Comparison of spherical harmonics and moment equations for electrons in semiconductors

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Abstract

The semiclassical Boltzmann equation for electrons in semiconductors is considered together with the parabolic band approximation and interaction terms for elastic scattering with acoustic phonons and inelastic scattering with optical phonons.
Taking only scalar and vectorial moments into account, two sets of equations are derived from the Boltzmann equation: spherical harmonics equations and equations for full moments.
The equations are solved for two simple processes in an infinite semiconductor in a homogeneous electric field. The results show that both moment systems agree, if the number of full moments exceeds the usual choice of hydrodynamical models. .
Keywords: Electron transport, Boltzmann equation, Spherical harmonics, Moments

1 Introduction

Moment equations derived from the electron Boltzmann equation are an important tool in semiconductor physics, owing to the fact that the computing times for their numerical solution are much smaller than for the Boltzmann equation.

The best known example for the moment method is the hydrodynamic model [1][2][3]. The moment equations contain transport coefficients and relaxation times which are typically fitted to Monte Carlo simulations of some simple processes [4].

This paper deals with two moment systems which have been presented and analyzed recently by Liotta and Majorana [5] and Struchtrup [6] and we compare their results for simple homogeneous processes.

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The energy-kinetic equations of [5] correspond to a spherical harmonics expansion with two moments [7][8][9] [10] - a scalar and a vector integral of the electron phase density with respect to the electrons directions which are functions of space-time and the electron energy.

The energy-kinetic equations are confronted with a set of equations for an arbitrary number of full moments, where only scalar and vectorial functions are considered. The full moments are integrals of the phase density with respect to the electron momentum, i.e. functions of space-time only.

In the system of full moments all relaxation times and transport coefficients are computed directly from the collision term of the Boltzmann equation. Thus, in opposition to usual hydrodynamic models [1][2][4], there are no free parameters for the fitting to Monte Carlo data. Moreover, the full collision operator is considered and not a relaxation time approach[1][4]. As will be seen, all moment equations are coupled through explicit matrices of mean collision frequencies. Due to this coupling the results for all moments depend on the number of moments chosen; in particular the results for electron density, energy and drift velocity will change with the number of moments.

Therefore the most important question in the use of moment systems is, how many moments are needed to describe the physics of a problem accurately, in the sense that the moment equations give a result close to a solution of the Boltzmann equation. In the present paper we accept the choice of only two spherical harmonics moments without asking whether this is a good approximation for the Boltzmann equation. In fact, we consider the results of the spherical harmonics as a benchmark for the full moments and ask how many full moments - scalar and vectorial - are needed to reproduce the results of the spherical harmonics equations.

As test problems we consider an infinite semiconductor in a homogeneous electric field, both in the transient and the stationary case where we compare the results for the drift velocity. Both moment systems give the same results, if the number of full moments exceeds the usual choice of hydrodynamic models.

Our examination is based on a simplified physical picture of the semiconductor, i.e. the parabolic band approximation with interaction terms for collisions of electrons with acoustical and optical phonons [11] [12]. This simplified description, although inaccurate for high electric fields, describes all interesting features of electron transport in semiconductors, e.g. velocity saturation and overshoot.

In the present paper we want to test whether a full moment method is capable of giving results in accordance to those of the spherical harmonics method. Thus, the emphasis of the paper lies on the influence of the moment number on the results and not on the physics. We think that it is appropriate to start with the simplified picture in this first study of multi-moment methods for electrons.

This present paper is a shortened version of [13].

2 Boltzmann equation for parabolic bands

The basic quantity in the kinetic theory of electron transport is the phase density f, defined such that $fd\mathbf{x}d\mathbf{c}$ gives the number of electrons in the space element $d\mathbf{x}$ with velocities in the element $d\mathbf{c}$ at time t. The phase density is governed by the Boltzmann equation which reads [14][6]

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} - \frac{e}{m} E_k \frac{\partial f}{\partial c_k} = Q_{ac} + Q_{op} \tag{1}$$

where e is the elementary charge, E_k denotes the electric field and m denotes the effective mass which differs from the electron mass m_e; for silicon we have $m = 0.32 m_e = 2.915\ 10^{-31} kg$. Here and in the following summation is understood for two equal Cartesian indices in a term.

