2}\,(m^*_A)^{\frac{3}{2}}}{\hbar^4}K_p$ and $\mathscr{E}^{\pm p}_A = \mathscr{E}_A \pm \hbar\omega_p$, while the functions R, S, R_i, S_i can be found in Appendix A.

Therefore the production terms for the density, energy, crystal momentum and energy flux are given by

$$C^{(p)}_{n_A} = 0,$$
$$C^{(p)}_{W_A} = \frac{N^{(p)}\overline{K}^p_A}{d^A_0}\, e^{\frac{\lambda_A}{k_B}}\left\{\int_{\overline{\mathscr{E}}^{-p}_A}^{\infty} R(\mathscr{E}_A, \mathscr{E}_A^{+p})\mathscr{E}_A\sqrt{\mathscr{E}_A\left(1 + \alpha_A\,\mathscr{E}_A\right)}\,\left(1 + 2\,\alpha_A\,\mathscr{E}_A\right) d\,\mathscr{E}_A\right.$$
$$\left. + \int_{\overline{\mathscr{E}}^{+p}_A}^{\infty} S(\mathscr{E}_A, \mathscr{E}_A^{-p})\mathscr{E}_A\sqrt{\mathscr{E}_A\left(1 + \alpha_A\,\mathscr{E}_A\right)}\,\left(1 + 2\,\alpha_A\,\mathscr{E}_A\right) d\,\mathscr{E}_A\right\},$$

with $\overline{\mathscr{E}}^{\,\pm p}_A = max(0, \pm\hbar\omega_p)$, and

$$C^{(p)}_{\mathbf{P}_A} = c^{(p)}_{A\,11}(W_A)\mathbf{V}_A + c^{(p)}_{A\,12}(W_A)\mathbf{S}_A, \tag{32}$$

$$C^{(p)}_{\mathbf{S}_A} = c^{(p)}_{A\,21}(W_A)\mathbf{V}_A + c^{(p)}_{A\,22}(W_A)\mathbf{S}_A. \tag{33}$$

As usual the production matrix

$$\hat{C}_A^{(p)} = \begin{pmatrix} c_{A\,11}^{(p)} & c_{A\,12}^{(p)} \\ c_{A\,21}^{(p)} & c_{A\,22}^{(p)} \end{pmatrix}$$

is given by

$$\hat{C}_A^{(p)} = \hat{Q}_A^{(p)} \hat{B}_A,$$

and the components of the matrix $\hat{Q}_A^{(p)}$ by

$$q_{A\,11}^{(p)} = \frac{2}{3} \frac{N^{(p)} \overline{K}_A^p}{d_0^A} \left[\phi_0^{V+} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,-p} \right) + \phi_0^{V-} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,+p} \right) \right], \tag{34}$$

$$q_{A\,12}^{(p)} = \frac{2}{3} \frac{N^{(p)} \overline{K}_A^p}{d_0^A} \left[\phi_1^{V+} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,-p} \right) + \phi_1^{V-} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,+p} \right) \right], \tag{35}$$

$$q_{A\,21}^{(p)} = \frac{2}{3\, m_A^*} \frac{N^{(p)} \overline{K}_A^p}{d_0^A} \left[\phi_0^{S+} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,-p} \right) + \phi_0^{S-} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,+p} \right) \right], \tag{36}$$

$$q_{A\,22}^{(p)} = \frac{2}{3\, m_A^*} \frac{N^{(p)} \overline{K}_A^p}{d_0^A} \left[\phi_1^{S+} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,-p} \right) + \phi_1^{S-} \left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,+p} \right) \right], \tag{37}$$

$$A = \varGamma \text{ and } L\,.$$

The functions $\phi_k^{V\pm}$, and $\phi_k^{S\pm}$ are in Appendix A.

6.4 Scattering with impurities

If we insert f_A^{ME}, $A = \varGamma$, L, into the expression of the collision operator relative to the scattering with impurities, this assumes the relaxation form

$$C_A^{(imp)}[f] \simeq -\frac{1}{\tau_A^{imp}} \left[f_A^{ME}(\mathbf{k}_A) - f_{0A}^{ME}(\mathscr{E}_A) \right],$$

where f_{0A}^{ME} is the isotropic part of f_A^{ME}, $f_{0A}^{ME} = \exp\left(-\frac{\lambda_A}{k_B} - \lambda_A^W \mathscr{E}_A\right)$, and the relaxation times are

$$\tau_A^{imp} = \left(\overline{K}_{imp}^A \right)^{-1} \frac{\mathscr{E}_A^2 \left(1 + \alpha_A \mathscr{E}_A\right)}{\chi(\mathscr{E}_A) \mathscr{N}(\mathscr{E}_A)},$$

with $\overline{K}_{imp}^A = \frac{\hbar}{4\sqrt{2\, m_A^*}} K_{imp}$, $\chi(\mathscr{E}_A) = \log\left[\frac{8\, m_A^*}{\hbar^2 \beta^2} \mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right) + 1 \right] - \frac{\frac{8\, m_A^*}{\hbar^2 \beta^2} \mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right)}{\frac{8\, m_A^*}{\hbar^2 \beta^2} \mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right) + 1}$ and $\mathscr{N}(\mathscr{E}_A) = \sqrt{\mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right)} \left(1 + 2\alpha_A \mathscr{E}_A\right)$, $A = \varGamma$, L.

