



Moment equations for electrons in semiconductors: comparison of spherical harmonics and full moments

S.F. Liotta*, H. Struchtrup

Dipartimento di Matematica, Università di Catania, Viale A. Doria 6, I-95125 Catania, Italy

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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. © 2000 Elsevier Science Ltd. All rights reserved.

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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 [1–3], see also Refs. [4,5]. The moment equations contain transport coefficients and relaxation times which are typically fitted to Monte Carlo simulations of some simple processes [6].

This paper deals with two moment systems which have been presented and analyzed recently by Liotta and Majorana [7] and Struchtrup [8] and we compare their results for simple homogeneous processes.

The energy-kinetic equations of Ref. [7] correspond to a spherical harmonics expansion with two moments [9–14] — 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. Usually these equations are solved only for stationary cases, below, however, we shall present results for the transient case in bulk silicon.

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 [1,2,6], 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 [1,6]. As

* Corresponding author. Tel.: +39-95-330-094.

E-mail addresses: liotta@dipmat.unict.it (S.F. Liotta), henning@dipmat.unict.it (H. Struchtrup).

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 the 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.

The equations for the full moments rely on a closure with a Grad type phase density [15,16], i.e. a Maxwellian times a polynomial. While we have chosen a Maxwellian which is based on the electron temperature [8], one may also consider a Maxwellian with the lattice temperature [18,19]. In accordance with the findings in Ref. [18], we show that the latter choice is numerically less expensive, but gives good results for small fields only.

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. The spherical harmonics can be computed from the Grad phase density and we compare the results for the stationary case. Both moment systems give the same results, if the number of full moments exceeds the usual choice of hydrodynamic models. The velocity curves for the full moments are presented in [8], all other curves are shown for the first time.

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 [20,21]. 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 multimoment methods for electrons.

Spherical harmonics codes with full band structure

are available in the literature, e.g. Refs. [10,22]. The incorporation of a full band structure into the moment method, however, is only at its beginnings. A moment system with 13 moments on the basis of the Kane dispersion relation [21] was just presented [23] and the study of an arbitrary moment number with the Kane law is planned for the future.

2. Boltzmann equation for parabolic bands

The basic quantity in the kinetic theory of electron transport is the phase density f , defined such that $f dx dc$ gives the number of electrons in the space element dx with velocities in the element dc at time t . The phase density is governed by the Boltzmann equation which reads [8,17]

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

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 $m = 0.32m_e = 2.915 \times 10^{-31}$ 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 [8,20]

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

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

where the abbreviations stand for

$$\mathcal{A} = \frac{1}{\pi} \frac{m^2 k_B \epsilon_1^2}{\hbar^4 \rho U_1^2} T_0,$$

$$\mathcal{B} = \frac{1}{2\pi} \frac{m^2 (D_t K)^2}{\hbar^2 \rho k_B \theta} \frac{1}{\exp(\theta/T_0) - 1},$$

$$\chi = \frac{2\hbar\omega}{m} = \frac{2k_B\theta}{m},$$

$$f^{(\pm)} = f(\sqrt{c^2 \pm \chi}, n_i),$$

$$\sqrt{(c^2 - \chi)_{|+}} = \begin{cases} \sqrt{(c^2 - \chi)_{|+}} & c^2 \geq \chi \\ 0 & c^2 < \chi \end{cases}.$$

$\mathcal{E}_l = 9 \text{ eV}$ is a deformation potential, $\rho = 2330 \text{ kg/m}^3$ is the crystal density and $U_l = 9040 \text{ m/s}$ is the longitudinal sound speed. Moreover, $D_l K = 11.4 \times 10^{10} \text{ eV/m}$ is another deformation potential, $\hbar\omega = 0.063 \text{ eV}$ is the energy of optical phonons and $\theta = \hbar\omega/k_B$ is an equivalent temperature. All values are for silicon [21]. 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 $T_0 = 300 \text{ K}$. 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,

$$f_{|E} = n \sqrt{\frac{m}{2\pi k_B T_0}}^3 e^{-(m/2k_B T_0)c^2}. \quad (2)$$

$n = \int f dc$ 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

$$u_{(i_1, i_2, \dots, i_n)} = \int n_{(i_1, i_2, \dots, i_n)} f d\Omega, \quad (3)$$

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

$$f = \sum_{n=0}^{\infty} \frac{(2n+1)!!}{4\pi n!} u_{(i_1, i_2, \dots, i_n)} n_{(i_1, i_2, \dots, i_n)}. \quad (4)$$

In practice, one considers not an infinite series, but only the first terms of Eq. (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 [8,9,14].

