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Non-parabolic macroscopic transport models for semiconductor device simulation

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Abstract

We present a formulation of non-parabolic macroscopic transport models which avoids the commonly used relaxation time approximation by using an expansion of the scattering integral into the odd moments of the distribution function. The parameters of this expansion and the closure relations required in the final transport model are directly calculated via analytical models of the distribution function. These models are obtained by displacing an isotropic distribution function with an energy-dependent displacement and expanding the displaced distribution function up to second-order. This allows, for instance, to investigate the commonly neglected second-order contributions to the energy tensor in more detail. In addition, new models for the non-parabolicity corrections of the streaming terms are suggested. In a detailed discussion non-parabolic macroscopic transport models of order four and six are compared.

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1. Introduction

Boltzmann's transport equation describes the motion of carriers in a solid subject to external and internal forces and is of fundamental importance for the modeling of

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semiconductor devices. Its solution is the microscopic distribution function $f(\mathbf{k}, \mathbf{r}, t)$. Since the distribution function provides information about a particle's momentum and position simultaneously, the distribution function is a classical concept neglecting Heisenberg's uncertainty principle. Carrier scattering is modeled using Fermi's Golden Rule.

From the distribution function macroscopically observable quantities such as the electrical current density can be calculated. In addition to the current various other quantities of interest can be obtained from the distribution function such as the particles' concentration and average carrier energy. However, direct solution of Boltzmann's equation is very time-consuming even with modern computers. Approximate solutions can be obtained from macroscopic transport models which determine a certain number of moments of the distribution function. These models are derived from Boltzmann's equation by applying the method of moments, transforming Boltzmann's equation into an infinite set of equations. To obtain a tractable equation set, this hierarchy has to be truncated after N equations. When only the first two moment equations are used, the drift-diffusion model is obtained [1]. From the first three moment equations one gets the hydrodynamic model [2] whereas the first four moment equations (and some additional assumptions) give an energy-balance model [3,4].

Independent of their order N, all macroscopic transport models are based on some more or less stringent approximations introduced in their derivation. This issue is fundamentally related to the fact that the truncated equation set contains more moments than equations. After deciding on a set of unknowns the additional moments have to be expressed as a function of those unknowns to close the equation system. Since this is not exactly possible, macroscopic transport models differ basically in the assumptions used for relating the additional moments to the unknowns of the equation system.

The most obvious problem is that the highest-order equation determining the Nth moment contains the $(N+1)$th moment. This $(N+1)$th moment provides the coupling to all higher-order equations and thus contains the information missing in the lower-order equations. Following the argumentation used in gas-dynamics [5], where for instance Grad's model assumes that the system is sufficiently described by the thirteen moments occurring in the first three moment equations, one assumes that the contribution of the higher-order moments is small. This issue is of fundamental importance as it justifies the truncation of the equation system. Up to now it is still not clear how many moments are really required to accurately describe carrier transport in modern semiconductor devices. We will show in the sequel that some commonly used assumptions are rather crude.

Another crucial step is the modeling of the moments of the scattering operator, particularly the odd moments. Conventionally, these moments are expressed using a macroscopic relaxation time approximation. Written in terms of mobilities this approach maintains the familiar form of the current relations known from the drift-diffusion equations. In the relaxation time approximation the mobilities are normally expressed as a function of the average carrier energy, which is an even moment of the distribution function. A rigorous treatment reveals, however, that the

mobilities as odd moments of the scattering integral depend on the odd moments of the distribution function such as the current and the energy flux [6,7]. By assuming that the ratios of these fluxes approximately behave as observed under homogeneous conditions, this flux dependence is commonly transformed into an average energy dependence. This might impair the quality of the model and we present an alternative formulation which avoids this assumption.

Finally, there is the issue of the band structure. It is commonly agreed upon that the assumption of a parabolic band structure is insufficient for the description of hot-carrier effects. In particular, it has been shown that a non-parabolic band structure modifies the driving forces [4]. Since these non-parabolicity factors cannot be exactly expressed as a function of the available moments, various approaches have been considered. They range from simple constant approximations [8] and average energy dependent expressions [9] to models based on data extracted from homogeneous Monte Carlo simulations [10].