The collision terms Q_{ac}, Q_{op} describe the collisions with acoustical and optical phonons respectively. We have [11][6]

$$Q_{ac} = -\mathcal{A} c \left[f - \frac{1}{4\pi} \int f d\Omega \right] ,$$

$$Q_{op} = -\mathcal{B} \left\{ \sqrt{c^2 + \chi} \left[f - \frac{e^{\frac{\theta}{T_0}}}{4\pi} \int f^{(+)} d\Omega \right] + \sqrt{(c^2 - \chi)_{|+}} \left[e^{\frac{\theta}{T_0}} f - \frac{1}{4\pi} \int f^{(-)} d\Omega \right] \right\} ,$$

where the abbreviations stand for

$$\mathcal{A} = \frac{1}{\pi} \frac{m^2 k_B \mathcal{E}_l^2}{\hbar^4 \varrho U_l^2} T_0 \quad , \quad \mathcal{B} = \frac{1}{2\pi} \frac{m^2 \left(D_t K\right)^2}{\hbar^2 \varrho k_B \theta} \frac{1}{\exp \frac{\theta}{T_0} - 1} \quad , \quad \chi = \frac{2\hbar\omega}{m} = \frac{2 k_B \theta}{m}$$

$$f^{(\pm)} = f\left(\sqrt{c^2 \pm \chi}, n_i \right) \quad , \quad \sqrt{(c^2 - \chi)_{|+}} = \begin{cases} \sqrt{(c^2 - \chi)_{|+}} & , \ c^2 \geq \chi \\ 0 & \ c^2 < \chi \end{cases}$$

$\mathcal{E}_l = 9\, eV$ is a deformation potential, $\varrho = 2330\, kg/m^3$ is the crystal density and $U_l = 9040\, m/s$ is the longitudinal sound speed. Moreover, $D_t K = 11.4\ 10^{10} \frac{eV}{m}$ is another deformation potential, $\hbar\omega = 0.063 eV$ is the energy of optical phonons and $\theta = \hbar\omega / k_B$ is an equivalent temperature. All values are for silicon [12]. T_0 denotes the temperature of the lattice which is assumed to be constant in the context of this paper. For the examples we chose $T_0 = 300K$. Finally k_B and $\hbar$ are Boltzmann's and Planck's constants, respectively, and $d\Omega$ denotes the element of solid angle.

In equilibrium - where the production terms vanish - the phase density is a Maxwellian,

$$f_{|E} = n \sqrt{\frac{m}{2\pi k_B T_0}}^3 e^{-\frac{m}{2 k_b T_0} c^2} . \tag{2}$$

$n = \int f d\mathbf{c}$ denotes the number density of electrons.

3 Spherical harmonics

Spherical harmonics moments are moments of the phase density with respect to the direction vector $n_i = c_i/c = \{\sin\vartheta\sin\varphi, \sin\vartheta\cos\varphi, \cos\vartheta\}$ defined as

$$u_{\langle i_1 i_2 \cdots i_n\rangle} = \int n_{\langle i_1} n_{i_2} \cdots n_{i_n\rangle} f d\Omega \tag{3}$$

where the brackets denote a symmetric trace-free tensor, see [6] for details. With the moments (3) we can write the phase density as an infinite series

$$f = \sum_{n=0}^{\infty} \frac{(2n+1)!!}{4\pi n!} u_{\langle i_1 i_2 \cdots i_n\rangle} n_{\langle i_1} n_{i_2} \cdots n_{i_n\rangle} \ . \tag{4}$$

In practice, one considers not an infinite series, but only the first terms of (4) and in the present paper we shall consider only the first two terms and set all higher terms equal to zero. This choice is appropriate when the elastic scattering dominates, so that the phase density is almost isotropic [7][6][10].