Such an expression for $C_A^{(imp)}$ is valid also under the more general assumption that the distribution function is weakly anisotropic. We note that, in the parabolic approximation, one recovers the same expression as in [15], (see page 67, formula 2.6.14).

Since this scattering is intravalley and elastic, computing the moments of $C_A^{(imp)}[f^{ME}]$, one gets

$$C_{n_A}^{(imp)} = 0, \qquad C_{W_A}^{(imp)} = 0\,, \tag{38}$$

while the production terms of the crystal momentum and energy flux are respectively given by

$$C_{\mathbf{P}_A}^{(imp)} = c_{A\,11}^{(imp)}(W_A)\mathbf{V}_A + c_{A\,12}^{(imp)}(W_A)\mathbf{S}_A, \tag{39}$$

$$C_{\mathbf{S}_A}^{(imp)} = c_{A\,21}^{(imp)}(W_A)\mathbf{V}_A + c_{A\,22}^{(imp)}(W_A)\mathbf{S}_A. \tag{40}$$

The production matrix

$$\hat{C}_A^{(imp)} = \begin{pmatrix} c_{A\,11}^{(imp)} & c_{A\,12}^{(imp)} \\ c_{A\,21}^{(imp)} & c_{A\,22}^{(imp)} \end{pmatrix}$$

decomposes as

$$\hat{C}_A^{(imp)} = \hat{Q}_A^{(imp)} \hat{B}_A,$$

and the components of the matrix $\hat{Q}_A^{(imp)}$ read

$$q_{A\,11}^{(imp)} = \frac{2\,\overline{K}_{imp}^{A}}{3\,d_0^A} \int_0^\infty \left(1 + 2\,\alpha_A\,\mathscr{E}_A\right)\,\chi(\mathscr{E}_A)\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)\,d\,\mathscr{E}_A, \tag{41}$$

$$q_{A\,12}^{(imp)} = \frac{2\,\overline{K}_{imp}^{A}}{3\,d_0^A} \int_0^\infty \overline{\mathscr{E}}_A\left(1 + 2\,\alpha_A\,\mathscr{E}_A\right)\,\chi(\mathscr{E}_A)\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)\,d\,\mathscr{E}_A, \tag{42}$$

$$q_{A\,21}^{(imp)} = \frac{2\,\overline{K}_{imp}^{A}}{3\,m_A^*\,d_0^A} \int_0^\infty \mathscr{E}_A\,\chi(\mathscr{E}_A)\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)\,d\,\mathscr{E}_A, \tag{43}$$

$$q_{A\,22}^{(imp)} = \frac{2\,\overline{K}_{imp}^{A}}{3\,m_A^*\,d_0^A} \int_0^\infty \mathscr{E}_A^2\,\chi(\mathscr{E}_A)\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)\,d\,\mathscr{E}_A, \tag{44}$$

$$A = \Gamma \text{ and } L\,.$$

7 Applications to the case of bulk GaAs

In this section we test the model in the case of bulk GaAs. The physical situation is represented by a GaAs semiconductor with uniform doping. Two different impurity concentrations, $N_+ = 10^{14}\text{cm}^{-3}$, 10^{17}cm^{-3} are considered, and all the above-mentioned scattering mechanisms are taken into account.

Simulating bulk semiconductors represents a basic preliminary step in the analysis of semiconductor devices. Usually from the results obtained in this case, one figures out the transport coefficients used in hydrodynamical models based on phenomenological assumptions.

From a physical point of view, the main features, common also to other types of semiconductors like silicon, revealed by measurements and MC simulations are the following:

- during the transient period the average velocity overshoots its asymptotic value, that is the value attained in the stationary case. This effect is observed when the applied electric field is increased and it is due to the fact that the velocity relaxation time is smaller than the energy relaxation time;
- by increasing the electric field, the asymptotic value of the velocity (V-E curves) shows a *saturation effect*.

Besides these, other phenomena are present which are typical of GaAs:

- an electron transfer from the Γ-valley to the L-valleys at the increase of the electric field;
- in the V-E curves one observes a decrease of the electron velocity when the electric field overcomes a certain threshold value. Such a phenomenon, known as *negative differential conductivity*, is the consequence of the transfer of electrons from the Γ-valley to the L-valleys, where their effective mass is much larger. It is also observed that at higher impurity concentrations both the low field mobility, the slope of the V-E curves at low fields, and the electron peak velocity decrease.

