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Extended moment method for electrons in semiconductors

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Abstract

The semiclassical Boltzmann equation for electrons in semiconductors with the Kane dispersion law or the parabolic band approximation is considered and systems of moment equations with an arbitrary number of moments are derived. First, the paper deals with spherical harmonics in the formalism of symmetric trace-free tensors. The collision frequencies are carefully studied for the physical properties of silicon. Then, for the parabolic band approximation, the hierarchy of equations for full moments of the phase density and the corresponding closure problem is discussed. In particular, a set of $2R$ scalar and vectorial moments is considered. To answer the question which number R one has to chose in order to retain the physical contents of the Boltzmann equation, the moment equations are examined in the drift-diffusion limit and in an infinite crystal in a homogeneous electric field (transient and stationary cases) for increasing number of moments R. The number R must be considered to be sufficient, if its further increase does not change the result considerably and the appropriate numbers for the processes are given.

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1. Introduction

This paper deals with the simulation of the transport of electrons in semiconductors which is an important task for the development of new semiconductor devices.

The suitable mathematical model for this task depends on the size of the device. For relatively large devices, the drift-diffusion equation [1,2] is the method of choice. Most of today's small devices are sufficiently described by the semi-classical Boltzmann

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equation, which accounts for quantum effects in an overall manner. Only extremely small devices with an extension of few atomic diameters must be tackled with a full quantum mechanical treatment, i.e. the Schroedinger equation.

The solution of the Boltzmann equation must be done numerically. Here, the common method is the Monte-Carlo method [3–5] which is very accurate nowadays, but requires computing times which are measured in hours or days. For this reason one derives simplified models from the Boltzmann equation, in the hope to meet the physical behavior of a semiconductor at lower computational cost. Most of these models are based on moment equations [6–10] and also this paper is devoted to these.

In particular, we shall deal with two types of moments, spherical harmonics and full moments. The spherical harmonics are moments of the phase density with respect to the direction vector of the electrons [11–13] and may be written as trace-free symmetric tensors [14–16]. The full moments are moments of the phase density with respect to the electron momentum [7,6,17]. In both cases, one derives an infinite set of coupled partial differential equations for an infinite number of moments. Thus the question arises, which and how many moments are needed for the proper description of a given process.

Only in few cases one finds proper asymptotic limits which allow the reduction of the number of moments. One of these is the afore mentioned drift-diffusion limit [1], where only one moment, the number density n, has to be considered. Another interesting limit is the so-called SHE-model [18–20,12], where the phase density is almost isotropic.

In general, however, there is not an easy answer to the above question and the only method to find an answer is as follows: if the increase of the number of moments changes the result, one has to increase further until the result does not change significantly. We shall demonstrate this method for simple examples.

In our 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 hydrodynamical models [7,6,12], there are no free parameters for the fitting to Monte Carlo data or experiments. 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.

Since our main interest lies in development and use of multi-moment methods, we restrict ourselves to a simplified physical picture of the semiconductor. Thus, we shall use the Kane dispersion law [5] or the parabolic band approximation [2] and consider the interaction of electrons with acoustical and optical phonons only [4,22]. This simplified physical picture, although inaccurate for high electric fields, describes all interesting features of electron transport in semiconductors, e.g. velocity saturation and overshoot. The emphasis of the paper lies on the influence of the moment number on the results and not on the physics. Therefore, it seems to be appropriate to start with the simplified picture in this first study of multimoment methods for electrons.

Spherical harmonics codes with full band effects are available in the literature, e.g. Ref. [12]. 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 was just presented [9].

The plan of the paper is as follows: In the next section we present the Boltzmann equation with the terms for the interaction of electrons with acoustical and optical phonons.

Section 3 considers the spherical harmonics expansion of the Boltzmann equation in the formalism of trace-free symmetric tensors [14,16]. The derivations of the SHE-model and the drift-diffusion equation are performed as limits for the collision frequencies [18,19].

In Section 4 we introduce the full moments and their equations. These contain additional quantities which are not related to the moments a priori. Here, one has to introduce a closure assumption in order to find constitutive relations and we outline the closure by the entropy maximum method [23,24] and the Grad expansion method [25,26].

Specific moment equations for scalar and vectorial moments are derived in Section 5. The system is closed with the Grad method for an arbitrary number of moments. In order to find criteria for the proper number of moments we consider the drift-diffusion limit and an infinite homogeneous semiconductor in a stationary or transient electric field. In all cases, we use the above-mentioned method and compare the results with an increasing number of moments.

2. Boltzmann equation

An electron at space–time coordinates x_i,t is described by the wave vector k_i which assumes values in the first Brillouin zone of the reciprocal lattice [2,5]. The phase density f is defined such that

$$f\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{k}$$

gives the number of electrons in the element of phase space $\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{k}$. The phase density is governed by the Boltzmann equation

$$\frac{\partial f}{\partial t}+c_k\frac{\partial f}{\partial x_k}-\frac{e}{\hbar}E_k\frac{\partial f}{\partial k_k}=Q\,, \tag{1}$$

where e is the elementary charge and $\hbar$ is Planck's constant. E_i denotes the electric field and Q is the collision term.

The energy ε of the electron depends on the band structure and is a function of the wave vector, the dispersion relation $\varepsilon=\varepsilon(k_i)$. $c_k(k_i)$ is the velocity of an electron which follows from the electron energy $\varepsilon(k_i)$ by (group velocity)

$$c_i=\frac{1}{\hbar}\frac{\partial\varepsilon}{\partial k_i}\,. \tag{2}$$

Throughout this paper we restrict ourselves to dispersion relations with spherical symmetry, where $\varepsilon(k_i) = \varepsilon(k)$. For detailed calculations we shall rely on the Kane dispersion law [5]

$$\varepsilon = \frac{1}{2\alpha}\left(-1 + \sqrt{1 + 2\alpha\frac{\hbar^2 k^2}{m}}\right) \tag{3}$$

and the parabolic band approximation

$$\varepsilon = \frac{\hbar^2 k^2}{2m}\,. \tag{4}$$

Here, m denotes the effective mass which differs from the electron mass m_e; for silicon we have $m = 0.32 m_e = 2.915 \times 10^{-31}$kg. For silicon the constant α has a value of $0.5\ \mathrm{eV}^{-1}$, the parabolic band approximation follows from the Kane dispersion by setting $\alpha = 0$.

For symmetric dispersion relations like (3,4), the velocity points in the direction $n_i = k_i/k$ of the crystal momentum. For the Kane dispersion we find

$$c_i = c n_i = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k} n_i = \sqrt{\frac{2}{m}\varepsilon(1 + \alpha\varepsilon)}\frac{1}{1 + 2\alpha\varepsilon} n_i\,. \tag{5}$$

Again, the corresponding formulae for the parabolic band approximation follow by setting $\alpha = 0$.

In the sequel, we shall also need the density of states $N(\varepsilon)$ defined by

$$k^2 \mathrm{d}k = N(\varepsilon)\mathrm{d}\varepsilon \quad \text{so that } N(\varepsilon) = k^2\frac{\mathrm{d}k}{\mathrm{d}\varepsilon} = \frac{1}{\hbar}\frac{k^2}{c}\,. \tag{6}$$

For the Kane law and parabolic bands we have, respectively,

$$N(\varepsilon) = \sqrt{\frac{m}{\hbar^2}}^3 \sqrt{2\varepsilon(1 + \alpha\varepsilon)}(1 + 2\alpha\varepsilon) \quad \text{and} \quad N(\varepsilon) = \sqrt{\frac{m}{\hbar^2}}^3 \sqrt{2\varepsilon}\,. \tag{7}$$

The Kane dispersion law approximately reduces to the parabolic band approximation (4) if $2\alpha\varepsilon < 0.1$, i.e. for energies below 0.1 eV. When we study the full moments later in this paper the parabolic band approximation is applied for much larger electron energies, though, so that the results at large energies do not represent the proper physics. As we have said in the introduction, this is a first study of multi-moment methods for electrons and it seems appropriate to start with the simplified picture in order to examine the influence of the moment number on the results.

The phase density is defined in the first Brillouin zone only. We shall assume that the electron energies not to large, so that the phase density goes to zero towards the boundary of the Brillouin zone. Then we can extend the definition of the phase density to the whole velocity space. In particular, this will allow us to calculate integrals of the phase density more easily.

For the examples, we shall assume constant electric fields, so that we do not need the Poisson equation for the determination of the electric field.