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

$$u_{|E} = \frac{4}{\sqrt{\pi}} n \sqrt{\frac{m}{2k_B T_0}} e^{-(m/2k_B T_0)c^2}, \quad u_{(i_1, i_2, \dots, i_n)|E} = 0. \quad (5)$$

The equations for the spherical harmonics follow by multiplication of the Boltzmann equation with $n_{(i_1, i_2, \dots, i_n)}$ and subsequent integration over all direc-

tions. For the first two moments we find the equations

$$\begin{aligned} \frac{\partial u}{\partial t} + c \frac{\partial u_k}{\partial x_k} - \frac{e}{m} E_k \frac{1}{c^2} \frac{\partial}{\partial c} [c^2 u_k] \\ = -\mathcal{B} \{ \sqrt{c^2 + \chi} [u - e^{\theta/T_0} u(\sqrt{c^2 + \chi})] \\ + \sqrt{(c^2 - \chi)_{|+}} [e^{\theta/T_0} u - u(\sqrt{c^2 - \chi})] \} \end{aligned} \quad (6)$$

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

These are the spherical harmonics equations for the model of Section 2, see Ref. [7] and — for the stationary case — Refs. [9–13].

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 [8]

$$\begin{aligned} q^r &= m \int c^{2r} f d\mathbf{c} = m \int c^{2r+2} u d\mathbf{c}, \\ q_i^r &= m \int c^{2r} c_i f d\mathbf{c} = m \int c^{2r+3} u_i d\mathbf{c}, \end{aligned} \quad (7)$$

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

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

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

Note, that the second equation defines the electron temperature. The usual choice of variables for hydrodynamic models consists in these eight moments plus the deviator of the pressure tensor $q_{(ij)} = m \int c_{(i} c_{j)} f d\mathbf{c} = m \int c^4 c_{(ij)} f d\mathbf{c}$ [1,6,24]. The latter is not considered here due to the neglect of the higher spherical harmonics struch. 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 $m c^{2r}$ and $m c^{2r} c_i$, respectively and subsequent integration. These

equations do not form a closed set for the variables in Eq. (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 [15,16]

$$f = f_{|T} \left[1 - \sum_{s=0}^R \lambda^2 c^{2s} - \sum_{s=0}^R \lambda_i^s c^{2s} c_i \right] \quad (8)$$

with $f_{|T} = n \sqrt{\frac{m}{2\pi k_B T}} \exp \left[-\frac{m}{2k_B T} c^2 \right];$

see Ref. [8] for a discussion. The main feature of the closure (8) is the choice of the local Maxwellian with the electron temperature T . The quality of the moment method depends considerably on the phase density which is chosen for the closure; e.g. one may use a closure with the global equilibrium phase density $f_{|E} = f_{|T_0}$ which is formed with the lattice temperature T_0 ; see Refs. [18,19] and Section 6.

Moreover, one may consider other functions for the closure, e.g. the maximum entropy method [24]. In each case one has to check for the proper number of moments — our results are restricted to the closure with the phase density (8).

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 Eq. (8) follow from Eq. (7) by inversion as functions of the moments,

$$\lambda^t = -\frac{\sqrt{\pi}}{2} \sum_{s=2}^R \mathcal{C}_{ts}^{-1} \frac{q^s - q_{|T}^s}{q^0 (2k_B T/m)^{s+t}}, \quad (9)$$

$$\lambda_i^t = -\frac{3\sqrt{\pi}}{2} \sum_{s=0}^R \hat{\mathcal{C}}_{ts}^{-1} \frac{q_i^s}{q^0 (2k_B T/m)^{s+t+1}}$$

with

$$q_{|T}^r = q^0 \left(\frac{2k_B T}{m} \right)^r \frac{2}{\sqrt{\pi}} \Gamma \left(r + \frac{3}{2} \right), \quad (10)$$

$$\mathcal{C}_{rs} = \Gamma \left(r + s + \frac{3}{2} \right), \quad \hat{\mathcal{C}}_{rs} = \Gamma \left(r + s + \frac{5}{2} \right).$$

$u_{|T}^r$ 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 harmonic moments of the phase density (8) as

$$u = \int f d\Omega = 4\pi f_{|T} \left(1 - \sum_{s=0}^R \lambda^s c^{2s} \right), \quad (11)$$

$$u_i = \int n_i f d\Omega = -\frac{4\pi}{3} f_{|T} \sum_{s=0}^R \lambda_i^s c^{2s+1}.$$