The parameters that appear in the scatterings rates can be expressed in terms of physical quantities characteristic of the considered material

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

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

$$K_p = \frac{\hbar\omega_p\, q^2}{8\pi^2\hbar}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon}\right),$$

$$K_{imp} = \frac{N_I\, Z^2\, q^4}{4\pi\hbar\,\epsilon^2}, \quad \beta = \left[\frac{q^2\, N_I}{\epsilon\, k_B\, T_L}\right]^{1/2},$$

where Ξ_d is the deformation potential of acoustic phonons, ρ the mass density of the semiconductor, v_s the sound velocity of the longitudinal acoustic mode, D_tK the deformation potential for non-polar optical phonons, ϵ_∞ the dielectric constant at optical frequency range and N_I and $Z\,q$ are respectively the impurity concentration and charge. Among these quantities, the deformation potentials cannot be deduced by means of first principles. In fact the perturbation theory employed to evaluate the transition probabilities is not able to calculate them from the quantum theory of scattering. In all the simulators, even the Monte Carlo ones, these quantities are considered as fitting parameters. Their values depend on the approximation used for the energy bands, on the specific characteristics of the material and on the energy range of interest in the applications.

We have adopted for them the same values as in [19]. For the sake of completeness all the physical parameters are summarized in Table 1.

Table 1. Values of the physical parameters used for GaAs

m_e	electron rest mass	9.1095×10^{-28} g
m^*_Γ	effective electron mass in the Γ-valley	$0.067 \times m_e$
m^*_L	effective electron mass in the L-valley	$0.35 \times m_e$
T_L	lattice temperature	300 K
ρ_0	density	5.360 g/cm^3
v_s	longitudinal sound speed	5.24×10^5 cm/sec
α_Γ	non parabolicity factor in the Γ-valley	0.611 eV^{-1}
α_L	non parabolicity factor in the L-valley	0.242 eV^{-1}
ϵ_r	relative dielectric constant	12.90
ϵ_∞	relative dielectric constant at optical frequency range	10.92
ϵ_0	vacuum dieletric constant	1.24×10^{-22} C^2/(eV cm)
Ξ_d	acoustic-phonon deformation potential	7 eV
D_tK	non-polar optical phonon deformation potential	10^9 eV/cm
$\hbar\omega_{np}$	non-polar optical phonon energy	0.03 eV
$\hbar\omega_p$	polar optical phonon energy	0.03536 eV
$\overline{\mathscr{E}}_\Gamma$	Γ-valley bottom energy	0 eV
$\overline{\mathscr{E}}_L$	L-valley bottom energy	0.32 eV
$Z_{\Gamma L}$	degeneracy from Γ to L valleys	4
$Z_{L\Gamma}$	degeneracy from L to Γ valley	1
Z_{LL}	degeneracy from L to L valleys	3

Concerning the evolution equations, taking into account the symmetry with respect to space translations, we can drop the spatial dependence. Therefore the balance equations reduce to the following set of ordinary differential equations

$$\frac{d}{dt} n_\Gamma = n_L\, C^{(np)+}_{n\ \Gamma L}(W_L) - n_\Gamma\, C^{(np)-}_{n\ \Gamma L}(W_\Gamma), \tag{45}$$

$$m^*_\Gamma \frac{d}{dt} n_\Gamma (V^i_\Gamma + 2\alpha_\Gamma S^i_\Gamma) = -q n_\Gamma E^i + c^\Gamma_{11}\, n_\Gamma V^i_\Gamma + c^\Gamma_{12}\, n_\Gamma S^i_\Gamma, \tag{46}$$

$$\frac{d}{dt} n_\Gamma W_\Gamma = -q n_\Gamma V^k_\Gamma E_k + n_L C^{(np)+}_{W\ \Gamma L}(W_L) + n_\Gamma \left[C^{(p)}_{W_\Gamma}(W_\Gamma) - C^{(np)-}_{W\ \Gamma L}(W_\Gamma) \right], \tag{47}$$

$$\frac{d}{dt} n_\Gamma S^i_\Gamma = -q\, n_\Gamma E_k G^{ik}_\Gamma + c^\Gamma_{21} n_\Gamma V^i_\Gamma + c^\Gamma_{22} n_\Gamma S^i_\Gamma, \tag{48}$$

$$\frac{d}{dt} n_L = -n_L\, C^{(np)-}_{n\ L\Gamma}(W_L) + n_\Gamma\, C^{(np)+}_{n\ L\Gamma}(W_\Gamma), \tag{49}$$

$$m^*_L \frac{d}{dt} n_L (V^i_L + 2\alpha_L S^i_L) = -q n_L E^i + c^L_{11}\, n_L V^i_L + c^L_{12}\, n_L S^i_L, \tag{50}$$

$$\frac{d}{dt} n_L W_L = -q n_L V_L^k E_k + n_\varGamma C^{(np)+}_{W\ L\varGamma}(W_\varGamma) + n_L \Big[C^{(p)}_{W_L}(W_L) + C^{(np)}_{W\ LL}(W_L) \\ - C^{(np)-}_{W\ L\varGamma}(W_L) \Big] , \qquad (51)$$

$$\frac{d}{dt} n_L S_L^i = -q\, n_L E_k G_L^{ik} + c_{21}^L n_L V_L^i + c_{22}^L n_L S_L^i , \qquad (52)$$

where

$$c_{ij}^A = c^{(ac)}_{A\,ij}(W_A) + c^{(np)}_{A\,ij}(W_A) + c^{(p)}_{A\,ij}(W_A) + c^{(imp)}_{A\,ij}(W_A) \quad A = \varGamma\,, L\,.$$