The spherical harmonics are functions of space x_i, time t and the absolute electron speed c. The spherical harmonics moments of the Maxwellian (2) are

$$u_{|E} = \frac{4}{\sqrt{\pi}} n \sqrt{\frac{m}{2k_B T_0}}^{3} e^{-\frac{m}{2k_B T_0}c^2} \quad , \quad u_{\langle i_1 i_2 \cdots i_n\rangle|E} = 0 \tag{5}$$

The equations for the spherical harmonics follow by multiplication of the Boltzmann equation with $n_{\langle i_1} n_{i_2} \cdots n_{i_n\rangle}$ and subsequent integration over all directions. For the first two moments we find the equations

$$\begin{aligned} \frac{\partial u}{\partial t} + c\frac{\partial u_k}{\partial x_k} - \frac{e}{m}E_k \frac{1}{c^2}\frac{\partial}{\partial c}\left[c^2 u_k\right] = -\mathcal{B}\Big\{ & \sqrt{c^2+\chi}\left[u - e^{\theta/T_0} u\left(\sqrt{c^2+\chi}\right)\right] + \\ & \sqrt{(c^2-\chi)_{|+}}\left[e^{\theta/T_0} u - u\left(\sqrt{c^2-\chi}\right)\right]\Big\} \\ \frac{\partial u_i}{\partial t} + \frac{1}{3}c\frac{\partial u}{\partial x_i} - \frac{1}{3}\frac{e}{m}E_i \frac{\partial u}{\partial c} = -\Big\{\mathcal{A}c + \mathcal{B} & \left[\sqrt{c^2+\chi} + e^{\theta/T_0}\sqrt{(c^2-\chi)_{|+}}\right]\Big\} u_i \end{aligned} \tag{6}$$

These are the spherical harmonics equations for the model of Section 2, see [5] and – for the stationary case – [7][8][9].

4 Full Moments

Next, we consider full moments of the phase density, and also here we restrict ourselves to scalar and vectorial moments. Thus, the full moments under consideration are [6]

$$\varrho^r = m\int c^{2r} f d\mathbf{c} = m\int c^{2r+2} u dc \ , \quad \varrho_i^r = m\int c^{2r} c_i f d\mathbf{c} = m\int c^{2r+3} u_i dc \ , \tag{7}$$

$r = 0, 1, \ldots, R$, with an arbitrary number R. Our interest in the remainder of the paper lies in the question, which number R one has to chose in order to retain the physical contents of the energy-kinetic equations (6).

Among the set (7), we have the number density n, the electron temperature T, the drift-velocity v_i and the energy flux q_i by

$$n = \frac{\varrho^0}{m} \quad , \quad \frac{3}{2}\varrho^0 \frac{k_B}{m} T = \frac{1}{2}\varrho^1 \quad , \quad \varrho^0 v_i = \varrho_i^0 \quad , \quad q_i = \frac{1}{2}\varrho_i^1 \, .$$

Note, that the second equation *defines* the electron temperature. The usual choice of variables for hydrodynamic models consists in these 8 moments plus the deviator of the pressure tensor $\varrho_{\langle ij \rangle} = m \int c_{\langle i} c_{j \rangle} f d\mathbf{c} = m \int c^4 u_{\langle ij \rangle} f dc$ [1][4][15]. The latter is not considered here due to the neglect of the higher spherical harmonics [6]. Thus, for $R = 1$, our equations below correspond to hydrodynamic models. We emphasize again that we shall consider the full collision term so that there are no fitting parameters in our model.

The equations for the full moments follow by multiplication of the Boltzmann equation with mc^{2r} and $mc^{2r} c_i$, respectively, and subsequent integration. These equations do not form a closed set for the variables (7), but contain additional quantities. In order to express these through the variables, we need a closure assumption, i.e. an expression for the phase density as a function of the variables. Here, we choose a Grad type function [16][17]

$$f = f_{|T} \left[1 - \sum_{s=0}^{R} \lambda^s c^{2s} - \sum_{s=0}^{R} \lambda_i^s c^{2s} c_i \right] \quad \text{with} \quad f_{|T} = n \sqrt{\frac{m}{2\pi k_B T}}^3 \exp\left[-\frac{m}{2k_B T} c^2 \right] \, , \tag{8}$$

see [6] for a discussion.