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

$$\frac{\partial q^r}{\partial t} + \frac{\partial q_k^r}{\partial x_k} + 2r \frac{e}{m} E_k q_k^{r-1} = -\Pi^r - \sum_{s=2}^R \Theta_{rs} (q^s - q_{|T}^s) \quad (12)$$

$$\frac{\partial q_i^r}{\partial t} + \frac{1}{3} \frac{\partial q^{r+1}}{\partial x_i} + \frac{2r+3}{3} \frac{e}{m} E_i q^r = -\sum_{s=0}^R \hat{\Theta}_{rsqi}^s$$

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

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

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

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

with the integrals

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

and the temperature ratios

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

The integrals $J_{r,s}$ may be expressed through the modified Bessel functions of the second kind; see Ref. [8] 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

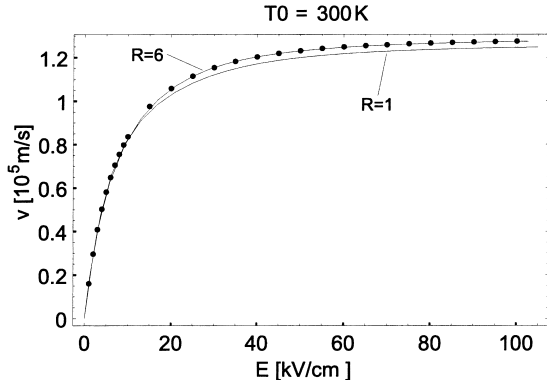


Fig. 1. Stationary homogeneous process: drift velocity as a function of the electric field calculated with spherical harmonics (dots) and full moments with $R = 1, 6$ (lines).

$$q^{R+1} = q_T^{R+1} + \sum_{s=0}^R \sum_{l=2}^R \mathcal{C}_{st}^{-1} \Gamma\left(R + s + \frac{5}{2}\right) \frac{q^l - q_T^l}{(2k_B T/m)^{l-R-1}}.$$

In equilibrium, the right hand sides of Eq. (12) must vanish, and we have $\gamma = 0$ or $T = T_0$; moreover, the moments assume their equilibrium values $q^l = q_{T_0}^l = q_{lE}^l$ and $q_{iE}^l = 0$.

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. Q_i^0/Q^0 — for a stationary electric field E as a function of its strength. The dotted line are the results obtained from the spherical harmonics Eq. (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 [20,21]. 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 Fig. 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 [20,21]. 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.

We compare the spherical harmonics (11) computed with the full moments with the numerical solution of Eq. (6). Following Ref. [7], we consider the functions of the electron energy $\varepsilon = (m/2)c^2$

$$N(\varepsilon) = \frac{1}{n} \sqrt{\frac{2\varepsilon}{m^3}} u(\varepsilon) \quad \text{and} \quad V_i(\varepsilon) = \frac{2\varepsilon}{nm^2} u_i(\varepsilon)$$

which are defined such that

$$1 = \int N(\varepsilon) d\varepsilon \quad \text{and} \quad v_i = \int V_i(\varepsilon) d\varepsilon$$

hold. Figure 3 shows these functions for the stationary homogeneous case with $E = 10$ kV/cm and $E = 50$ kV/cm in suitable units. In both cases, we have a