All these issues can be rigorously dealt with by using a self-consistent analytical description of the distribution function. The parameters of this analytical distribution function model are determined by the unknowns of the transport model. With this distribution function model the closure relations for the additional moments can then be calculated in a more or less straightforward manner. Obviously, the quality of this distribution function model has a strong impact on the quality of the resulting closure relations and thus on the macroscopic transport model. Here, we compare six moments descriptions [11] with models based on a heated Maxwellian distribution.

To quantify the accuracy of macroscopic transport models it is mandatory to compare their results with more rigorous solutions of Boltzmann's equation, for instance with results obtained from Monte Carlo models. It is of course important not to limit the comparison to the homogeneous case but to also consider realistic device structures which display non-homogeneity effects which have been the main motivation for the development of higher-order macroscopic transport models in the first place. To capture the two-dimensional electrostatics of MOS transistors we use a one-dimensional cut along the surface through the potential resulting from a two-dimensional energy-transport [4] solution. This one-dimensional cut is then used for a non-selfconsistent Monte Carlo simulation to give a one-dimensional approximation of carrier transport. As an example device we use the 90 nm well-tempered MOS [12] with the bias conditions $V_D = V_G = 1\,V$. The issue of self-consistency, which is important for realistic simulations [13], is neglected here since it further complicates the comparison. It is assumed that when a non-selfconsistent solution of a macroscopic transport model agrees better with a non-selfconsistent Monte Carlo simulation than another macroscopic transport model, that this improved accuracy is preserved in the self-consistent simulation. Of primary importance is the velocity profile which determines the carrier concentration in a one-dimensional simulation and is thus the primary coupling parameter to Poisson's equation.

In the Monte Carlo code we use a single equivalent isotropic but non-parabolic band described by Kane's dispersion relation to capture the main contribution of non-parabolicity. We assume a linear scattering operator and consider phonon and

impurity scattering based on Fermi's Golden Rule. The expressions derived for the distribution function and the relations derived therefrom are evaluated with the moments obtained from the Monte Carlo simulation and not in a self-consistent way. However, we only take the moments $\langle \mathscr{E}^i \rangle$ and $\langle \mathscr{E}^i \mathbf{u} \rangle$ which would be obtained from a corresponding macroscopic transport model. Such an evaluation can, therefore, be considered a consistency test and leaves some uncertainty as to the quality of the actual implementation. However, since from these consistency tests many characteristic properties of the relations can be identified, we consider them a useful tool to supplement any theoretical derivation.

The main purpose of this article is to investigate how the wealth of information provided by Boltzmann's equation can be approximated by higher-order moment equation systems. Particular emphasis will be put on the derivation of the closure relations which significantly determine the accuracy of the final macroscopic transport model. Therefore, the discussion will be limited to a single equivalent band which is expected to serve as a realistic example. If several bands are of importance and the equivalent band approximation is not justified, the theory has to be extended to multiple coupled moment equation systems [2].

2. Boltzmann's equation

We start our derivation from the single particle Boltzmann transport equation [14]

$$\partial_t f + \mathbf{u} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = Q[f] \,. \tag{1}$$

Boltzmann's equation is a semi-classical kinetic equation, which assumes that the motion of carriers follows the classical Newton laws. The scattering operator Q represents the rate of change of f due to collisions and is modeled via Fermi's Golden Rule. We limit the discussion to the non-degenerate case and neglect electron–electron scattering which results in a linear scattering operator. The solution of Boltzmann's equation is the time dependent carrier distribution function $f(\mathbf{k}, \mathbf{r}, t)$ in the six-dimensional phase space. The group velocity $\mathbf{u}$ appearing in (1) can be obtained from perturbation theory as [15]

$$\mathbf{u}(\mathbf{k}, \mathbf{r}) = \nabla_{\mathbf{p}} \mathscr{E}(\mathbf{k}, \mathbf{r}) \,, \tag{2}$$