2.1. Collision terms

The electron gas in semiconductors is rarefied, so that contributions from the Pauli exclusion principle may be ignored. Then, the collision term Q of the Boltzmann equation is of the form [1]

$$Q = \int [s(\mathbf{k}', \mathbf{k}) f' - s(\mathbf{k}, \mathbf{k}') f] \, d\mathbf{k}' \,. \tag{8}$$

The first term describes interactions where the wave vector changes from $\mathbf{k}'$ to $\mathbf{k}$ while the second term describes the inverse processes; $s(\mathbf{k}, \mathbf{k}')$ is the collision probability. The corresponding equilibrium distribution is the Maxwellian [1] which reads for the Kane dispersion law,

$$f_{|E} = n \sqrt{\frac{\hbar^2/m}{2\pi k_B T_0}}^{3} \frac{\sqrt{\pi \alpha k_B T_0} \exp[-1/2\alpha k_B T_0]}{K_2(1/2\alpha k_B T_0)} \exp\left[-\frac{\varepsilon}{k_B T_0}\right] , \tag{9}$$

$K_\nu(x)$ denotes the modified Bessel functions of the second kind. The factor in front of the exponential follows from the requirement, that the integral of f in k-space gives the number density n,

$$n = \int f \, d\mathbf{k} \,. \tag{10}$$

For the parabolic band approximation ($\alpha \to 0$) the Maxwellian reads

$$f_{|E} = n \sqrt{\frac{\hbar^2/m}{2\pi k_B T_0}}^{3} \exp\left[-\frac{\hbar^2/m}{2 k_B T_0} k^2\right] . \tag{11}$$

2.1.1. Elastic scattering at acoustic phonons

For the elastic scattering of electrons with acoustic phonons one finds the collision probability [4]

$$s_{\mathrm{ac}}(\mathbf{k}, \mathbf{k}') = \mathscr{A} \delta(\varepsilon' - \varepsilon) \quad \text{with } \mathscr{A} = \frac{k_B T_0 \mathscr{E}_l^2}{4\pi^2 \hbar \varrho U_l^2} \,. \tag{12}$$

$\mathscr{E}_l = 9\,\mathrm{eV}$ is the deformation potential, $\varrho = 2330\,\mathrm{kg/m^3}$ is the crystal density and $U_l = 9040$ m/s is the longitudinal sound speed; all values for silicon.

With an isotropic dispersion relation like (3,4) it is easy to calculate Q_{ac} from (8) as

$$Q_{\mathrm{ac}} = -4\pi \mathscr{A} N(\varepsilon) \left[f - \frac{1}{4\pi} \int f \, d\Omega \right] , \tag{13}$$

where $d\Omega = \sin\vartheta \, d\vartheta \, d\varphi$ is the element of solid angle. The collision term Q_{ac} leads to an isotropic phase density and every isotropic function of the crystal momentum is a conserved quantity, in particular we have for all $r \geqslant 0$

$$\int k^r Q_{\mathrm{ac}} \, d\mathbf{k} = 0 \quad \text{and} \quad \int \varepsilon^r Q_{\mathrm{ac}} \, d\mathbf{k} = 0 \,.$$

Table 1
Z_η, $\theta_\eta = \hbar\omega^\eta / k_B$ and $D_t K_\eta$ for silicon

	Z_η	$\theta_\eta[K]$	$D_t K_\eta[10^{10}\mathrm{eV/m}]$
g_1	1	140	0.5
g_2	1	215	0.8
g_3	1	720	11
f_1	4	220	0.3
f_2	4	550	2.0
f_3	4	685	2.0

2.1.2. Inelastic collisions with optical phonons

The collision probability for collisions among electrons and optical phonons reads [1,4]

$$s^\eta_{\mathrm{op}}(\mathbf{k}, \mathbf{k}') = \mathscr{B}^\eta [N^\eta_{\mathrm{op}}\, \delta(\varepsilon' - \varepsilon - \hbar\omega^\eta) + (N^\eta_{\mathrm{op}} + 1)\, \delta(\varepsilon' - \varepsilon + \hbar\omega^\eta)] \tag{14}$$

with the phase density of optical phonons with frequency ω^η

$$N^\eta_{\mathrm{op}} = \frac{1}{\exp[\hbar\omega^\eta / k_b T_0] - 1} \quad \text{and} \quad \mathscr{B}^\eta = Z_\eta \frac{(D_t K_\eta)^2}{8\pi^2 \varrho \omega^\eta}$$

with numbers Z_η and the deformation potential $D_t K_\eta$. For silicon, one has six contributions (intervalley scattering) $\eta = g_1, g_2, g_3, f_1, f_2, f_3$ [4] and the corresponding values for the constants can be read from Table 1, where we do not print the frequencies ω^η but the corresponding temperatures $\theta_\eta = \hbar\omega^\eta / k_B$.

We insert (14) in (8), compute the integrals and find

$$\begin{aligned} Q_\eta = {} & -4\pi \mathscr{B}_\eta N^\eta_{\mathrm{op}} \left\{ N(\varepsilon + \hbar\omega^\eta) \left[f - \frac{e^{\theta_\eta / T_0}}{4\pi} \int f^{(+)}\, \mathrm{d}\Omega \right] + N(\varepsilon - \hbar\omega^\eta)_{|+} \right. \\ & \left. \times \left[e^{\theta_\eta / T_0} f - \frac{1}{4\pi} \int f^{(-)}\, \mathrm{d}\Omega \right] \right\}, \end{aligned} \tag{15}$$

with the abbreviations

$$f^{(\pm)} = f(\varepsilon \pm \hbar\omega, n_i), \quad N(\varepsilon - \hbar\omega)_{|+} = \begin{cases} N(\varepsilon - \hbar\omega, & \varepsilon \geqslant \hbar\omega\,, \\ 0, & \varepsilon < \hbar\omega\,. \end{cases}$$

In the last equations, we have introduced the notation $f(k_i) = f(k, n_i) = f(\varepsilon, n_i)$ for the phase density, $n_i = c_i / c$ is the direction of propagation of the electrons.

The overall collision term for inelastic collisions is given by $Q_{\mathrm{op}} = \sum_\eta Q_\eta$. The equilibrium phase density for Q_η – determined by setting $Q_\eta = 0$ – is given by a Maxwellian times a function which is periodic in $\hbar\omega^\eta$ [27]. The overall equilibrium function of Q_{op}, however, is the Maxwellian (9), since the periods $\hbar\omega^\eta$ are incommensurable. The only conserved quantity is the particle number n,

$$\int Q_\eta\, \mathrm{d}\mathbf{k} = 0\,.$$

3. Spherical harmonics

3.1. Moments

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

$$u_{\langle i_1 i_2 \cdots i_n\rangle} = \int n_{\langle i_1} n_{i_2} \cdots n_{i_n\rangle} f \, \mathrm{d}\Omega \, . \tag{16}$$

The brackets denote a symmetric trace-free tensor [14,16], see Appendix A for details.

With the moments (16) the phase density can be written as a series

$$f = \sum_{n=0}^{\infty} \frac{(2n+1)!!}{4\pi n!} u_{\langle i_1 i_2 \cdots i_n\rangle} n_{\langle i_1} n_{i_2} \cdots n_{i_n\rangle} \, . \tag{17}$$

In practice, one considers not an infinite series, but only the first terms of (17). The spherical harmonics are functions of space x_i, time t and the electron energy ε or the absolute value k of the crystal momentum, alternatively. The moments of the Maxwellian are

$$u_{|E} = 4\pi f_{|E}, \quad u_{\langle i_1 i_2 \cdots i_n\rangle |E} = 0 \tag{18}$$

3.2. Equations for spherical harmonics

The equations for the spherical harmonics (16) 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 scalar u we find the equation

$$\begin{aligned}\frac{\partial u}{\partial t} + c\left[\frac{\partial u_k}{\partial x_k} - eE_k \frac{1}{k^2}\frac{\partial}{\partial \varepsilon}[k^2 u_k]\right] = -4\pi \sum_{\eta} \mathscr{B}_\eta N_{\mathrm{op}}^{\eta} \{ & N(\varepsilon + \hbar\omega^\eta)\,[u - \mathrm{e}^{\theta_\eta/T_0} u^{(+)}] \\ & + N(\varepsilon - \hbar\omega^\eta)_{|+}[\mathrm{e}^{\theta_\eta/T_0} u - u^{(-)}]\}\end{aligned} \tag{19}$$

with $u^{(\pm)} = u(\varepsilon \pm \hbar\omega)$. The tensorial equations read

$$\begin{aligned}&\frac{\partial u_{\langle i_1 \cdots i_n\rangle}}{\partial t} + c\left\{\frac{n}{2n+1}\frac{\partial u_{\langle i_1 \cdots i_{n-1}}}{\partial x_{i_n\rangle}} + \frac{\partial u_{\langle i_1 \cdots i_n k\rangle}}{\partial x_k} - eE_k \frac{1}{k^{n+2}}\frac{\partial}{\partial \varepsilon}[k^{n+2} u_{\langle i_1 \cdots i_n k\rangle}]\right. \\ &\left. - \frac{n}{2n+1} eE_{\langle i_1} k^{n-1} \frac{\partial}{\partial \varepsilon}\frac{u_{i_2 \cdots i_n\rangle}}{k^{n-1}}\right\} = -\kappa_n u_{\langle i_1 \cdots i_n\rangle} \, .\end{aligned} \tag{20}$$

The newly introduced quantity

$$\kappa_n = 4\pi \mathscr{A} N(\varepsilon) + 4\pi \sum_{\eta} \mathscr{B}_\eta N_{\mathrm{op}}^{\eta} [N(\varepsilon + \hbar\omega^\eta) + \mathrm{e}^{\theta_\eta/T_0} N(\varepsilon - \hbar\omega^\eta)_{|+}] \tag{21}$$

denotes the collision frequency for the tensorial spherical harmonics. κ_n is independent of the number of indices n, thus all $u_{\langle i_1 \cdots i_n\rangle}, n = 1, 2, \ldots$ decay with the same rate.

Eqs. (19), (20) for the spherical harmonics form an infinite set of equations, since the equation for $u_{\langle i_1\cdots i_n\rangle}$ contains also the higher moment $u_{\langle i_1\cdots i_n k\rangle}$.