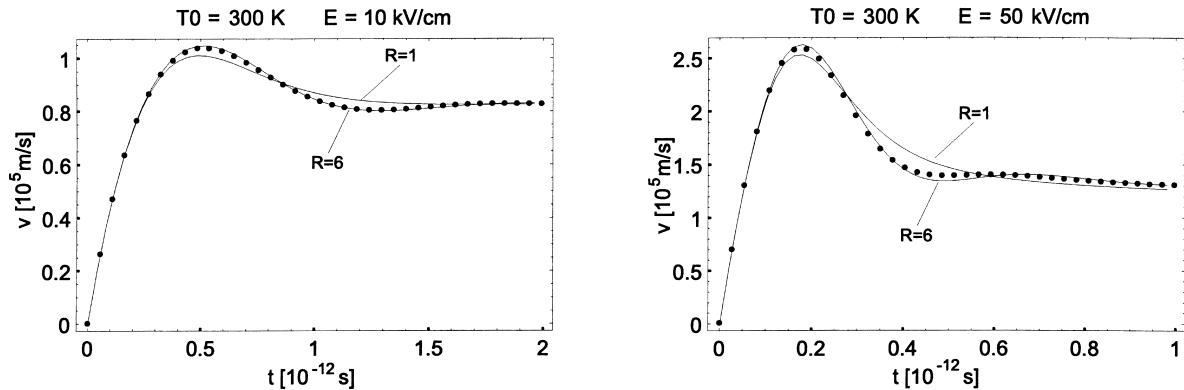


Fig. 2. Transient homogeneous process: drift velocity as a function of time with $E = 10$ kV/cm, 50 kV/cm calculated with spherical harmonics (dots) and full moments with $R = 1, 6$ (lines).

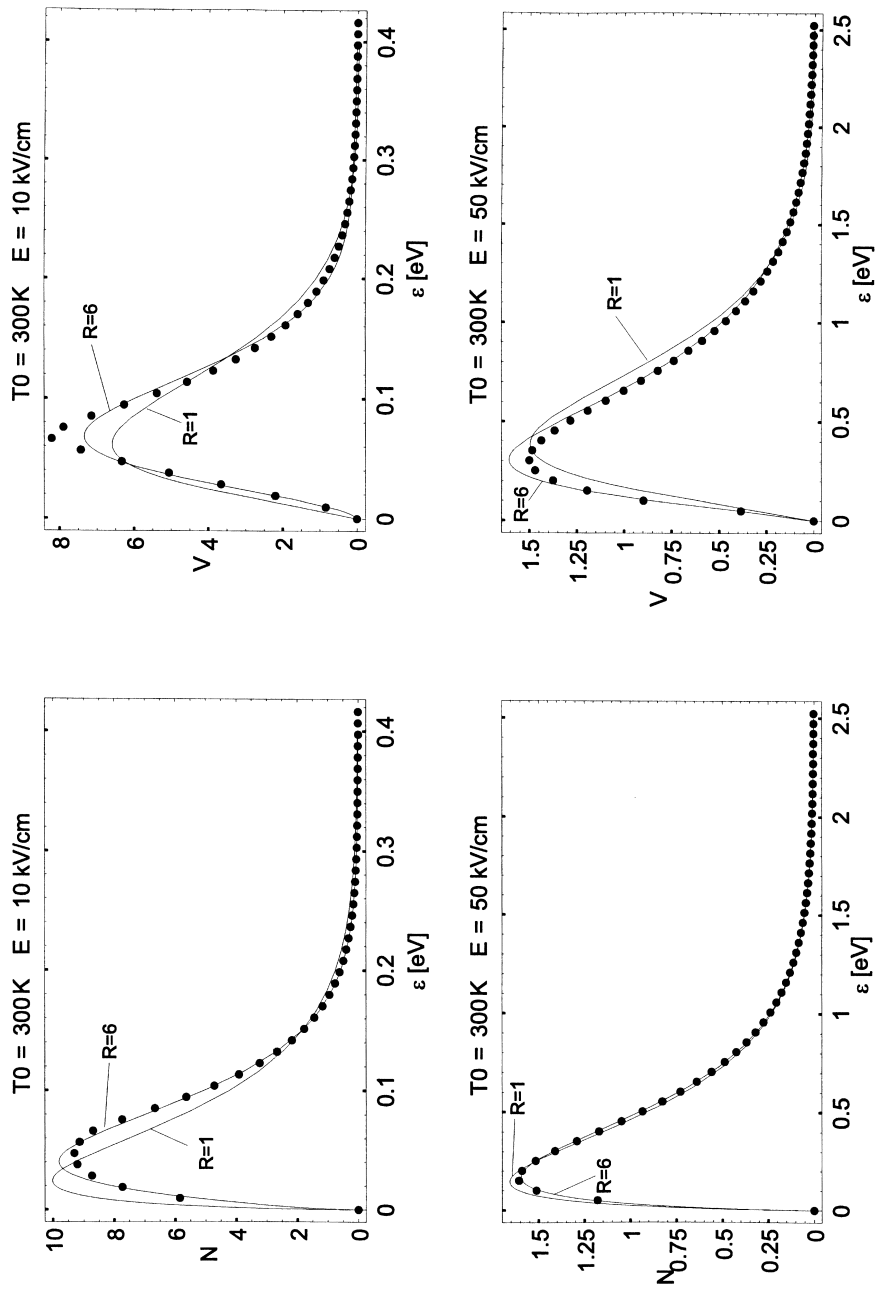


Fig. 3. The functions N , $V = V_1$ in suitable units calculated from the full moments (lines) and the spherical harmonics equations (dots) for $E = 10$ kV/cm, 50 kV/cm.