where $\mathscr{E} = \mathscr{E}(\mathbf{k}, \mathbf{r})$ represents the kinetic carrier energy which is given by the band structure. The force $\mathbf{F}$ exerted on the electrons in the presence of electric and magnetic fields and inhomogeneous material properties is for electrons generally given as

$$\mathbf{F}(\mathbf{k}, \mathbf{r}, t) = -\nabla_{\mathbf{r}}(E_{\mathrm{c},0}(\mathbf{r}) + \mathscr{E}(\mathbf{k}, \mathbf{r})) - \mathrm{q}(\mathbf{E}(\mathbf{r}, t) + \mathbf{u}(\mathbf{k}, \mathbf{r}) \times \mathbf{B}(\mathbf{r}, t)) \tag{3}$$

and depends on $\mathbf{k}$, $\mathbf{r}$, and the time t. The two spatial gradients ($\nabla_{\mathbf{r}}$) account for changes in the bottom of the conduction band edge $E_{\mathrm{c},0}$ and the shape of the band structure. Here, we only consider materials with position-independent band structures $\mathscr{E} = \mathscr{E}(\mathbf{k})$ and omit the influence of magnetic fields which reduces the

external force $\mathbf{F}$ to the electrostatic force $\mathbf{F}(\mathbf{r},t) = -\mathrm{q}\mathbf{E}(\mathbf{r},t)$ and the group velocity to $\mathbf{u} = \mathbf{u}(\mathbf{k})$.

2.1. Band structure model

In the following we will restrict ourselves to isotropic band structures with the dispersion relation $\mathscr{E}(\mathbf{k})$ defined implicitly through the bandform function $\gamma(\mathscr{E})$

$$\gamma(\mathscr{E}) = \frac{\hbar^2 k^2}{2m^*} \,. \tag{4}$$

Here, m^* is the effective isotropic carrier mass and $\gamma(\mathscr{E}) = \mathscr{E}$ for an isotropic parabolic band. The extension of the model to anisotropic band structures of the form

$$\gamma(\mathscr{E}) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x^*} + \frac{k_y^2}{m_y^*} + \frac{k_z^2}{m_z^*}\right) \tag{5}$$

by means of the Herring–Vogt transformation [16] is straightforward.

To bring the final model into as much a compact form as possible, the dispersion relation and the relations derived from it will be separated into their parabolic and non-parabolic contributions by introducing non-parabolicity correction functions $H_\xi(\mathscr{E})$. This gives

$$\gamma(\mathscr{E}) = \mathscr{E} H_{\mathscr{E}}(\mathscr{E}) \tag{6}$$

for the dispersion relation

$$g(\mathscr{E}) = g_0 \sqrt{\mathscr{E}} H_{\mathrm{g}}(\mathscr{E}) \tag{7}$$

for the density-of-states and

$$\mathbf{u}(\mathbf{k}) = \nabla_{\mathbf{p}} \mathscr{E}(|\mathbf{k}|) = \frac{\hbar \mathbf{k}}{m^*} H_{\mathrm{u}}(\mathscr{E}) \tag{8}$$

for the group velocity. Note that only for isotropic bands the group velocity is parallel to the crystal momentum $\hbar\mathbf{k}$ and allows for a definition of $H_{\mathrm{u}}(\mathscr{E})$ as in (8). The functions $H_{\mathscr{E}}(\mathscr{E})$, $H_{\mathrm{g}}(\mathscr{E})$, and $H_{\mathrm{u}}(\mathscr{E})$ equal unity for the simplest case of a parabolic band structure. An alternative way of expressing the relationship between the group velocity and the crystal momentum is via an energy-dependent mass [17] as

$$\mathbf{u}(\mathbf{k}) = \frac{\hbar \mathbf{k}}{m(\mathscr{E})} \,, \tag{9}$$

with $m(\mathscr{E}) = m^*/H_{\mathrm{u}}(\mathscr{E})$, which is of course equivalent to (8).