For one-dimensional processes, say in direction $x = x_1$, so that $E_i = \{E, 0, 0\}$, only the components

$$u_{\langle n\rangle} = u_{\langle \underbrace{1\cdots 1}_{n\ \text{times}}\rangle}$$

are of concern and the corresponding moment equations read

$$\frac{\partial u_{\langle n\rangle}}{\partial t} + c\left\{\frac{n^2}{4n^2-1}\frac{\partial u_{\langle n-1\rangle}}{\partial x} + \frac{\partial u_{\langle n+1\rangle}}{\partial x}\right.$$
$$\left. - eE\frac{1}{k^{n+2}}\frac{\partial}{\partial \varepsilon}[k^{n+2}u_{\langle n+1\rangle}] - \frac{n^2}{4n^2-1}eEk^{n-1}\frac{\partial}{\partial \varepsilon}\frac{u_{\langle n-1\rangle}}{k^{n-1}}\right\} = -\kappa_n u_{\langle i_1\cdots i_n\rangle}\,. \tag{22}$$

In order to reduce the infinite system (19), (20) to tractable finite systems one may truncate the infinite hierarchy of moment equations, i.e. consider only the equations for the spherical harmonics $u_{\langle i_1\cdots i_n\rangle}$, $n = 0, 1, 2, \ldots, M$ with $u_{\langle i_1\cdots i_{M+j}\rangle} = 0$ $(j \geqslant 1)$. This yields the question, which value M one has to take into account. Unfortunately, there is no easy answer since the number M will depend on the process under consideration, in particular on the initial and boundary data.

Thus, one has to calculate the same process with increasing moment number M until the results do not change considerably, if M is further increased. Then, one should have the proper moment number. We shall use this idea later, not for the spherical harmonics but for the full moments.

3.3. Mean free paths and collision frequencies

The interaction between electrons and acoustic or optical phonons leads to two different tendencies: (i) the tendency towards an isotropic phase density, described by the collision frequency κ_n given by (21) and (ii) the tendency towards thermal equilibrium, i.e. the Maxwellian phase density, described by the r.h.s. of (19), which we denote by P in the following.

Unfortunately, P is not easily described by one single-collision frequency. Let us consider first a situation close to equilibrium, where the phase density is almost Maxwellian. By a standard argument of kinetic theory [26], we replace u in the gain terms of P by the Maxwellian (18) to obtain the relaxation time approximation [1]

$$P = -\kappa_0(u - u_{|E}) \tag{23}$$

with the inverse relaxation time – or collision frequency –

$$\kappa_0 = 4\pi\sum_\eta \mathscr{B}_\eta N_{\text{op}}^\eta[N(\varepsilon + \hbar\omega^\eta) + \mathrm{e}^{\theta_\eta/T_0}N(\varepsilon - \hbar\omega^\eta)_{|+}] = \kappa_n - 4\pi\mathscr{A}N(\varepsilon)\,. \tag{24}$$

The relaxation time approximation (23) is appropriate for relatively low energetic electrons: In each collision with optical phonons the electron gains or looses the energy $\hbar\omega^\eta$. If its own energy is of the same order of magnitude, few collisions will suffice to

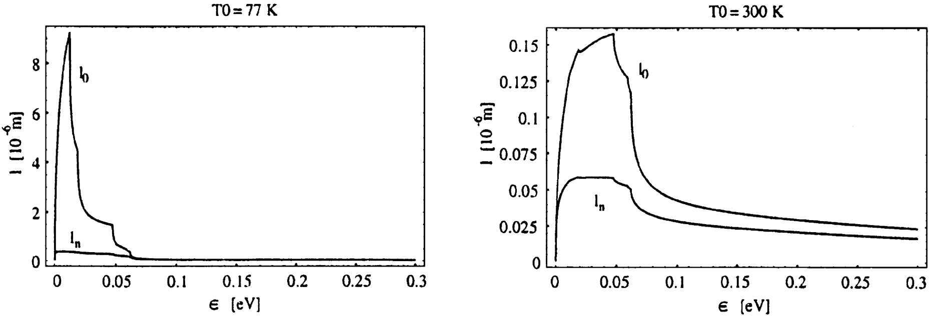

Fig. 1. Mean free paths l_0, l_n for $T_0 = 77$ K (left) and 300 K (right).

thermalize the electrons. The corresponding mean free paths, i.e. the average distances between interactions, are given by

$$l_0 = \frac{c}{\kappa_0}, \qquad l_n = \frac{c}{\kappa_n} \, . \tag{25}$$

These depend on the electron energy ε and the functions for the Kane dispersion law are shown in Fig. 1 for the lattice temperatures 77 and 300 K. The corresponding curves for the parabolic band approximation are very similar and are not shown here.

In particular, we read from the figures, that l_0 and l_n – or κ_0 and κ_n – are of the same order of magnitude at room temperature (300 K). At the temperature of liquid nitrogen (77 K) l_0 is one order of magnitude larger than l_n, but only for moderate electron energies. For high energies, both mean free paths are almost equal, $l_0/l_n = 1.115$.

For large electric fields, where the electrons gain a large amount of energy between the collisions, the energy of the electrons does not change considerably in one single collision. It needs many collisions with phonons to relax the electrons to equilibrium and we have to expect an effective mean free path – or relaxation length - which is larger than the mean free path l_0. In this case one can expand the right-hand side P of (19) for small values of $\hbar\omega^\eta/\varepsilon$ to find

$$P = 4\pi \sum_\eta \mathscr{B}_\eta N_{\mathrm{op}}^\eta \hbar\omega^\eta \left\{ \left[2\frac{\mathrm{d}N(\varepsilon)}{\mathrm{d}\varepsilon} u + N(\varepsilon)\frac{\partial u}{\partial \varepsilon} \right] (\mathrm{e}^{\theta_\eta/T_0} - 1) + \mathcal{O}\left(\frac{\hbar\omega^\eta}{\varepsilon}\right) \right\} .$$

For lack of something better, we consider the factor of u as the effective collision frequency – or inverse relaxation time – for hot electrons, viz.

$$\kappa_\infty = 8\pi \sum_\eta \mathscr{B}_\eta N_{\mathrm{op}}^\eta \hbar\omega^\eta \frac{\mathrm{d}N(\varepsilon)}{\mathrm{d}\varepsilon} (\mathrm{e}^{\theta_\eta/T_0} - 1) \quad \text{and} \quad l_\infty = \frac{c}{\kappa_\infty} \tag{26}$$

is the effective mean free path.

Fig. 2 shows the ratio l_∞/l_n in comparison to the former value l_0/l_n for the Kane dispersion. For large energies, the mean free path between interactions with optical phonons is much larger than the mean free path between collisions with acoustic phonons. We do not show the corresponding curves for parabolic bands, but state that for these l_∞/l_n increases faster with energy.

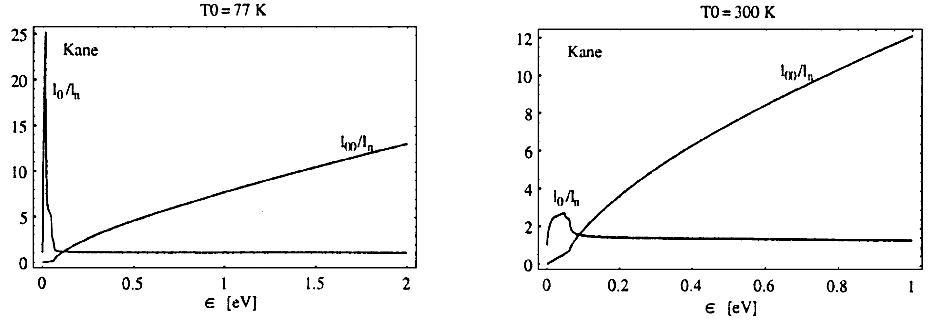

Fig. 2. Ratios l_∞/l_n and l_0/l_n for $T_0=77$ K (left) and 300 K (right) for the Kane dispersion law.

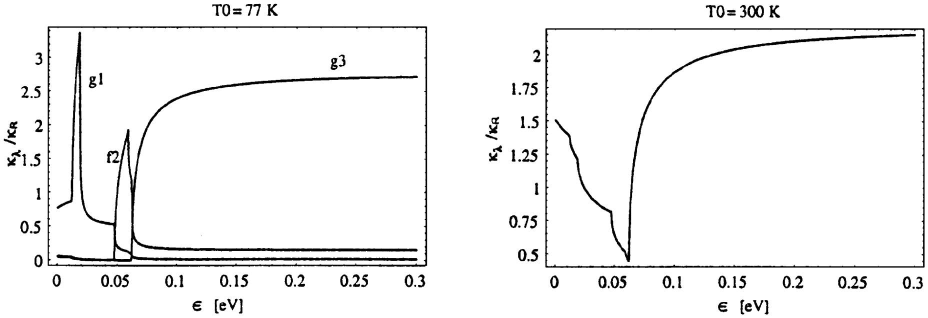

Fig. 3. κ_λ/κ_R for $\lambda=g_1,g_3,f_2$ at $T_0=77$ K and for $\lambda=g_3$ at $T_0=300$ K.

Thus, at low temperatures or high electric fields, the tendency towards an isotropic phase density predominates the tendency towards the Maxwellian.

At the end of this section, we ask whether one of the terms

$$\kappa_\lambda = 4\pi\mathscr{B}_\lambda N_{\mathrm{op}}^{\lambda}[N(\varepsilon+\hbar\omega^\eta)+\mathrm{e}^{\theta_\eta/T_0}N(\varepsilon-\hbar\omega^\eta)_{|+}]$$

in κ_0 dominates the remainder $\kappa_R=\kappa_0-\kappa_\lambda$. If this were the case, one had a tendency towards a Maxwellian times a periodic function, see Section 2.1.2. Fig. 3 shows the ratios κ_λ/κ_R for those λ where the ratio is bigger than 1 at least for some values of the energy. However, κ_λ/κ_R is almost of order one and we conclude that periodic equilibrium functions play no role.