From (45), (49) and the expressions of the production terms, one has that $n = n_\varGamma + 4\, n_L = \text{const}$, so that the total electron number is conserved, as it must be. In cases when a constant bias voltage is applied to the semiconductor, the Poisson equation $(3)_2$ is satisfied with n equal to the value of the doping concentration and **E** constant. The motion is along the direction of the electric field and, if we take this as the x-direction, the system (45)-(52) reads

$$\frac{d}{dt} n_\varGamma = n_L\, C^{(np)+}_{n\ \varGamma L}(W_L) - n_\varGamma\, C^{(np)-}_{n\ \varGamma L}(W_\varGamma), \qquad (53)$$

$$\frac{d}{dt} n_\varGamma V_\varGamma = \left(2\alpha_\varGamma G_\varGamma - \frac{1}{m_\varGamma^*} \right) q\, E\, n_\varGamma + \left(\frac{c_{11}^\varGamma}{m_\varGamma^*} - 2\,\alpha_\varGamma\, c_{21}^\varGamma \right) n_\varGamma V_\varGamma + \\ + \left(\frac{c_{12}^\varGamma}{m_\varGamma^*} - 2\,\alpha_\varGamma\, c_{22}^\varGamma \right) n_\varGamma S_\varGamma , \qquad (54)$$

$$\frac{d}{dt} n_\varGamma W_\varGamma = -q n_\varGamma V_\varGamma E + n_L C^{(np)+}_{W\ \varGamma L}(W_L) + n_\varGamma \Big[C^{(p)}_{W_\varGamma}(W_\varGamma) - C^{(np)-}_{W\ \varGamma L}(W_\varGamma) \Big] , \qquad (55)$$

$$\frac{d}{dt} n_\varGamma S_\varGamma = -q\, n_\varGamma E\, G_\varGamma + c_{21}^\varGamma n_\varGamma V_\varGamma + c_{22}^\varGamma n_\varGamma S_\varGamma , \qquad (56)$$

$$\frac{d}{dt}\, (n_\varGamma + 4\, n_L) = 0, \qquad (57)$$

$$\frac{d}{dt} n_L V_L = \left(2\alpha_L G_L - \frac{1}{m_L^*} \right) q\, E\, n_L + \left(\frac{c_{11}^L}{m_L^*} - 2\,\alpha_L\, c_{21}^L \right) n_L V_L + \\ + \left(\frac{c_{12}^L}{m_L^*} - 2\,\alpha_L\, c_{22}^L \right) n_L S_L , \qquad (58)$$

$$\frac{d}{dt} n_L W_L = -q n_L V_L E + n_\varGamma C^{(np)+}_{W\ L\varGamma}(W_\varGamma) + n_L \Big[C^{(p)}_{W_L}(W_L) + C^{(np)}_{W\ LL}(W_L) \\ - C^{(np)-}_{W\ L\varGamma}(W_L) \Big] , \qquad (59)$$

$$\frac{d}{dt} n_L S_L = -q\, n_L E\, G_L + c_{21}^L n_L V_L + c_{22}^L n_L S_L\, , \qquad (60)$$

where V_A and S_A are the x-components of $\mathbf{V}_A$ and $\mathbf{S}_A$ and G_A is the xx-component of G_A^{ij}, $A = \varGamma,\ L$. In the evolution equations the x-component E of the electric field enters as a parameter.

As initial conditions for (53)-(60), we take, in suitable units,

$$\begin{array}{rcl} n_\varGamma(0) + 4\, n_L(0) & = & 1, \\ \dfrac{n_\varGamma(0)}{n_L(0)} & = & \dfrac{\int_{\Re^3} f_\varGamma^{(eq)} d\mathbf{k}_\varGamma}{\int_{\Re^3} f_L^{(eq)} d\mathbf{k}_L} = \left(\dfrac{m_\varGamma^*}{m_L^*} \right)^{3/2} \dfrac{d_0^\varGamma(\frac{1}{k_B T_L})}{d_0^L(\frac{1}{k_B T_L})}, \\ V_A(0) & = & 0, \\ W_A(0) & = & g_A \left(\dfrac{1}{k_B T_L} \right), \\ S_A(0) & = & 0, \qquad\qquad\qquad\qquad A = \varGamma\,, L\,. \end{array}$$

The crystal temperature, T_L, is assumed to be 300 K.

The solutions of (53)-(60) for electric fields respectively equal to $0.2, 0.5, 1, 2$ and $6\,\frac{V}{\mu m}$, are reported in Fig. 4. The stationary regime is reached in a few picoseconds.