Note that the closure problem for the full moments is more involved than for the spherical harmonics where the closure consists simply in setting all higher spherical harmonics equal to zero.

The expansion coefficients λ, λ_i in (8) follow from (7) by inversion as functions of the moments,

$$\lambda^t = -\frac{\sqrt{\pi}}{2} \sum_{s=2}^{R} \mathcal{C}_{ts}^{-1} \frac{\varrho^s - \varrho_{|T}^s}{\varrho^0 \left(\frac{2k_B T}{m} \right)^{s+t}} \quad , \quad \lambda_i^t = -\frac{3\sqrt{\pi}}{2} \sum_{s=0}^{R} \hat{\mathcal{C}}_{ts}^{-1} \frac{\varrho_i^s}{\varrho^0 \left(\frac{2k_B T}{m} \right)^{s+t+1}} \tag{9}$$

with

$$\varrho_{|T}^r = \varrho^0 \left(\frac{2k_B T}{m} \right)^r \frac{2}{\sqrt{\pi}} \Gamma\left(r + \frac{3}{2} \right) \quad , \quad \mathcal{C}_{rs} = \Gamma\left(r + s + \frac{3}{2} \right) \quad , \quad \hat{\mathcal{C}}_{rs} = \Gamma\left(r + s + \frac{5}{2} \right) \, . \tag{10}$$

$u_{|T}^r$ are the moments of $f_{|T}$ with $u_{|T}^0 = u^0$ and $u_{|T}^1 = u^1$; $\Gamma(r)$ denotes the gamma function.

It is an easy task to compute the spherical harmonics moments of the phase density (8) as

$$u = \int f d\Omega = 4\pi f_{|T} \left(1 - \sum\nolimits_{s=0}^{R} \lambda^s c^{2s} \right) \quad , \quad u_i = \int n_i f d\Omega = -\frac{4\pi}{3} f_{|T} \sum\nolimits_{s=0}^{R} \lambda_i^s c^{2s+1} \, . \tag{11}$$

With the phase density (8) we obtain from the Boltzmann equation a closed set of equations for the moments (7),

$$\frac{\partial \varrho^r}{\partial t} + \frac{\partial \varrho^r_k}{\partial x_k} + 2r\frac{e}{m}E_k\varrho^{r-1}_k = -\Pi^r - \sum_{s=2}^{R}\Theta_{rs}\left(\varrho^s - \varrho^s_{|T}\right)$$

$$\frac{\partial \varrho^r_i}{\partial t} + \frac{1}{3}\frac{\partial \varrho^{r+1}}{\partial x_i} + \frac{2r+3}{3}\frac{e}{m}E_i\varrho^r = -\sum_{s=0}^{R}\hat{\Theta}^s_{rs\varrho i} \tag{12}$$

for $r = 0, 1, \ldots, R$. The production vector Π^r and the matrices of mean collision frequencies Θ_{rs}, $\hat{\Theta}_{rs}$ are given by

$$\Pi^r = \frac{2}{\sqrt{\pi}}n\sqrt{\frac{2k_BT}{m}}\left(\frac{2k_BT}{m}\right)^r \mathcal{B}\left(1-e^{\gamma}\right)\left(J_{r,0} - J_{0,r}\right)$$

$$\Theta_{rs} = \sqrt{\frac{2k_BT}{m}}\left(\frac{2k_BT}{m}\right)^{r-s}\sum_t \mathcal{C}^{-1}_{ts}\mathcal{B}\left[J_{r+t,0} - J_{t,r} + e^{\gamma}\left(J_{0,r+t} - J_{r,t}\right)\right] \tag{13}$$

$$\hat{\Theta}_{rs} = \sqrt{\frac{2k_BT}{m}}\left(\frac{2k_BT}{m}\right)^{r-s}\sum_t \hat{\mathcal{C}}^{-1}_{ts}\left[\mathcal{A}\Gamma\left(r+t+3\right) + \mathcal{B}\left[J_{r+t+1,0} + e^{\gamma}J_{0,r+t+1}\right]\right]$$

with the integrals

$$J_{r,s} = 2\int_0^\infty x^{2+2r}\sqrt{x^2+\alpha}^{\,1+2s}e^{-x^2}dx \tag{14}$$

and the temperature ratios

$$\alpha = \frac{\theta}{T} \quad , \quad \gamma = \theta\left(\frac{1}{T_0} - \frac{1}{T}\right) .$$

The integrals $J_{r,s}$ may be expressed through the modified Bessel functions of the second kind, see [6] for details.