3.4. Truncation at order 1 (SHE)

There exits a proper asymptotic limit [18,19] in case that the collision frequency towards isotropy dominates,

$$\kappa_n \gg \kappa_{0,\infty}\,. \tag{27}$$

As we have seen before in Section 3.3, this condition is fulfilled at low temperatures or large electric fields. Moreover, we assume that the mean free path l_n is much smaller than a macroscopic length L,

$$l_n \ll L \, .$$

At $T_0 = 77$ K we have $l_n \simeq 0.35 \times 10^{-6}$ m for small energies and $l_n \leqslant 0.05 \times 10^{-6}$ m for energies above 0.1 eV, so that – for the interesting case of high fields – the condition is fulfilled for $L \geqslant 0.5 \times 10^{-6}$ m. At $T_0 = 300$ K, we have for large energies $l_n \leqslant 0.02 \times 10^{-6}$ m, allowing for smaller $L \geqslant 0.2 \times 10^{-6}$ m.

We expand formally

$$u_{\langle i_1 \cdots i_n \rangle} = u^{(0)}_{\langle i_1 \cdots i_n \rangle} + \frac{1}{\kappa_n} u^{(1)}_{\langle i_1 \cdots i_n \rangle} + \mathcal{O}\left(\frac{1}{(\kappa_n)^2} \right), \quad n = 1, 2, \ldots \, , \tag{28}$$

insert this in (20) and obtain by comparison of the factors at $(\kappa_n)^0, (\kappa_n)^1$

$$u^{(0)}_{\langle i_1 \cdots i_n \rangle} = 0, \quad n = 1, 2, \ldots, \qquad u^{(1)}_{\langle i_1 \cdots i_n \rangle} = 0, \quad n = 2, 3, \ldots$$

and

$$\frac{c}{3} \left[\frac{\partial u}{\partial x_i} - e E_i \frac{\partial u}{\partial \varepsilon} \right] = -u^{(1)}_i \, . \tag{29}$$

Thus, in the limit (27) we have the equations

$$\frac{\partial u}{\partial t} + \frac{1}{N(\varepsilon)} \left[\frac{\partial}{\partial x_k} [N(\varepsilon) c u_k] - e E_k \frac{\partial}{\partial \varepsilon} [N(\varepsilon) c u_k] \right] = P \, ,$$

$$\frac{c}{3} \left[\frac{\partial u}{\partial x_i} - e E_i \frac{\partial u}{\partial \varepsilon} \right] = -\kappa_n u_i \, , \tag{30}$$

where we have used (6). In the literature, these equations are denoted as “spherical harmonics expansion model”, or SHE-model, [18,19,12,13]. Eq. (30) holds for all bands with spherical symmetry.

3.5. The drift-diffusion equation

Now, we assume that *both* mean free paths, l_0 and l_n, are considerably smaller than the macroscopic length L,

$$l_0 \ll L, \quad l_n \ll L \, . \tag{31}$$

From the discussion of Section 3.3 and its figures, it follows that the second condition can be met at low electric fields, if $L \geqslant 5 \times 10^{-5}$ m ($T_0 = 77$) or $L \geqslant 10^{-6}$ m ($T_0 = 300$ K), respectively.

When (31) is valid, we can formally expand u in (30) according to

$$u = u^{(0)} + \mathcal{O}\left(\frac{1}{\kappa_0} \right)$$

which yields, together with (10) and (16), the Maxwellian

$$u^{(0)} = 4\pi f_{|E} \tag{32}$$

so that the number density n is the only variable in the present limit. The evolution equation for n – the well-known continuity equation – follows by integration of the Boltzmann equation over k-space as

$$\frac{\partial n}{\partial t} + \frac{\partial J_k}{\partial x_k} = 0 \tag{33}$$

with the particle flux

$$J_k = \int c_k f \, \mathrm{d}\mathbf{k} = \int u_k c N(\varepsilon) \, \mathrm{d}\varepsilon \, . \tag{34}$$

From $(30)_2$, (32) and (34) follows the drift-diffusion law

$$J_k = -D \left[\frac{\partial n}{\partial x_k} + \frac{n e E_k}{k_B T_0} \right] , \tag{35}$$

where the diffusion coefficient D is determined by the collision frequency κ_n as

$$D = \frac{4}{3} \sqrt{\frac{2 k_B T_0}{\pi m}} \frac{\sqrt{\pi \alpha k_B T_0} \exp[-1/2\alpha k_B T_0]}{K_2(1/2\alpha k_B T_0)} \int \frac{c^2}{\kappa_n} N(\varepsilon) \mathrm{e}^{-\varepsilon / k_B T_0} \, \mathrm{d}\varepsilon \, . \tag{36}$$

The continuity equation (33) with the particle flux (35) forms the drift-diffusion equation, which is the most used macroscopic model in semiconductor physics. However, as we have seen, its use is limited to relatively large devices.

In Section 5.3 we shall compute the drift diffusion coefficient from the equations for the full moments; the coefficient (36) will be considered as a benchmark for comparison.

4. Full moments and the closure problem

4.1. Moments

For our considerations on the full moments we shall use the parabolic band approximation only. The corresponding calculations for the Kane dispersion are more involved, to involved, indeed, for a first study on multi moment methods [9].

Full moments of the phase density are defined as

$$u^r_{\langle i_1 i_2 \cdots i_n \rangle} = m \int c^{2r} c_{\langle i_1} c_{i_2} \cdots c_{i_n \rangle} f \, \mathrm{d}\mathbf{k} \, , \tag{37}$$

so that the $u^r_{\langle i_1 i_2 \cdots i_n \rangle}$ are the irreducible parts of traces of the moments $m \int c_{i_1} c_{i_2} \cdots c_{i_m} f \, \mathrm{d}\mathbf{k}$. Some of the moments have a physical interpretation on the macroscopic scale. In particular, we have

$u^0 = mn$ mass density ,

$u^0_i = mnv_i$ momentum density ,

$\frac{1}{2} u^1 = \frac{3}{2} n k_B T + \frac{mn}{2} v^2$ energy density ,

$$u^0_{ij} = \frac{1}{3} u^1 \delta_{ij} + u^0_{\langle ij\rangle} \qquad \text{momentum flux}\,,$$

$$\frac{1}{2} u^1_i \qquad \text{energy flux}\,, \tag{38}$$

n is the number density and v_i is the macroscopic velocity of the electrons; T is the electron temperature. The full moments depend on space and time only.

The hydrodynamic model [7,8,21,17,22] considers only the moments with physical interpretation, i.e. the set of 13 moments (38); sometimes the momentum flux is not considered as a variable [21]. Here, we do not restrict the attention to the moments with physical interpretation, but shall consider an *arbitrary* number of moments.

In equilibrium, where $f = f_{|E}$ holds, the moments assume the values

$$u^r_{|E} = u^0 \left(\frac{2k_B T_0}{m}\right)^r \frac{2}{\sqrt{\pi}} \Gamma\left(r + \frac{3}{2}\right), \quad u^r_{\langle i_1 i_2 \cdots i_n\rangle} = 0 \ (n \geqslant 1)\,. \tag{39}$$

4.2. Moment equations

Multiplication of the Boltzmann equation with $c^{2r} c_{\langle i_1} c_{i_2} \cdots c_{i_n\rangle}$ and integration over velocity space yields the equations for the moments $u^r_{\langle i_1 \cdots i_n\rangle}$. For the scalar moment u^r we obtain

$$\frac{\partial u^r}{\partial t} + \frac{\partial u^r_k}{\partial x_k} + 2r \frac{e}{m} E_k u^{r-1}_k = P^r \tag{40}$$

with the production

$$P^r = -\sum_\eta \hat{\mathscr{B}}_\eta \int \sqrt{c^2 + \chi_\eta}\, c^2 [c^{2r} - (c^2 + \chi_\eta)^r][u - \mathrm{e}^{\theta_\eta/T_0} u^{(+)}]\, \mathrm{d}c\,, \tag{41}$$

where $u(c) = m^3/\hbar^3 \int f\, \mathrm{d}\Omega$ is the first spherical harmonics moment and $u^{(+)} = u(\sqrt{c^2 + \chi_\eta})$. In (41) we have introduced the abbreviations

$$\hat{\mathscr{B}}_\eta = \frac{Z_\eta}{2\pi} \frac{m^2 (D_t K_\eta)^2}{\hbar^2 \varrho k_B \theta_\eta} N^\eta_{\mathrm{op}}, \quad \chi_\eta = \frac{2k_B \theta_\eta}{m}\,.$$

The choice $r=0$ gives the continuity equation (33). The moment equation for tensorial moments reads

$$\frac{\partial u^r_{\langle i_1 \cdots i_n\rangle}}{\partial t} + \frac{n}{2n+1} \frac{\partial u^{r+1}_{\langle i_1 \cdots i_{n-1}\rangle}}{\partial x_{i_n}} + \frac{\partial u^r_{\langle i_1 \cdots i_n k\rangle}}{\partial x_k}$$
$$+ 2r \frac{e}{m} E_k u^{r-1}_{\langle i_1 \cdots i_n k\rangle} + \frac{n(2r + 2n + 1)}{2n+1} \frac{e}{m} E_{\langle i_1} u^r_{i_2 \cdots i_n\rangle} = P^r_{\langle i_1 \cdots i_n\rangle} \tag{42}$$

with the productions

$$P^r_{\langle i_1 \cdots i_n\rangle} = -\hat{\mathscr{A}} u^{r+1/2}_{\langle i_1 \cdots i_n\rangle} - \sum_\eta \hat{\mathscr{B}}_\eta \int \sqrt{c^2 + \chi_\eta}\, c^2$$
$$\times \left[c^{2r+n} u_{\langle i_1 \cdots i_n\rangle}(c) + \sqrt{c^2 + \chi_\eta}^{\,2r+n} \mathrm{e}^{\theta_\eta/T_0} u^{(+)}_{\langle i_1 \cdots i_n\rangle} \right] \mathrm{d}c\,, \tag{43}$$

where

$$\hat{\mathscr{A}} = 4\pi\mathscr{A}\frac{m^2}{\hbar^3} = \frac{1}{\pi}\frac{m^2 k_B \mathscr{E}_l^2}{\hbar^4 \varrho U_l^2} T_0 .$$

Moreover, $u_{\langle i_1 \cdots i_n \rangle}(c) = m^3/\hbar^3 \int n_{\langle i_1} n_{i_2} \cdots n_{i_n \rangle} f \, \mathrm{d}\Omega$ is the nth spherical harmonics moment and $u^{(+)}_{\langle i_1 \cdots i_n \rangle} = u_{\langle i_1 \cdots i_n \rangle}(\sqrt{c^2 + \chi_\eta})$.