In this article Kane's first-order correction [18] will be used where the bandform function is given as

$$\gamma(\mathscr{E}) = \mathscr{E}(1 + \alpha\mathscr{E}) \,. \tag{10}$$

We are perfectly aware that Kane's relation is only valid for energies smaller than 1 eV [19]. However, for the sake of demonstrating the basic correction terms that

appear in the flux relations as a result of non-parabolicity this approximation is sufficient. In addition, it allows us to use the same band structure and parameters in both the microscopic Monte Carlo model and the macroscopic transport model. Thus, any differences observed between the two must result from the approximation of the distribution function through its moments and the closure relations derived therefrom.

For Kane's model we get the following relationships:

$$H_{\mathscr{E}}(\mathscr{E}) = 1 + \alpha\mathscr{E}\,, \tag{11}$$

$$H_{\mathrm{g}}(\mathscr{E}) = \sqrt{1+\alpha\mathscr{E}}(1+2\alpha\mathscr{E})\,, \tag{12}$$

$$H_{\mathrm{u}}(\mathscr{E}) = \frac{1}{1+2\alpha\mathscr{E}} = \left(1+\frac{2\alpha\hbar^2\mathbf{k}^2}{m^*}\right)^{-1/2} \tag{13}$$

with α being the non-parabolicity factor. We will also need the inverse effective mass tensor, which is the second-order term of the expansion of the dispersion relation and is defined as [15]

$$\hat{\mathrm{m}}^{-1}(\mathbf{k}) = \nabla_{\mathbf{p}} \otimes \mathbf{u}(\mathbf{k}) = \nabla_{\mathbf{p}} \otimes \nabla_{\mathbf{p}}\mathscr{E}(\mathbf{k})\,, \tag{14}$$

where $\otimes$ denotes the tensor product [20]. For Kane's relation one obtains

$$\hat{\mathrm{m}}^{-1}(\mathbf{k}) = \frac{H_{\mathrm{u}}(\mathscr{E})}{m^*}\left(\hat{\mathrm{I}} - \frac{2\alpha\hbar^2}{m^*}H_{\mathrm{u}}^2(\mathscr{E})\mathbf{k}\otimes\mathbf{k}\right)\,. \tag{15}$$

More accurate analytic band structures and full-band structures can be used in a similar manner as it is done for models based on a spherical-harmonic expansion of the distribution function [21–23]. The band structures are, however, subject to the same limitations, most notably, they have to be isotropic. In particular, isotropic numerical 'full-band' structures can be introduced via numerically tabulating the functions $H_{\mathscr{E}}(\mathscr{E})$, $H_{\mathrm{g}}(\mathscr{E})$, and $H_{\mathrm{u}}(\mathscr{E})$ at the expense of replacing the analytical expressions derived in this article by results based on numerical integration.

2.2. Moments of the distribution function

As Boltzmann's equation is difficult to solve directly, simplifications are commonly sought. A common simplification is to investigate only a few moments of the distribution function, such as the carrier concentration and the average carrier energy. A moment is obtained by multiplying the distribution function with a suitable weight function $\phi = \phi(\mathbf{k})$ and integrating over $\mathbf{k}$-space as

$$\langle\phi\rangle(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\int \phi(\mathbf{k})f(\mathbf{k},\mathbf{r},t)\,\mathrm{d}^3\mathbf{k}\,, \tag{16}$$

which is normalized with the carrier concentration $n(\mathbf{r},t)$ given by

$$n(\mathbf{r},t) = \int f(\mathbf{k},\mathbf{r},t)\,\mathrm{d}^3\mathbf{k}\,. \tag{17}$$

Thus, the three k-coordinates are eliminated at the expense of information loss concerning the details of the distribution function. In the following, the explicit space and time dependence of the moments is omitted for notational convenience.