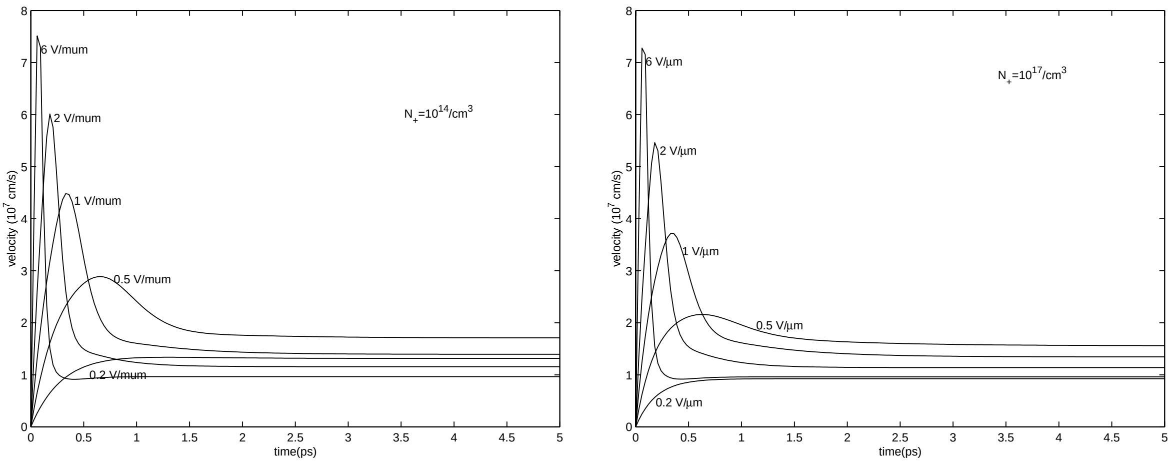

Fig. 4. The time evolution of the electron average velocity for different values of the electric field and for $N_+ = 10^{14}/\text{cm}^3$ and $10^{17}/\text{cm}^3$ respectively

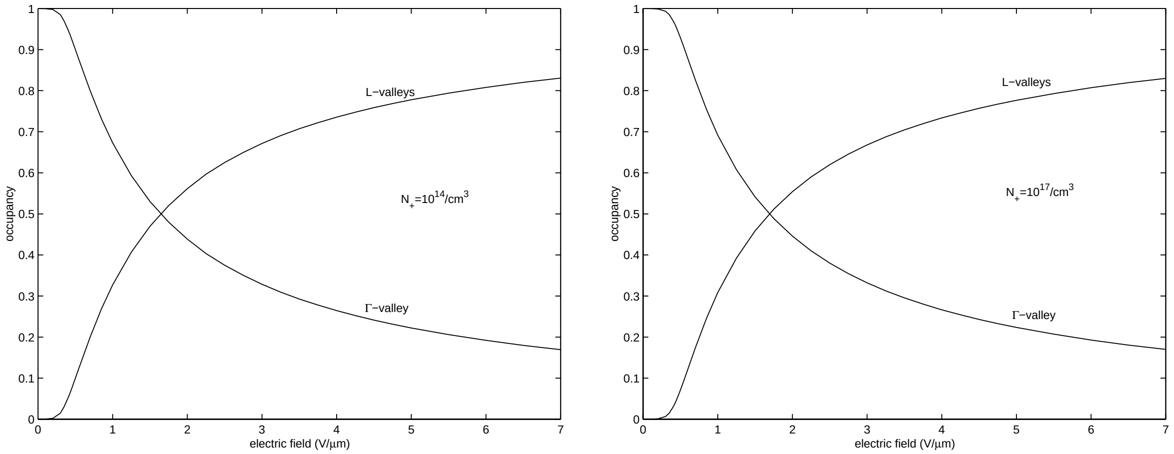

Fig. 5. Electron occupancy in the Γ- and L-valleys for $N_+ = 10^{14}/\text{cm}^3$ and $10^{17}/\text{cm}^3$ respectively

The typical phenomena of overshoot and saturation of the velocity are both qualitatively and quantitatively well described, see [19] page 111, Fig. 3.23 for a comparison with results obtained by MC simulations. We also report the curves representing the electron valley occupancy, $\frac{n_\Gamma}{n_\Gamma + 4n_L}$ and $\frac{4n_L}{n_\Gamma + 4n_L}$, and average velocity as functions of the electric field (see Figs. 5 and 6) for the above impurity concentrations. Figure 5 clearly shows the electron transfer from the Γ-valley to the L-valleys. The population inversion is observed at electric fields of about $1.8V/\mu m$.

Figure 6 shows that the low field mobility and the electron peak velocity decrease with the increase of the impurity concentration, see [19] Figs. 3.16 and 3.17 for a comparison with results obtained by MC simulations.

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Appendix A

In this Appendix we report some functions entering into the expressions of the scattering mechanisms we have taken into account.

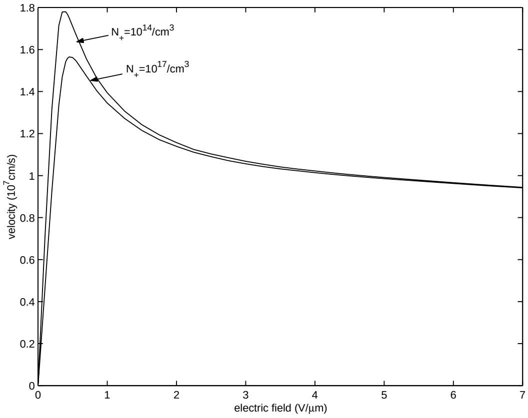

Fig. 6. Electron velocity versus electric field characteristics for $N_+ = 10^{14}/\mathrm{cm}^3$ and $10^{17}/\mathrm{cm}^3$ respectively