Unlike the spherical harmonics Eqs. (19), (20), the equations for the full moments (40), (42) do not form a proper set of equations. Indeed, the productions $P^r_{\langle i_1 \cdots i_n \rangle}$ are not related to the variables $u^r_{\langle i_1 \cdots i_n \rangle}$ but only to the spherical harmonics $u_{\langle i_1 \cdots i_n \rangle}(c)$. The corresponding closure problem will be discussed now.

4.3. The closure problem

In order to find a closed set of equations one has to consider a finite number of moments, and in this paper we consider the variables

$$u^r_{\langle i_1 i_2 \cdots i_n \rangle}, \quad n = 0, 1, \ldots, M, \quad r = 0, 1, \ldots, R . \tag{44}$$

The choice of the numbers M and R depends on the process under consideration. The moment equations (40) and (42) for moments (44) do not form a closed set of equations, since they contain the additional quantities

$$u^r_{\langle i_1 i_2 \cdots i_{M+1} \rangle}, \quad r = 0, 1, \ldots, R \text{ and } P^r_{\langle i_1 \cdots i_n \rangle}, \quad n = 0, 1, \ldots, M, \quad r = 0, 1, \ldots, R \tag{45}$$

which are a priori not related to the set of variables (44). Thus, constitutive functions are required which relate the unknowns (45) to the variables.

Since the unknowns are integrals of the phase density, the closure problem is solved when we have a phase density which is determined by the values of the variables. We consider the so-called normal solutions which have the form

$$f = \mathscr{F}(u^r_{\langle i_1 i_2 \cdots i_n \rangle}(x_i, t), c_i) . \tag{46}$$

f depends on space–time only through the moments and there is no dependence on gradients and time derivatives of the moments. For consistency the phase density (46) must fulfill the relations

$$u^r_{\langle i_1 i_2 \cdots i_n \rangle} = m \int c^{2r} c_{\langle i_1} c_{i_2} \cdots c_{i_n \rangle} \mathscr{F} \, \mathrm{d}\mathbf{k}, \quad n = 0, 1, \ldots, M, \quad r = 0, 1, \ldots, R . \tag{47}$$

4.4. Entropy maximum closure

Among all phase densities of the form (46) which fulfill (47), it seems to be natural to choose that function $\mathscr{F}_{\max}$ which is most probable in the sense that it corresponds to the maximum number of microscopic realizations. This distinguished function is that phase density which maximizes the entropy of the electrons [23,24]. As before the contributions of the Pauli principle can be ignored for the thin gas of electrons in semiconductors so that we can use the Boltzmann entropy density

$$s = -k_B \int f \ln f \, d\mathbf{k} \, . \tag{48}$$

Maximising the entropy density with the constraints of given values for moments (44) gives by a standard procedure

$$\mathscr{F}_{\max} = \exp\left[1 - \sum_{r,n} \Lambda^r_{\langle i_1 \cdots i_n \rangle} c^{2r} c_{\langle i_1} c_{i_2} \cdots c_{i_n \rangle}\right] \, . \tag{49}$$

By (47) the Lagrange multipliers $\Lambda^r_{\langle i_1 \cdots i_n \rangle}$ are functions of the moments and the relations $\Lambda^r_{\langle i_1 \cdots i_n \rangle}(u^s_{\langle j_1 \cdots j_m \rangle})$ are invertible [23]. Moreover, the closure with $\mathscr{F}_{\max}$ gives a system of symmetric hyperbolic type with convex extension and guarantees well-posedness for Cauchy problems as well as finite wave and shock speeds, see [23,24,28] for details.

Unfortunately, one cannot find analytic solutions of the integrals of $\mathscr{F}_{\max}$ in general. A fully analytic treatment is only possible if one considers the five variables u^0, u^1 and u^0_i, i.e. number density n, energy density $\frac{3}{2} n k_B T$ and velocity v_i. The corresponding maximized phase density is the shifted Maxwellian

$$\mathscr{F}^{(5)}_{\max} = n \sqrt{\frac{\hbar^2/m}{2\pi k_B T}}^{\,3} \exp\left[-\frac{m}{2k_B T}(c_i - v_i)^2\right] \tag{50}$$

with the temperature of the electron gas T. $\mathscr{F}^{(5)}_{\max}$ is the phase density of the energy transport model [29] which can be justified by an asymptotic limit in case that the collision frequency of electron–electron collisions dominates. This result is only of theoretical interest, however, since these collisions play no role in the rarefied electron gas in a semiconductor.

One may also expand the maximized phase density into a series in the Lagrange multipliers $\Lambda^r_{\langle i_1 \cdots i_n \rangle}$. This cumbersome procedure was until now performed for the 13 moment case which considers the variables (38) with expansions to second and third order [21,17,22]. The evaluation of $\mathscr{F}_{\max}$ by numerical integration is very cumbersome, up to now this was done for ideal gases only [30].

4.5. Grad expansion

For the motivation of Grad's phase density [25] we recall that the equilibrium phase density is given by the Maxwellian (9) so that the equilibrium values of the Lagrange multipliers are given by

$$\Lambda^0_{|E} = 1 - \ln\left[n \sqrt{\frac{\hbar^2/m}{2\pi k_B T_0}}^{\,3}\right], \qquad \Lambda^1_{|E} = \frac{m}{2k_B T_0}, \quad \Lambda^r_{\langle i_1 \cdots i_n \rangle |E} = 0 \, .$$

We introduce the non-equilibrium parts λ of the Lagrange multipliers by

$$\lambda^r_{\langle i_1 \cdots i_n \rangle} = \Lambda^r_{\langle i_1 \cdots i_n \rangle} - \Lambda^r_{\langle i_1 \cdots i_n \rangle |E}$$

with $\lambda^r_{\langle i_1\cdots i_n\rangle|E}=0$ and expand $\mathscr{F}_{\max}$ to the first order in λ to obtain

$$\mathscr{F}=f_{|E}\left[1-\sum_{r,n}\lambda^r_{\langle i_1\cdots i_n\rangle}c^{2r}c_{\langle i_1}c_{i_2}\cdots c_{i_n\rangle}\right]. \tag{51}$$

Now, $\mathscr{F}$ is a series in spherical harmonics and powers of the velocity with the Maxwellian as integration kernel. For small values of the λ's, this phase density coincides with the maximized phase density $\mathscr{F}_{\max}$ but for larger values of the λ's the phase density (51) is an approximation of the phase density in its own right [31,10,32].

Clearly, the usefulness of approximation (51) for the phase density depends on the number of expansion coefficients and the choice of the kernel. In fact, the use of the shifted Maxwellian (50) as kernel is the better choice for systems far from equilibrium [8,9,17,22,20], and we shall use it in the sequel so that we consider the approximation

$$\mathscr{F}_G=\mathscr{F}^{(5)}_{\max}\left[1-\sum_{r,n}\lambda^r_{\langle i_1\cdots i_n\rangle}c^{2r}c_{\langle i_1}c_{i_2}\cdots c_{i_n\rangle}\right]. \tag{52}$$

The kernel of the expansion must be chosen so that the phase density reduces to the Maxwellian $f_{|E}$ in equilibrium – this requirement is met by $\mathscr{F}^{(5)}_{\max}$.

It might well be that one needs a lower number of expansion coefficients – or Lagrange multipliers – if one chooses $\mathscr{F}_{\max}$ instead of $\mathscr{F}_G$. However, the additional expenditure for the numerical integration of $\mathscr{F}_{\max}$ cannot be compared with the much lower numerical cost of taking a larger number of moments into account.

5. Moments for the SHE model

5.1. Moments and phase density

From now on, we restrict ourselves to crystals where conditions (27) for the SHE model are fulfilled. Then, only scalar and vectorial moments play a role, see (30), and, by (28), the latter should be small. Accordingly, we consider the set of full moments

$$u^r=m\int c^{2r}f\,\mathrm{d}\mathbf{k},\qquad u^r_i=m\int c^{2r}c_i f\,\mathrm{d}\mathbf{k},\quad r=0,1,\ldots,R\,. \tag{53}$$

The corresponding moment equations build an approximation for the SHE model (30), and the quality of the approximation depends on the 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 Boltzmann equation or the SHE model, respectively.