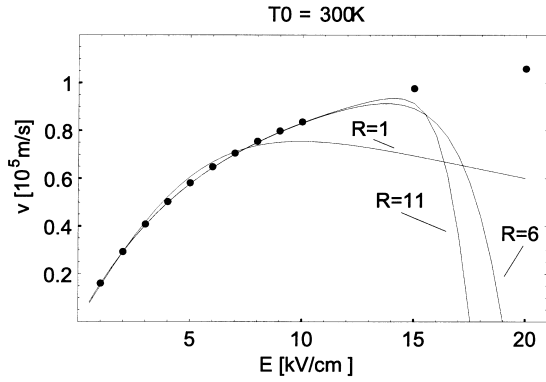


Fig. 4. Homogeneous stationary process: drift velocity as a function of the electric field calculated with spherical harmonics (dots) and full moments with global equilibrium closure for $R = 1, 6$ or 11 (lines).

better agreement between the numerical solution of Eq. (6) and the moment theory with $R = 6$. However, while the agreement in the function $N(\varepsilon)$ is good, there is a clear difference in the function V , which is most marked close to its maximum.

6. Global equilibrium closure

In this last section, we consider the closure of the moment equations with the global Maxwellian [18,19], i.e. with the phase density

$$f = f_{|E} \left[1 - \sum_{s=0}^R \lambda^s c^{2s} - \sum_{s=0}^R \lambda_i^s c^{2s} c_i \right] \quad (15)$$

instead of Eq. (8).

In this case, the moment equations read

$$\begin{aligned} \frac{\partial \varrho^r}{\partial t} + \frac{\partial \varrho_k^r}{\partial x_k} + 2r \frac{e}{m} E_k \varrho_k^{r-1} &= - \sum_{s=1}^R \Theta_{rs}(T_0) (\varrho^s - \varrho_{|E}^s) \\ \frac{\partial \varrho_i^r}{\partial t} + \frac{1}{3} \frac{\partial \varrho^{r+1}}{\partial x_i} + \frac{2r+3}{3} \frac{e}{m} E_i \varrho^r &= - \sum_{s=0}^R \hat{\Theta}_{rs}(T_0) \varrho_i^s \end{aligned} \quad (16)$$

with the same matrices of mean collision frequencies as above in Eq. (13), but evaluated at the lattice temperature T_0 . Thus, the set of moment equations is linear in the moments and may be solved at lower computational cost as the set (12), which is strongly nonlinear in the electron temperature $T = \frac{1}{3} \varrho^1 / (\varrho^0 (k_B/m))$. Indeed, in the linear case, one has to compute the matrices $\Theta_{rs}(T_0)$ and $\hat{\Theta}_{rs}(T_0)$ only once, while the nonlinear case requires the evaluation of the matrices for all values of the temperature.

Figure 4 shows the velocity-field characteristics com-

puted with the linear equations for moment numbers $R = 1, 6$ and 11 in comparison to the results of the spherical harmonics. For fields $E \leq 12.5$ kV/cm the results from the linearized equations match very well. Above this value, however, we were not able to find convergence (note that the numerical inversion of the matrices $\mathcal{C}_{rs}, \hat{\mathcal{C}}_{rs}$ requires high precision calculations in order to be accurate).

This results are in accordance with Ref. [18] where it was shown that the closure (15) gives bad results at large electric fields.

We conclude that the linear equations should be used in the case of low fields, since they give good results at low computational cost. High fields, however, require the use of the nonlinear closure, i.e. Eq. (12), or of the spherical harmonics Eq. (6).