Table 2. Values of $\overline{\mathscr{E}}^{\,\pm}_{AB}$

		absorption	emission
initial valley	final valley	$\overline{\mathscr{E}}^{\,+}_{AB}$	$\overline{\mathscr{E}}^{\,-}_{AB}$
Γ	L	$\overline{\mathscr{E}}_L - \hbar\omega_{np}$	$\overline{\mathscr{E}}_L + \hbar\omega_{np}$
L	Γ	0	0
L	L	0	$\hbar\omega_{np}$

In the production terms relative to the non-polar optical phonon scattering the following functions appear (the values of $\overline{\mathscr{E}}^{\,\pm}_{AB}$ are given in Table 2 for each different type of interaction)

$$\begin{aligned}\eta_k^{\pm}\left(\lambda_C^W,\alpha_A,\alpha_B,\overline{\mathscr{E}}^{\,\pm}_{AB}\right) &= \int_{\overline{\mathscr{E}}^{\,\pm}_{AB}}^{\infty} \mathscr{E}_A^k\left[\mathscr{E}_A\left(1+\alpha_A\,\mathscr{E}_A\right)\right]^{1/2}\left(1+2\alpha_A\,\mathscr{E}_A\right)\left[\mathscr{E}_A^{\pm}\left(1+\alpha_B\,\mathscr{E}_A^{\pm}\right)\right]^{1/2}\\ &\qquad \left(1+2\alpha_B\,\mathscr{E}_A^{\pm}\right)\exp\left(-\lambda_C^W\,\mathscr{E}_A\right)d\,\mathscr{E}_A,\end{aligned}$$

$$\begin{aligned}\zeta_k^V\left(\lambda_A^W,\alpha_A,\alpha_B,\overline{\mathscr{E}}^{\,\pm}_{AB}\right) &= \int_{\overline{\mathscr{E}}^{\,\pm}_{AB}}^{\infty} \mathscr{E}_A^k\left[\mathscr{E}_A\left(1+\alpha_A\,\mathscr{E}_A\right)\right]^{3/2}\left[\mathscr{E}_A^{\pm}\left(1+\alpha_B\,\mathscr{E}_A^{\pm}\right)\right]^{1/2}\\ &\qquad \left(1+2\alpha_B\,\mathscr{E}_A^{\pm}\right)\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)d\,\mathscr{E}_A,\\ \zeta_k^S\left(\lambda_A^W,\alpha_A,\alpha_B,\overline{\mathscr{E}}^{\,\pm}_{AB}\right) &= \int_{\overline{\mathscr{E}}^{\,\pm}_{AB}}^{\infty} \mathscr{E}_A^k\left[\mathscr{E}_A^{\pm}\left(1+\alpha_B\,\mathscr{E}_A^{\pm}\right)\right]^{1/2}\frac{\left(1+2\alpha_B\,\mathscr{E}_A^{\pm}\right)}{1+2\,\alpha_A\,\mathscr{E}_A}\left[\mathscr{E}_A\,(1+\right.\\ &\qquad \left.+\alpha_A\,\mathscr{E}_A)\right]^{3/2}\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)d\,\mathscr{E}_A.\end{aligned}$$

As regards the polar optical scattering, we have [4]

$$\begin{aligned}R(\mathscr{E}_A,\mathscr{E}_A^+) &= g_0(\mathscr{E}_A,\mathscr{E}_A^+)\mathscr{N}\left(\mathscr{E}_A^+\right)e^{-\frac{\lambda_A}{k_B}}\left\{\exp\left(\frac{\hbar\omega_p}{k_BT_L}\right)\exp\left(-\lambda_A^W\,\mathscr{E}_A^+\right)-\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)\right\},\\ S(\mathscr{E}_A,\mathscr{E}_A^-) &= g_0(\mathscr{E}_A,\mathscr{E}_A^-)\mathscr{N}\left(\mathscr{E}_A^-\right)e^{-\frac{\lambda_A}{k_B}}\left\{\exp\left(-\lambda_A^W\,\mathscr{E}_A^-\right)-\exp\left(\frac{\hbar\omega_p}{k_BT_L}\right)\exp\left(-\lambda_A^W\,\mathscr{E}_A\right)\right\},\\ R_i(\mathscr{E}_A,\mathscr{E}_A^+) &= \mathscr{N}(\mathscr{E}_A^+)\left\{\exp\left(\frac{\hbar\omega_p}{k_BT_L}\right)\frac{\left[\mathscr{E}_A^+\left(1+\alpha_A\mathscr{E}_A^+\right)\right]^{1/2}}{1+2\alpha_A\mathscr{E}_A^+}g_1(\mathscr{E}_A,\mathscr{E}_A^+)f_{A\,i}(\mathscr{E}_A^+)+\right.\\ &\qquad \left.-\frac{\left[\mathscr{E}_A\left(1+\alpha_A\mathscr{E}_A\right)\right]^{1/2}}{1+2\alpha_A\mathscr{E}_A}g_0(\mathscr{E}_A,\mathscr{E}_A^+)f_{A\,i}(\mathscr{E}_A)\right\},\end{aligned}$$