Since all vectorial moments are small in the SHE limit, we need to consider only linear contributions in the vectors. This implies the omission of the kinetic energy $(u^0/2)v^2$ in the energy density $\frac{1}{2}u^1$ and the use of the phase density

$$f=f_{|T}\left[1-\sum_{s=0}^{R}\lambda^s c^{2s}-\sum_{s=0}^{R}\lambda^s_i c^{2s}c_i\right] \tag{54}$$

for the closure. $f_{|T}$ is the Maxwellian with the electron temperature T, viz.

$$f_{|T} = n\sqrt{\frac{\hbar^2/m}{2\pi k_B T}}^{3} \exp\left[-\frac{m}{2k_B T}c^2\right] ,$$

Eq. (54) is obtained by linearizing (52) in v_i.

The expansion coefficients λ, λ_i follow as

$$\lambda^t = -\frac{\sqrt{\pi}}{2}\sum_{s=2}^{R} \mathscr{C}_{ts}^{-1}\frac{u^s - u^s_{|T}}{u^0(2k_B T/m)^{s+t}}, \quad \lambda_i^t = -\frac{3\sqrt{\pi}}{2}\sum_{s=0}^{R} \hat{\mathscr{C}}_{ts}^{-1}\frac{u_i^s}{u^0(2k_B T/m)^{s+t+1}} \tag{55}$$

with

$$u^r_{|T} = u^0\left(\frac{2k_B T}{m}\right)^r \frac{2}{\sqrt{\pi}}\Gamma\left(r+\frac{3}{2}\right), \quad \mathscr{C}_{rs} = \Gamma\left(r+s+\frac{3}{2}\right),$$
$$\hat{\mathscr{C}}_{rs} = \Gamma\left(r+s+\frac{5}{2}\right) . \tag{56}$$

$u^r_{|T}$ are the moments of $f_{|T}$ with $u^0_{|T} = u^0$ and $u^1_{|T} = u^1$.

5.2. Moment equations

With the phase density (54) we obtain from (41) and (42) a closed set of equations for the moments (53),

$$\frac{\partial u^r}{\partial t} + \frac{\partial u^r_k}{\partial x_k} + 2r\frac{e}{m}E_k u_k^{r-1} = -\Pi^r - \sum_{s=2}^{R}\Theta_{rs}(u^s - u^s_{|T}) ,$$
$$\left[\frac{\partial u_i^r}{\partial t}\right] + \frac{1}{3}\frac{\partial u^{r+1}}{\partial x_i} + \frac{2r+3}{3}\frac{e}{m}E_i u^r = -\sum_{s=0}^{R}\hat{\Theta}_{rs}u_i^s \tag{57}$$

for $r = 0, 1, \ldots, R$. The brackets around the time derivative of u_i^r indicate that it can be ignored in the SHE limit, see $(30)_2$.

The production vector Π^r and the matrices of mean collision frequencies Θ_{rs}, $\hat{\Theta}_{rs}$ are given by

$$\Pi^r = \frac{2}{\sqrt{\pi}}n\sqrt{\frac{2k_B T}{m}}\left(\frac{2k_B T}{m}\right)^r \sum_\eta \hat{\mathscr{B}}_\eta(1 - \mathrm{e}^{\gamma_\eta})(J^\eta_{r,0} - J^\eta_{0,r}) ,$$

$$\Theta_{rs} = \sqrt{\frac{2k_B T}{m}}\left(\frac{2k_B T}{m}\right)^{r-s}\sum_t \mathscr{C}_{ts}^{-1}\sum_\eta \hat{\mathscr{B}}_\eta[J^\eta_{r+t,0} - J^\eta_{t,r} + \mathrm{e}^{\gamma_\eta}(J^\eta_{0,r+t} - J^\eta_{r,t})] , \tag{58}$$

$$\hat{\Theta}_{rs} = \sqrt{\frac{2k_B T}{m}}\left(\frac{2k_B T}{m}\right)^{r-s}\sum_t \hat{\mathscr{C}}_{ts}^{-1}\left[\hat{\mathscr{A}}\Gamma(r+t+3) + \sum_\eta \hat{\mathscr{B}}_\eta[J^\eta_{r+t+1,0} + \mathrm{e}^{\gamma_\eta}J^\eta_{0,r+t+1}]\right]$$

with the integrals

$$J^{\eta}_{r,s} = 2\int_0^{\infty} x^{2+2r} \sqrt{x^2 + \alpha_\eta}^{\,1+2s} \mathrm{e}^{-x^2}\,\mathrm{d}x \tag{59}$$

and the temperature ratios

$$\alpha_\eta = \frac{\theta_\eta}{T}, \quad \gamma_\eta = \theta_\eta\left(\frac{1}{T_0} - \frac{1}{T}\right).$$

The integrals $J^{\eta}_{r,s}$ may be expressed through the modified Bessel functions of the second kind $K_n(\alpha_\eta/2)$, see Appendix B for details.

The moment u^{R+1} in system (57) is related to variables (53) by a constitutive equation which follows from (54) as

$$u^{R+1} = u^{R+1}_{|T} + \sum_{s=0}^{R}\sum_{t=2}^{R} \mathscr{C}_{st}^{-1}\Gamma\left(R+s+\frac{5}{2}\right)\frac{u^t - u^t_{|T}}{(2k_B T/m)^{t-R-1}}\,.$$

In equilibrium, the right-hand sides of (57) must vanish, and we have $\gamma_\eta = 0$ or $T = T_0$; moreover, the moments assume their equilibrium values $u^r = u^r_{|T_0} = u^r_{|E}$ and $u^r_{i|E} = 0$.

5.3. Local equilibrium and drift-diffusion equation

As a first test for the moment method we consider the drift-diffusion limit (31) of Eq. (57) where the electron gas is in local equilibrium. The scalar moments assume their equilibrium values in this case, $u^r = u^r_{|E}$, so that $T = T_0$ holds.

For the calculation of the particle flux and the diffusion coefficient we proceed with the vectorial equation $(57)_2$, where we introduce the equilibrium values of the moments u^r and, as in (29), set $u^r_i = 0$ on the left-hand side to obtain

$$\frac{1}{3}\left(\frac{2k_B T_0}{m}\right)^{r+1}\frac{2}{\sqrt{\pi}}\Gamma\left(r+\frac{5}{2}\right)\left[\frac{\partial u^0}{\partial x_i} + \frac{u^0 e E_i}{k_B T_0}\right] = -\sum_{s=0}^{R}\hat{\Theta}_{rs}u^s_i\,.$$

Solving this for $J_i = (1/m)u^0_i$ yields the drift diffusion law (35) but now the diffusion coefficient is given by

$$\hat{D} = \frac{4}{3}\sqrt{\frac{2k_B T_0}{\pi m}}\sum_{r=0}^{R}\hat{\vartheta}_{0r}^{-1}\frac{1}{2}\Gamma\left(r+\frac{5}{2}\right) \tag{60}$$

with the matrix

$$\hat{\vartheta}_{rs} = \sum_{t=0}^{R}\hat{\mathscr{C}}_{ts}^{-1}\left[\hat{\mathscr{A}}\Gamma(r+t+3) + \sum_{\eta}\hat{\mathscr{B}}_\eta[J^{\eta}_{r+t+1,0} + J^{\eta}_{0,r+t+1}]\right],$$

the integrals J^{η} in $\hat{\vartheta}_{rs}$ must be evaluated with $T = T_0$.

The new diffusion coefficient $\hat{D}$ must be compared with the former result (36) which we use as a benchmark here (with $\alpha = 0$). Since $\hat{D}$ depends on the number of moments R, this comparison is an indicator for the choice of R: If $\hat{D}$ coincides with D from (36), the number of moments is sufficient – at least for the case of local equilibrium.

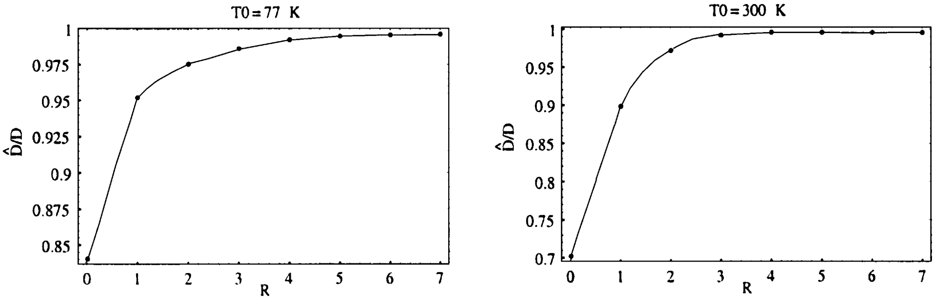

Fig. 4. Ratio $\hat{D}/D$ of the diffusion coefficients (36, 60) versus the moment number R for 77 and 300 K.

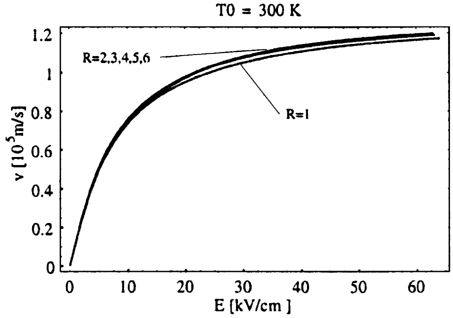

Fig. 5. Stationary homogeneous process ($T_0 = 300$ K): mean speed v as function of the electric field E with moment numbers $R = 1, 2, 3, 4, 5, 6$.