The moment u^{R+1} in the system (12) is related to the variables (7) by a constitutive equation which follows from (8) as

$$\varrho^{R+1} = \varrho^{R+1}_{|T} + \sum_{s=0}^{R}\sum_{t=2}^{R}\mathcal{C}^{-1}_{st}\Gamma\left(R+s+\frac{5}{2}\right)\frac{\varrho^t - \varrho^t_{|T}}{\left(\frac{2k_BT}{m}\right)^{t-R-1}} .$$

In equilibrium, the right hand sides of (12) must vanish, and we have $\gamma = 0$ or $T = T_0$; moreover, the moments assume their equilibrium values $\varrho^r = \varrho^r_{|T_0} = \varrho^r_{|E}$ and $\varrho^r_{i|E} = 0$.

5 Homogeneous processes

We compare the results of the two set of equations for two simple one-dimensional homogeneous processes. Figure 1 shows the drift velocity of the electrons - i.e. ϱ^0_i/ϱ^0 - for a

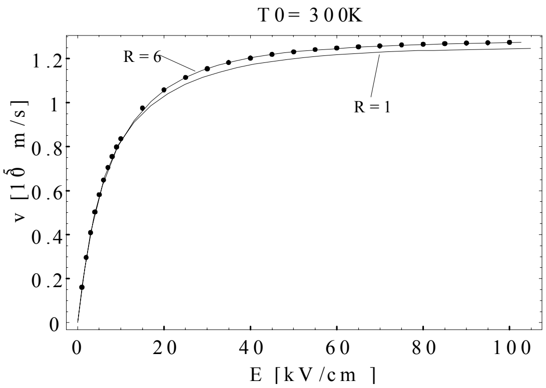

Figure 1: Stationary homogeneous process: drift velocity as a function of the electric field calculated with spherical harmonics (dots) and full moments with $R = 1, 6$ (lines).

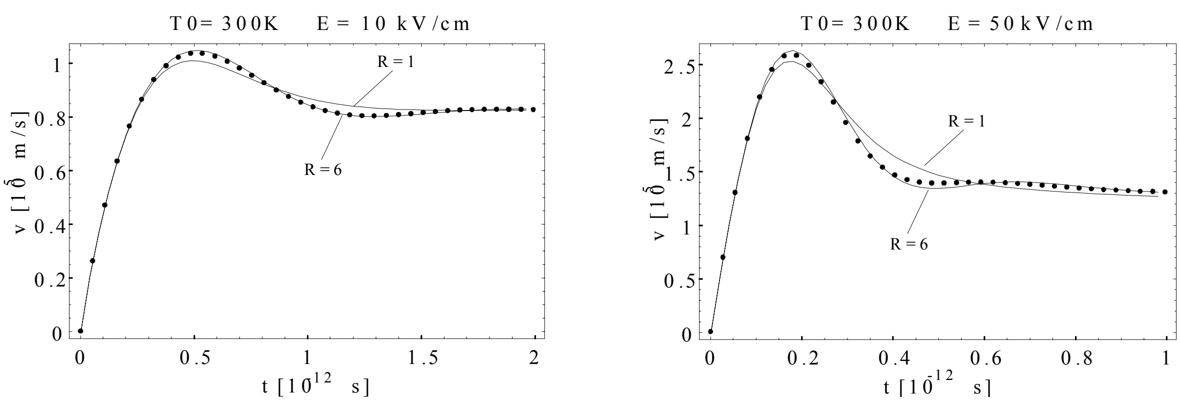

Figure 2: Transient homogeneous process: drift velocity as a function of time with $E = 10kV/cm, 50kV/cm$ calculated with spherical harmonics (dots) and full moments with $R = 1, 6$ (lines).

stationary electric field E as a function of its strength. The dots are the results obtained from the spherical harmonics equations (6) while the curves are obtained with the full moment equations with moment numbers $R = 1, 6$. All curves show the well-known saturation effect for high fields [11] [12]. However, it needs a moment number of $R = 6$ to obtain the curve of the spherical harmonics; with a number $R = 1$ of full moments the results differ in particular at high fields.