In the simplest case these weight functions are chosen to be ascending powers of $\mathbf{k}$. However, to obtain macroscopic quantities such as the average velocity and the average energy, commonly used weight functions are powers of the carrier energy $\mathscr{E}^i$ and the fluxes $\mathbf{p}\mathscr{E}^i$ and $\mathbf{u}\mathscr{E}^i$. Recall that only for parabolic bands the moments resulting from the latter two are related via the effective mass as $\langle \mathbf{p}\mathscr{E}^i \rangle = m^* \langle \mathbf{u}\mathscr{E}^i \rangle$. In general, a more complicated relationship exists between the two, which depends on higher-order moments of the distribution function. For Kane's relation we obtain

$$\langle \mathbf{p}\mathscr{E}^i \rangle = m^* \langle \mathbf{u}\mathscr{E}^i \rangle + 2\alpha m^* \langle \mathbf{u}\mathscr{E}^{i+1} \rangle \,, \tag{18}$$

$$\langle \mathbf{u}\mathscr{E}^i \rangle = \frac{1}{m^*} \left\langle \frac{\mathbf{p}\mathscr{E}^i}{1+2\alpha\mathscr{E}} \right\rangle = \frac{1}{m^*} \sum_{j=0}^{\infty} (-2\alpha)^j \langle \mathbf{p}\mathscr{E}^{i+j} \rangle \,. \tag{19}$$

In the following we consider the first N moment equations for the macroscopic transport models. These equations will be derived from the even weight functions $\mathscr{E}^i$ and the odd weight functions $\mathbf{p}\mathscr{E}^i$.

$$\phi = \begin{cases} \mathscr{E}^i, & i = 0, 1, \ldots, M_\mathrm{S} \,, \\ \mathbf{p}\mathscr{E}^i, & i = 0, 1, \ldots, M_\mathrm{A} \,. \end{cases} \tag{20}$$

The order of the expansion is thus given as $N = (M_\mathrm{S} + 1) + (M_\mathrm{A} + 1)$. Unless otherwise noted, however, M_A will be equal M_S with

$$M_\mathrm{A} = M_\mathrm{S} = M = N/2 - 1 \,. \tag{21}$$

Thus, for a four moments model with $N = 4$, $M_\mathrm{S} = 1$, and $M_\mathrm{A} = 1$ we use the weight functions 1, $\mathbf{p}$, $\mathscr{E}$, and $\mathbf{p}\mathscr{E}$. Cases where M_S and M_A differ are a three moments model with $N = 3$, $M_\mathrm{S} = 1$ and $M_\mathrm{A} = 0$ or a five moments model with $N = 5$, $M_\mathrm{S} = 2$ and $M_\mathrm{A} = 1$.

2.3. Diffusion scaling

To isolate dominant effects, Boltzmann's equation is commonly considered in a scaled dimensionless form. Various scalings have been considered to investigate limiting cases such as high- and low-field transport. Here we will use the by now classic diffusion scaling [24–26]. The scaling parameters ξ_0 that relate a quantity ξ to its scaled forms ξ_s as $\xi = \xi_0 \xi_\mathrm{s}$ are x_0, the characteristic device dimension, $k_0 = \sqrt{m^* \mathrm{k_B} T_\mathrm{L}}/\hbar$, the scaling parameter for the wave vector τ_0, a characteristic scattering rate which can be pulled out of the scattering operator $Q = Q_\mathrm{s}/\tau_0$, the velocity scale for the group velocity $u_0 = \sqrt{\mathrm{k_B} T_\mathrm{L}/m^*}$, and the scale for the electrostatic potential $\psi_0 = \hbar k_0 u_0 / q$

$$\frac{x_0}{u_0 t_0} \partial_{t_\mathrm{s}} f + \mathbf{u} \cdot \nabla_{\mathbf{r}_\mathrm{s}} f + \mathbf{F} \cdot \nabla_{\mathbf{k}_\mathrm{s}} f = \frac{x_0}{u_0 \tau_0} Q_\mathrm{s}[f] \,. \tag{22}$$

Diffusion scaling assumes the time scale of the system to be

$$t_0 = \frac{\tau_0}{\kappa^2}\,, \tag{23}$$

i.e., we assume the scattering frequency to be high compared to the considered time scale [25]. We obtain

$$\kappa\partial_{t_s} f + \mathbf{u}\cdot\nabla_{\mathbf{r}_s} f + \mathbf{F}\cdot\nabla_{\mathbf{k}_s} f = \tfrac{1}{\kappa} Q_s[f]\,, \tag{24}$$

where the Knudsen number

$$\kappa = \frac{\tau_0 u_0}{x_0} \tag{25}$$

appears as a scaling parameter which represents the mean free path $\tau_0 u_0$ relative to the device dimension. Since the Knudsen number is small in collision-dominated systems it will be interpreted as the order of the term it appears with. To allow a simple comparison of the relations derived in the following with expressions from literature we continue with the unscaled variables but keep the Knudsen number as an indicator for the order of each term. Of course, the unscaled Knudsen number equals unity.