---

[4] For simplicity, we have omitted the superscript p in $\mathscr{E}_A^{\pm(p)}$ and $\mathscr{E}_{A(0)}^{\pm(p)}$.

$$
\begin{aligned}
S_i(\mathscr{E}_A, \mathscr{E}_A^-) \quad = \quad & \mathscr{N}(\mathscr{E}_A^-) \left\{ \frac{\left[\mathscr{E}_A^- \left(1 + \alpha_A \mathscr{E}_A^-\right)\right]^{1/2}}{1 + 2\alpha_A \mathscr{E}_A^-} \, g_1(\mathscr{E}_A, \mathscr{E}_A^-) f_{A\,i}(\mathscr{E}_A^-) + \right. \\
& \left. - \exp\left(\frac{\hbar\omega_p}{k_B T_L}\right) \frac{\left[\mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right)\right]^{1/2}}{1 + 2\alpha_A \mathscr{E}_A} \, g_0(\mathscr{E}_A, \mathscr{E}_A^-) f_{A\,i}(\mathscr{E}_A) \right\},
\end{aligned}
$$

with

$$
\begin{aligned}
\mathscr{N}\left(\mathscr{E}_A\right) &= \sqrt{\mathscr{E}_A(1 + \alpha_A \mathscr{E}_A)}(1 + 2\alpha_A \mathscr{E}_A), \\
f_{A\,i}(\mathscr{E}_A) &= -\exp(-\frac{\lambda_A}{k_B} - \lambda_A^W \, \mathscr{E}_A) \left[\lambda_A^{V_i} + \mathscr{E}_A \lambda_A^{S_i}\right]
\end{aligned}
$$

and

$$
\begin{aligned}
g_0(x_A, y_A) \;=\; & 2\,\pi \left\{ \left[\frac{a(x_A, y_A)}{\delta(x_A, y_A)} - \frac{b(x_A, y_A)\,\lambda(x_A, y_A)}{\delta(x_A, y_A)^2} + \frac{c(x_A, y_A)\,\lambda(x_A, y_A)^2}{\delta(x_A, y_A)^3} \right] \right. \\
& \left. \times \log \frac{\lambda(x_A, y_A) + \delta(x_A, y_A)}{\lambda(x_A, y_A) - \delta(x_A, y_A)} + \frac{2\,b(x_A, y_A)}{\delta(x_A, y_A)} - \frac{2\,c(x_A, y_A)\,\lambda(x_A, y_A)}{\delta(x_A, y_A)^2} \right\}, \\
g_1(x_A, y_A) \;=\; & 2\,\pi \left\{ a(x_A, y_A) \left[\frac{2}{\delta(x_A, y_A)} + \frac{\lambda(x_A, y_A)}{\delta(x_A, y_A)^2} \log \frac{\lambda(x_A, y_A) - \delta(x_A, y_A)}{\lambda(x_A, y_A) + \delta(x_A, y_A)} \right] \right. \\
& + \frac{b(x_A, y_A)\lambda(x_A, y_A)}{\delta(x_A, y_A)^3} \left[\lambda(x_A, y_A) \log \frac{\lambda(x_A, y_A) + \delta(x_A, y_A)}{\lambda(x_A, y_A) - \delta(x_A, y_A)} - 2\delta(x_A, y_A) \right] \\
& + \frac{c(x_A, y_A)}{\delta(x_A, y_A)^4} \left[\frac{2}{3} \delta(x_A, y_A)^3 + 2\lambda(x_A, y_A)^2 \delta(x_A, y_A) \right. \\
& \left. \left. + \lambda(x_A, y_A)^3 \log \frac{\lambda(x_A, y_A) - \delta(x_A, y_A)}{\lambda(x_A, y_A) + \delta(x_A, y_A)} \right] \right\},
\end{aligned}
$$

where

$$
\begin{aligned}
a(x_A, y_A) &= \frac{(1 + \alpha_A x_A)(1 + \alpha_A y_A)}{(1 + 2\alpha_A x_A)(1 + 2\alpha_A y_A)}, \\
b(x_A, y_A) &= \frac{2\,\alpha_A \left[x_A\, y_A (1 + \alpha_A x_A)(1 + \alpha_A y_A)\right]^{1/2}}{(1 + 2\alpha_A x_A)(1 + 2\alpha_A y_A)}, \\
c(x_A, y_A) &= \frac{\alpha_A^2\, x_A\, y_A}{(1 + 2\alpha_A x_A)(1 + 2\alpha_A y_A)}, \\
\lambda(x_A, y_A) &= \frac{2\, m_A^*}{\hbar^2} \left[x_A(1 + \alpha_A x_A) + y_A(1 + \alpha_A y_A)\right], \\
\delta(x_A, y_A) &= -\frac{4\, m_A^*}{\hbar^2} \left[x_A\, y_A (1 + \alpha_A x_A)(1 + \alpha_A y_A)\right]^{1/2} .
\end{aligned}
$$