Also in the transient case, where the crystal is suddenly subjected to a constant homogeneous field, it needs a number of about $R = 6$ of full moments to obtain the same result as with the spherical harmonics equations, see Figure 2.

The two figures, for different values of the electric field, show the overshoot of velocity, which is also reported from Monte-Carlo solution of the Boltzmann equation [11][12]. These do not exhibit the minimum after the peak but give a monotony decreasing velocity after the peak. However, there is a lot of noise in the Monte Carlo results, and therefore it is not clear whether the minimum is an artefact of our choice of only two spherical harmonics or whether it has a physical meaning. Calculations with more spherical harmonics which will allow to answer this interesting question are in preparation.

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References

[1] Blotekjaer K. *Transport equations for electrons in two-valley semiconductors.* IEEE Trans. Electron Devices **17**, 38-47 (1970)

[2] Baccarani G. and Wordeman M.R. *An investigation of steady stae velocity overshoot in silicon.* Solid-State Electronics **28**, 407-416 (1985)

[3] A.M. Anile and M. Trovato *Non-linear closure for hydrodynamical semiconductor transport models.* Phys. Lett. A, **230**, 387-395 (1997)

[4] A.M.Anile and O. Muscato. *Extended thermodynamics tested beyond the linear regime: the case of electron transport in silicon semiconductors.* Cont. Mech. Thermodyn. **8**, 131-142 (1996)

[5] Liotta S.F., Majorana A. *Energy-kinetic equations modeling electron transport in semiconductors.* Preprint, Università di Catania, 1999

[6] Struchtrup H. *The moment method for electrons in semiconductors.* submitted

[7] Vecchi M.C. and Rudan M. *Modeling electron and hole transport with full-band structure effects by menas of the spherical-harmonics expansion of the BTE* IEEE Trans. ED **45**, 230-238 (1998)

[8] Gnudi A., Ventura D. and Baccarani G. *Modeling impact ionization on a BJT by means of spherical harmonics expansion of the Boltzmann transpot equation.* IEEE Trans. CAD **12**, 1706 (19xx)

[9] Rahmat K., White J. and Antonidias D.A. *Simulation of Semiconductor Devices Using a Galerkin/Spherical Harmonic Expansion Approach to Solving the Coupled Poisson-Boltzmann System.* IEEE Trans. CAD **15**, 1181-1196, (1996)

[10] N. Ben Abdallah and P. Degond *On a hierarchy of macroscopic models for semiconductors.* J. Math. Phys. **37**, 3306-3333 (1996)

[11] Jacoboni C., Reggiani L. *The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials.* Rev. Mod. Phys **55**, 645-705 (1983)

[12] Tomizawa K. *Numerical simulation of submicron semiconductor devices.* Boston: Artech House, 1993

[13] Liotta S.F. and Struchtrup H. *Moment equations for electrons in semiconductors: comparison of spherical harmonics and full moments.* accepted for publication in Solid-state Electronics (1999)

[14] Markowich P.A., Ringhofer C.A., Schmeiser C. *Semiconductor equations.* Wien: Springer, 1990

[15] M. Trovato and P. Falsaperla *Full nonlinear closure for a hydrodynamical model of transport in silicon.* Phys. Rev. B. **57**, 4456-4472, (1997)

[16] Grad H. *On the Kinetic Theory of Rarefied Gases.* Comm. Pure Appl. Math., Vol.2, Wiley, New Yorck (1949)

[17] Liboff R.L.*The Theory of Kinetic Equations*. Wiley and Sons, New York 1969