Fig. 4 shows the ratio $\hat{D}/D$ as a function of the moment numbers for $T_0 = 77$ and 300 K. For a moment number $R \geqslant 4$, both diffusion coefficients, $\hat{D}$ and D, have almost the same value. For lower R, however, the results differ. The choice $R = 0$, with number density n and particle flux J_k as sole moments, gives an error in the diffusion coefficient between 15% and 30%, depending on temperature. Also with $R = 1$, corresponding to the hydrodynamic model [8,17,22] the error is in the range of 5–10%.

5.4. Stationary homogeneous process

Our next test for the moment system (57) is a one-dimensional homogeneous stationary process in an infinite semiconductor with constant electric field $E_i = \{E, 0, 0\}$. In particular, we are interested in the velocity v_i in dependence of the electric field.

The field equations (57) reduce to algebraic equations, viz.

$$2r\frac{e}{m}Eu_1^{r-1} = -\Pi^r - \sum_{s=2}^{R}\Theta_{rs}(u^s - u^s_{|T}), \qquad \frac{2r+3}{3}\frac{e}{m}Eu^r = -\sum_{s=0}^{R}\hat{\Theta}_{rs}u_1^s \, . \qquad (61)$$

The solution of (61) is outlined in Appendix C, here we present only the results.

Fig. 5 shows the drift velocity v in dependence of the electric field for $T_0 = 300$ K with moment numbers $R = 1, \ldots, 6$. For large fields, the velocity goes to a constant

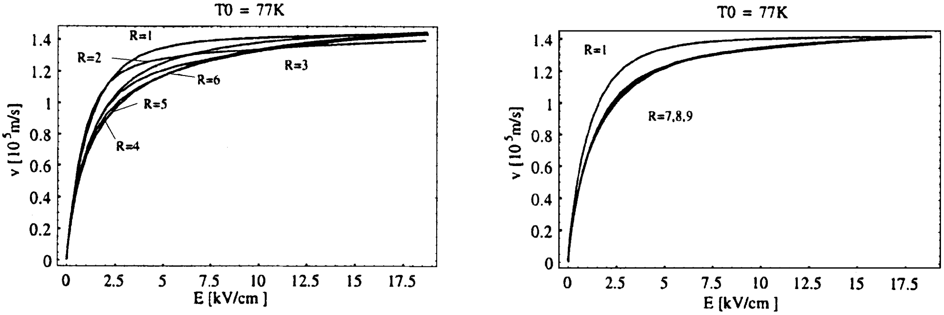

Fig. 6. Stationary homogeneous process ($T_0 = 77$ K): mean speed v as function of the electric field E with moment numbers $R = 1,2,3,4,5,6$ (left) and $R = 1,7,8,9$ (right).

limit, this is the well-known saturation effect [4,5]. All curves match very well, so that for the description of this process a moment number of $R = 1$ is sufficient.

At lower temperatures, this is not true anymore: Fig. 6 shows on the left the same curves for a lattice temperature $T_0 = 77$ K. The increase of the moment number changes the results considerably at fields below 20 kV/cm. For $R \geqslant 7$ the result does not change anymore, see the right part of Fig. 6.

The moment number has no influence at large fields, all choices of R lead to the same saturation velocity. This behavior reflects the high-energy solution of the SHE-model with parabolic bands, which yields a phase density of the form $f_{|T}(1 + \lambda_i n_i)$ [20].

5.5. Non-stationary homogeneous process

As last example for the influence of the moment number on the results, we consider a homogeneous crystal in thermal equilibrium which is suddenly subjected to a constant electric field E. The plots show the velocity as a function of time which exhibits the well-known velocity overshoot [4,5] for small times before the result reaches the saturation value of the last section.

For the calculation of the overshoot, one has to consider the time derivatives in $(57)_2$. However, these should play no role in the proper SHE-limit and in taking them into account we operate on an improper time scale. Note moreover, that the condition (27) is not well fulfilled since the electron energies are to small in the following calculations.

In Fig. 7 we show the result for room temperature $T = 300$ K for $E = 10$ kV/cm and $E = 50$ kV/cm. The peak value of v is the same for all moment numbers $R \geqslant 2$, but the results differ in the minimum after the peak, which becomes more pronounced with increasing moment number. For the higher field $E = 50$ kV/cm the differences between the curves are more marked.

The minimum after the peak is not observed in Monte-Carlo simulations [4], where the velocity is monotony decreasing after the peak. It may be that the minimum is an artefact of our equations due to the wrong time scale under consideration or insufficient choice of moments.

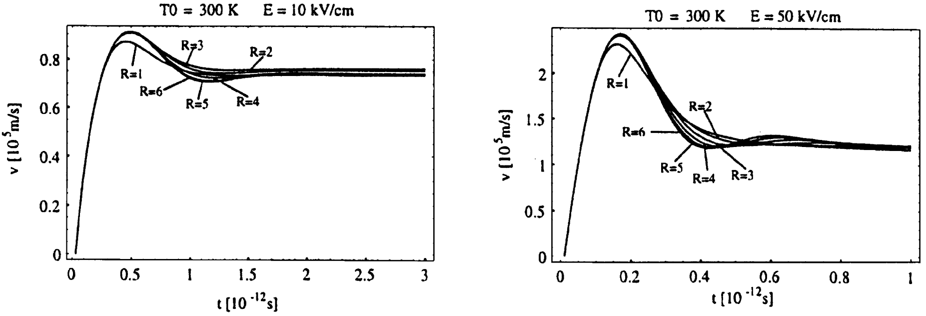

Fig. 7. Non-stationary homogeneous process: drift velocity v as a function of time t for $T_0 = 300$ K and electric fields $E = 10$ kV/cm (left) and 50 kV/cm (right) for various moment numbers R.

The minimum appears also when one considers the first two spherical harmonics equations (scalar and vectorial) with both time derivatives. Comparison between the spherical harmonics solution and the moment equations shows an excellent agreement for $R \geqslant 6$ [33].

6. Conclusions

In the present paper, we have examined moment equations for electrons in semiconductors. First, we studied spherical harmonics moments, where we laid emphasis on the discussion of collision frequencies and mean free paths. This allowed us to identify the ranges of applicability for the drift-diffusion model, where the local phase density is Maxwellian, and the SHE-model, where the phase density is almost isotropic.

Then, we presented the moment method for full moments with a discussion of the closure problem. Explicitly, we treated a case with scalar and vectorial moments, as is appropriate if the phase density is almost isotropic, i.e. in the range of validity of the SHE-model. The results of the moment method depend on the number of moments taken into account and we have shown for several model processes that the results converge for increasing moment number.

The required number of moments changes with the process under consideration and varies from $R=1$ or 2 (saturation velocity) to $R=6$ (velocity overshoot). This implies in particular that the hydrodynamic model with $R=1$ is not sufficient for the description of all processes.

It should be remembered that there are no free parameters in our moment equations. It is common to fit the constants in the production terms of the hydrodynamic model to Monte Carlo data, though, which ensures perfect results for the processes used for the fitting [21]. Whether the fitting is appropriate for other processes is not clear.

The solutions of our extended moment equations agree well with solutions of the corresponding spherical harmonics equations [33] and can be solved at lower numerical cost.

Until now, a high moment number is used only together with the parabolic band approximation. The use of more realistic models like the Kane dispersion law or the spherical full-band model of Ref. [12] is possible for the 13 moment case [9]. Future studies will show whether non-parabolic bands may be incorporated into an extended set of moment equations. If this were possible, the moment equations will a competitor for the full band spherical harmonics equations.

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Appendix A. Trace-free tensors and spherical harmonics

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

$$S_{i_1 i_2 \ldots i_j \ldots i_k \ldots i_n} \delta_{i_j i_k} = 0$$

holds for every pair i_j, i_k. The irreducible part of a symmetric tensor $A_{i_1 i_2 \ldots i_n}$ follows from [15]

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

where

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

$$\left|\left|\frac{n}{2}\right|\right| = \begin{cases} \frac{n}{2} & n \text{ even}, \\ \frac{n-1}{2} & n \text{ uneven}, \end{cases} \qquad n!! = \prod_{j=0}^{||(n-1)/2||} (n-2j) .$$

For the daily work, it is useful to write instead [16]

$$A_{\langle i_1 \cdots i_n \rangle} \sum_{k=0}^{||n/2||} b_{n,k} (\delta_{i_1 i_2} \cdots \delta_{i_{2k-1} i_{2k}} A^{(k)}_{i_{2k+1} \cdots i_n} + \cdots (P_{n,k} \text{ terms})) ,$$

where $A^{(k)}_{i_{2k+1} \cdots i_n}$ is the kth trace of $A_{i_1 \cdots i_n}$ and the sum in brackets extends over all P_{nk} different permutations of the indices. We have

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

The first few tensors $A_{\langle i_1\cdots i_n\rangle}$ read

$$\begin{aligned}A_{\langle i\rangle} &= A_i\,,\\ A_{\langle ij\rangle} &= A_{ij}-\tfrac{1}{3}A_{kk}\delta_{ij}\,,\\ A_{\langle ijk\rangle} &= A_{ijk}-\tfrac{1}{5}(A_{ill}\delta_{jk}+A_{jll}\delta_{ik}+A_{kll}\delta_{ij})\,.\end{aligned}$$

The tensor $A_{i_1\cdots i_n}$ may also be written as a sum of its trace-free parts [16],

$$A_{i_1\cdots i_n}=\sum_{k=0}^{||n/2||}\hat{b}_{n,k}(\delta_{i_1i_2}\cdots\delta_{i_{2k-1}i_{2k}}A^{(k)}_{\langle i_{2k+1}\cdots i_n\rangle}+\cdots(P_{nk}\text{ terms}))\,,$$

where $A^{(k)}_{\langle i_{2k+1}\cdots i_n\rangle}$ is the trace-free part of the kth trace of $A_{i_1\cdots i_n}$ and