In the end, we have

$$
\begin{aligned}
\phi_k^{V+}\left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,-}\right) \;=\; & \int_{\overline{\mathscr{E}}_A^{\,-}}^{\infty} \mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right) \left(1 + 2\,\alpha_A \mathscr{E}_A\right) \mathscr{N}\left(\mathscr{E}_A^+\right) \left\{ \mathscr{E}_A^k \frac{\left[\mathscr{E}_A(1 + \alpha_A \mathscr{E}_A)\right]^{1/2}}{1 + 2\,\alpha_A \mathscr{E}_A} \right. \\
& \times g_0\left(\mathscr{E}_A, \mathscr{E}_A^+\right) \exp\left(-\lambda^{W_A} \, \mathscr{E}_A\right) - \exp\left(\frac{\hbar\omega_p}{k_B\, T_L}\right) \left(\mathscr{E}_A^+\right)^k \\
& \left. \times \frac{\left[\mathscr{E}_A^+(1 + \alpha_A \mathscr{E}_A^+)\right]^{1/2}}{1 + 2\,\alpha_A \mathscr{E}_A^+} \, g_1\left(\mathscr{E}_A, \mathscr{E}_A^+\right) \exp\left(-\lambda_A^W \, \mathscr{E}_A^+\right) \right\} d\,\mathscr{E}_A, \\
\phi_k^{V-}\left(\lambda_A^W, \overline{\mathscr{E}}_A^{\,+}\right) \;=\; & \int_{\overline{\mathscr{E}}_A^{\,+}}^{\infty} \mathscr{E}_A \left(1 + \alpha_A \mathscr{E}_A\right) \left(1 + 2\,\alpha_A \mathscr{E}_A\right) \mathscr{N}\left(\mathscr{E}_A^-\right) \left\{ \mathscr{E}_A^k \frac{\left[\mathscr{E}_A(1 + \alpha_A \mathscr{E}_A)\right]^{1/2}}{1 + 2\,\alpha_A \mathscr{E}_A} \right.
\end{aligned}
$$

$$
\times g_0\left(\mathcal{E}_A, \mathcal{E}_A^-\right) \exp\left(\frac{\hbar\omega_p}{k_B\, T_L}\right) \exp\left(-\lambda_A^W\, \mathcal{E}_A\right) - \left(\mathcal{E}_A^-\right)^k
\times \frac{\left[\mathcal{E}_A^-(1+\alpha_A\mathcal{E}_A^-)\right]^{1/2}}{1+2\,\alpha_A\mathcal{E}_A^-}\, g_1\left(\mathcal{E}_A, \mathcal{E}_A^-\right) \exp\left(-\lambda_A^W\, \mathcal{E}_A^-\right)\Big\}\, d\,\mathcal{E}_A
$$

and

$$
\begin{aligned}
\phi_k^{S+}\left(\lambda_A^W, \mathcal{E}_{A(0)}^-\right) = & \int_{\overline{\mathcal{E}}_A^{\,-}}^{\infty} \mathcal{E}_A^2\left(1+\alpha_A\mathcal{E}_A\right)\mathcal{N}\left(\mathcal{E}_A^+\right)\Bigg\{\mathcal{E}_A^k\,\frac{\left[\mathcal{E}_A(1+\alpha_A\mathcal{E}_A)\right]^{1/2}}{1+2\,\alpha_A\mathcal{E}_A} \\
& \times g_0\left(\mathcal{E}_A, \mathcal{E}_A^+\right)\exp\left(-\lambda_A^W\,\mathcal{E}_A\right) - \exp\left(\frac{\hbar\omega_p}{k_B\,T_L}\right)\left(\mathcal{E}_A^+\right)^k \\
& \times \frac{\left[\mathcal{E}_A^+(1+\alpha_A\mathcal{E}_A^+)\right]^{1/2}}{1+2\,\alpha_A\mathcal{E}_A^+}\, g_1\left(\mathcal{E}_A, \mathcal{E}_A^+\right)\exp\left(-\lambda_A^W\,\mathcal{E}_A^+\right)\Big\}\, d\,\mathcal{E}_A, \\
\phi_k^{S-}\left(\lambda_A^W, \mathcal{E}_{A(0)}^+\right) = & \int_{\overline{\mathcal{E}}_A^{\,+}}^{\infty} \mathcal{E}_A^2\left(1+\alpha_A\mathcal{E}_A\right)\mathcal{N}\left(\mathcal{E}_A^-\right)\Bigg\{\mathcal{E}_A^k\,\frac{\left[\mathcal{E}_A(1+\alpha_A\mathcal{E}_A)\right]^{1/2}}{1+2\,\alpha_A\mathcal{E}_A} \\
& \times g_0\left(\mathcal{E}_A, \mathcal{E}_A^-\right)\exp\left(\frac{\hbar\omega_p}{k_B\,T_L}\right)\exp\left(-\lambda_A^W\,\mathcal{E}_A\right) - \left(\mathcal{E}_A^-\right)^k \\
& \times \frac{\left[\mathcal{E}_A^-(1+\alpha_A\mathcal{E}_A^-)\right]^{1/2}}{1+2\,\alpha_A\mathcal{E}_A^-}\, g_1\left(\mathcal{E}_A, \mathcal{E}_A^-\right)\exp\left(-\lambda_A^W\,\mathcal{E}_A^-\right)\Big\}\, d\,\mathcal{E}_A.
\end{aligned}
$$

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