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Appendix A. Trace-free tensors and spherical harmonics

A symmetric tensor S_{i_1, i_2, \dots, i_n} is trace-free, or irreducible, if

$$S_{i_1, i_2, \dots, i_j, \dots, i_k, \dots, i_n} \delta_{j, i_k} = 0$$

holds for every pair i_j, i_k . The irreducible part of a symmetric tensor A_{i_1, i_2, \dots, i_n} follows from Ref. [26]

$$A_{(i_1, i_2, \dots, i_n)} = \sum_{k=0}^{\lfloor n/2 \rfloor} a_{nk} \delta_{(i_1, i_2, \dots, i_{2k-1} i_{2k}} A_{i_{2k+1}, \dots, i_n) i_1, \dots, j_k j_1, \dots, j_k}$$

where

$$a_{nk} = (-1)^k \frac{n!(2n-2k-1)!!}{(n-2k)!(2n-1)!!(2k)!!}$$

$$\lfloor \frac{n}{2} \rfloor = \begin{cases} \frac{n}{2} & n \text{ even} \\ \frac{n-1}{2} & n \text{ uneven} \end{cases}, \quad n!! = \prod_{j=0}^{\lfloor (n-1)/2 \rfloor} (n-2j).$$

For the daily work, it is useful to write instead [25]

$$\begin{aligned} A_{(i_1, \dots, i_n)} &= \sum_{k=0}^{\lfloor n/2 \rfloor} b_{n,k} (\delta_{i_1 i_2}, \dots, \delta_{i_{2k-1} i_{2k}} A_{i_{2k+1}, \dots, i_n}^{(k)} \\ &+ \dots (P_{n,k} \text{ terms})) \end{aligned}$$

where $A_{i_2k+1, \dots, i_n}^{(k)}$ is the k th trace of A_{i_1, \dots, i_n} and the sum in brackets extends over all P_{nk} different permutations of the indices. We have

$$b_{n,k} = \frac{(-1)^k}{\prod_{j=0}^{k-1} (2(n-j) - 1)}, \quad P_{n,k} = \frac{n!}{(n-2k)!2^k k!}.$$

The first few tensors $A_{(i_1, \dots, i_n)}$ read

$$A_{(i)} = A_i, \quad A_{(ij)} = A_{ij} - \frac{1}{3} A_{kk} \delta_{ij},$$

$$A_{(ijk)} = A_{ijk} - \frac{1}{5} (A_{iil} \delta_{jk} + A_{jll} \delta_{ik} + A_{kll} \delta_{ij}).$$

The tensor A_{i_1, \dots, i_n} may also be written as a sum of its trace-free parts [25],

$$A_{i_1, \dots, i_n} = \sum_{k=0}^{\lfloor n/2 \rfloor} \hat{d}_{n,k} (\delta_{i_1 i_2}, \dots, \delta_{i_{2k-1} i_{2k}} A_{(i_{2k+1}, \dots, i_n)}^{(k)} + \dots (P_{n,k} \text{ terms})),$$

where $A_{(i_{2k+1}, \dots, i_n)}^{(k)}$ is the trace-free part of the k th trace of A_{i_1, \dots, i_n} and

$$\hat{d}_{n,k} = \frac{1}{\prod_{j=0}^{k-1} (2(n-k-j) + 1)}.$$

Spherical harmonics may be represented through the trace-free tensors

$$n_{(i_1, \dots, i_n)}$$

with a unit vector $n_i = \{\sin \vartheta \sin \varphi, \sin \vartheta \cos \varphi, \cos \vartheta\}_i$. Spherical harmonics form an orthogonal set with

$$\int n_{(i_1, \dots, i_n)} n_{(j_1, \dots, j_n)} d\Omega = \begin{cases} 0 & n \neq m \\ \frac{4\pi}{\prod_{j=0}^n (2j+1)} \delta_{(i_1, \dots, i_n)(j_1, \dots, j_n)} & n = m. \end{cases}$$

Here, $d\Omega = \sin \vartheta d\vartheta d\varphi$ is the element of solid angle and δ_{k_1, \dots, k_l} is an l -dimensional unit tensor with l even, defined by

$$\delta_{k_1, \dots, k_l} = \delta_{k_1 k_2}, \dots, \delta_{k_{l-1} k_l} + \dots + \left(\frac{l!}{(l/2)!2^{l/2}} \text{ terms} \right).$$

In particular, the following two identities hold and are used several times in this paper:

$$A_{i_1 i_2, \dots, i_n} \int n_{(i_1, \dots, i_n)} n_{(j_1, \dots, j_n)} d\Omega = \begin{cases} 0 & n \neq m \\ \frac{4\pi n!}{\prod_{j=0}^n (2j+1)} A_{(j_1, \dots, j_n)} & n = m \end{cases} \quad (17)$$

$$n_{(i_1, \dots, i_n)} n_k = n_{(i_1, \dots, i_n} n_k)$$

$$+ \frac{n}{2n+1} n_{((i_1, \dots, i_{n-1}) \delta_{i_n) k}}.$$

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