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

Spherical harmonics may be represented through the trace-free tensors [14]

$$n_{\langle i_1}\ldots n_{i_n\rangle}$$

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

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

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

$$\delta_{k_1\cdots k_l}=\delta_{k_1k_2}\cdots\delta_{k_{l-1}k_l}+\cdots+\left(\frac{l!}{(l/2)!2^{l/2}},\text{ terms}\right).$$

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

$$A_{i_1i_2\ldots i_n}\int n_{\langle i_1}\ldots n_{i_n\rangle}n_{\langle j_1}\ldots n_{j_m\rangle}\,\mathrm{d}\Omega=\begin{cases}0, & n\neq m\,,\\ \frac{4\pi n!}{\prod\limits_{j=0}^{n}(2j+1)}A_{\langle j_1\cdots j_n\rangle}, & n=m\,,\end{cases}\tag{A.1}$$

$$n_{\langle i_1}\ldots n_{i_n\rangle}n_k=n_{\langle i_1}\ldots n_{i_n}n_{k\rangle}+\frac{n}{2n+1}n_{\langle\langle i_1}\ldots n_{i_{n-1}\rangle}\delta_{i_n\rangle k}.$$

Appendix B. Integrals $J^{\eta}_{r,s}$ and Bessel functions

The integrals $J^{\eta}_{r,s}$ (59) can be expressed by the modified Bessel functions of the second kind

$$K_n\left(\frac{\alpha_\eta}{2}\right)=\frac{1}{(2n-1)!!}\frac{1}{(\alpha_\eta/2)^n}\int_{\alpha_\eta/2}^{\infty}\sqrt{z^2-\left(\frac{\alpha_\eta}{2}\right)^2}^{\,n-1/2}\mathrm{e}^{-z}\,\mathrm{d}z\,.$$

The substitution $z = x^2 + \alpha_\eta/2$ yields for the integrals

$$J^{\eta}_{r,s} = \mathrm{e}^{\alpha_\eta/2} \sum_{k=0}^{r-s} \binom{r-s}{k} \left(-\frac{\alpha_\eta}{2}\right)^{r-s-k} L_{s,k} \quad (r \geqslant s)$$

and

$$J^{\eta}_{r,s} = \mathrm{e}^{\alpha_\eta/2} \sum_{k=0}^{s-r} \binom{s-r}{k} \left(\frac{\alpha_\eta}{2}\right)^{s-r-k} L_{r,k} \quad (r \leqslant s)\,,$$

where $L_{s,k}$ stands for

$$L_{s,k} = \int_{\alpha_\eta/2}^{\infty} \left(z^2 - \frac{\alpha_\eta^2}{4}\right)^{s+1/2} z^k \mathrm{e}^{-z}\, \mathrm{d}z\,.$$

For the $L_{s,k}$ one shows easily, that

$$L_{s,k+2} = L_{s+1,k} + \frac{\alpha_\eta^2}{4} L_{s,k}, \quad L_{s,0} = (2s+1)!! \left(\frac{\alpha_\eta}{2}\right)^{s+1} K_{s+1}\left(\frac{\alpha_\eta}{2}\right)\,,$$

$$L_{s,0} = (2s+1)!! \left(\frac{\alpha_\eta}{2}\right)^{s+2} K_{s+2}\left(\frac{\alpha_\eta}{2}\right)$$

hold, where the last equality follows by partial integration. Going backwards through the formulae, one finds $J^{\eta}_{r,s}$ in terms of the Bessel functions.

Appendix C. Solution for the stationary homogeneous process

For the solution of (61) it is convenient to use dimensionless moments defined by

$$m^r = \frac{u^r}{u^0 (2k_B T/m)^r}, \qquad v^r = \frac{u_1^r}{u^0 \sqrt{2k_B T/m}(2k_B T/m)^r}\,,$$

for which the moment equations read

$$r\mathscr{E} v^{r-1} = -\hat{\Pi}^r - \sum_{s=2}^{R} \vartheta_{rs} \left(m^s - \frac{2\Gamma(s+\frac{3}{2})}{\sqrt{\pi}}\right)\,,$$

$$\frac{1}{3}\left(r + \frac{3}{2}\right) \mathscr{E} m^r = -\sum_{s=0}^{R} \hat{\vartheta}_{rs} v^s\,, \tag{C.1}$$

$r = 0, 1, \ldots, R$. Note that $m^0 = 1$ and $m^1 = \frac{3}{2}$ hold and that the first equation is an identity for $r = 0$. $\mathscr{E}$ is the dimensionless electric field

$$\mathscr{E} \frac{eE}{\hat{\mathscr{A}} k_B T}$$

and the dimensionless production vector $\hat{\Pi}^r$ and matrices of mean collision frequencies $\vartheta_{rs}, \hat{\vartheta}_{rs}$ are given by

$$\hat{\Pi}^r = \frac{2}{\sqrt{\pi}} \sum_{\eta} \frac{\hat{\mathscr{B}}_\eta}{\hat{\mathscr{A}}} (1 - \mathrm{e}^{\gamma_\eta})(J^{\eta}_{r,0} - J^{\eta}_{0,r})\,,$$

$$\vartheta_{rs} = \sum_t \mathscr{C}_{ts}^{-1} \sum_\eta \frac{\hat{\mathscr{B}}_\eta}{\hat{\mathscr{A}}} [J^\eta_{r+t,0} - J^\eta_{t,r} + \mathrm{e}^{\gamma_\eta}(J^\eta_{0,r+t} - J^\eta_{r,t})] ,$$

$$\hat{\vartheta}_{rs} = \sum_t \hat{\mathscr{C}}_{ts}^{-1} \left[\Gamma(r+t+3) + \sum_\eta \frac{\hat{\mathscr{B}}_\eta}{\hat{\mathscr{A}}} [J^\eta_{r+t+1,0} + \mathrm{e}^{\gamma_\eta} J^\eta_{0,r+t+1}] \right] .$$

The solution of the analytic equations (C.1) proceeds in several steps. In the first step, we rewrite $(\mathrm{C}.1)_1$ and invert $(\mathrm{C}.1)_2$ so that

$$r\mathscr{E}v^{r-1} = -\bar{\Pi}^r - \sum_{s=2}^R \vartheta_{rs} m^s ,$$

$$v^t = -\frac{\mathscr{E}}{3} \sum_{r=0}^R \hat{\vartheta}_{tr}^{-1} \left(r + \frac{3}{2} \right) m^r = -\frac{\mathscr{E}}{2} \hat{\vartheta}_{t0}^{-1} - \frac{5}{4} \mathscr{E} \hat{\vartheta}_{t1}^{-1} - \frac{\mathscr{E}}{3} \sum_{r=2}^R \hat{\vartheta}_{tr}^{-1} \left(r + \frac{3}{2} \right) m^r , \tag{C.2}$$

where $\bar{\Pi}^r$ stands for

$$\bar{\Pi}^r = \hat{\Pi}^r - \sum_{s=2}^R \vartheta_{rs} \frac{2}{\sqrt{\pi}} \Gamma \left(s + \frac{3}{2} \right) .$$

Now, the moments v^t can be eliminated and we find after little rearrangement the equations

$$\sum_{s=2}^R \left[\vartheta_{1s} - \frac{1}{3} \mathscr{E}^2 \hat{\vartheta}_{0s}^{-1} \left(s + \frac{3}{2} \right) \right] m^s = \tilde{\Pi}^1 \quad \text{and} \quad \sum_{s=2}^R A_{rs} m^s = \tilde{\Pi}^r$$

with the quadratic matrix A_{rs} and the vector $\tilde{\Pi}^r$ given by

$$A_{rs} = \left[\vartheta_{rs} - \frac{r}{3} \mathscr{E}^2 \hat{\vartheta}_{r-1s}^{-1} \left(s + \frac{3}{2} \right) \right] , \quad r, s = 2, \ldots, R ,$$

$$\tilde{\Pi}^r = \frac{r}{2} \mathscr{E}^2 \left(\hat{\vartheta}_{r-1,0}^{-1} + \frac{5}{2} \hat{\vartheta}_{r-1,1}^{-1} \right) - \bar{\Pi}^r , \quad r = 1, \ldots, R .$$

By inversion of A_{rs} we find

$$m^s = \sum_{t=2}^R A_{st}^{-1} \tilde{\Pi}^t \tag{C.3}$$

and

$$\sum_{s=2}^R \sum_{t=2}^R \left[\vartheta_{1s} - \frac{1}{3} \mathscr{E}^2 \hat{\vartheta}_{0s}^{-1} \left(s + \frac{3}{2} \right) \right] A_{st}^{-1} \tilde{\Pi}^t = \tilde{\Pi}^1 . \tag{C.4}$$

Inspection shows, that the last equation is a polynomial in $\mathscr{E}^2$ with coefficients that depend on the electron temperature T with the crystal temperature T_0 as parameter. For $R = 1$ the l.h.s of (C.4) vanishes, so that it reads $0 = \tilde{\Pi}^1$.

Eq. (C.4) has to be solved numerically. It is advantageous to prescribe the temperature T and to solve for the electric field. Due to the polynomial form, there are several solutions $\mathscr{E}(T)$, most of these, however, give complex values for $\mathscr{E}$ and are meaningless. Depending on the value of R we obtained several real solution curves and only one of these fulfills the equilibrium condition $\mathscr{E}(T_0) = 0$ and therefore is considered to be the physical solution. From the numerical solution follow the moments by (C.3) and (C.4).

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