For both the macroscopic transport models and the distribution function model it is advantageous to formally split the distribution function into its symmetric and anti-symmetric parts as

$$f(\mathbf{k},\mathbf{r},t) = f_S(\mathbf{k},\mathbf{r},t) + \kappa f_A(\mathbf{k},\mathbf{r},t)\,. \tag{26}$$

The Knudsen number that multiplies the anti-symmetric part in (26) is motivated as follows: For small electric fields the distribution function can be approximated by a displaced Maxwellian distribution $f(\mathbf{u}-\mathbf{V})$, where $\mathbf{V}$ is the average velocity of the electron gas [19]. The average velocity is related to the macroscopic length scale x_0 and the time scale of the system t_0 and thus scales with $V_0 = x_0/t_0$. We therefore obtain for the scaled form of the displaced Maxwellian distribution

$$f(\mathbf{u}-\mathbf{V}) = f\left(u_0\left(\mathbf{u}_s - \frac{x_0}{u_0 t_0}\mathbf{V}_s\right)\right) = f_s(\mathbf{u}_s - \kappa\mathbf{V}_s)\,, \tag{27}$$

where $x_0/(u_0 t_0)$ evaluates to κ. For a small displacement the distribution function (27) can be expanded to obtain

$$f_s(\mathbf{u}_s - \kappa\mathbf{V}_s) \approx f_s(\mathbf{u}_s) - \kappa\mathbf{V}_s\cdot\frac{\partial f_s(\mathbf{u}_s)}{\partial\mathbf{u}_s}\,. \tag{28}$$

The Maxwellian distribution $f(\mathbf{u})$ is symmetric and therefore the second term in (28) constitutes the anti-symmetric part of the distribution function.

Since κ is small in collision dominated systems, expansion (26) indicates that the anti-symmetric part is smaller than the symmetric part. Such a splitting is advantageous because only the symmetric part $f_S(\mathbf{k},\mathbf{r},t)$ contributes to averages with the even weight functions whereas only the anti-symmetric part $f_A(\mathbf{k},\mathbf{r},t)$ contributes to the averages related to odd weight functions. Without loss of generality, the symmetric and anti-symmetric parts of the distribution function

$f(\mathbf{k},\mathbf{r},t)$ with respect to $\mathbf{k}$ are obtained via the relations

$$f_{\mathrm{S}}(\mathbf{k},\mathbf{r},t)=\tfrac{1}{2}(f(\mathbf{k},\mathbf{r},t)+f(-\mathbf{k},\mathbf{r},t))\,, \tag{29}$$

$$\kappa f_{\mathrm{A}}(\mathbf{k},\mathbf{r},t)=\tfrac{1}{2}(f(\mathbf{k},\mathbf{r},t)-f(-\mathbf{k},\mathbf{r},t))\,. \tag{30}$$

By inserting (26) into (24) and equating symmetric and anti-symmetric terms Boltzmann's equation splits into two equations

$$\partial_t f_{\mathrm{S}}+\mathbf{u}\cdot\nabla_{\mathbf{r}} f_{\mathrm{A}}+\mathbf{F}\cdot\nabla_{\mathbf{p}} f_{\mathrm{A}}=\tfrac{1}{\kappa^2}Q_{\mathrm{S}}[f_{\mathrm{S}}]\,, \tag{31}$$

$$\kappa^2\partial_t f_{\mathrm{A}}+\mathbf{u}\cdot\nabla_{\mathbf{r}} f_{\mathrm{S}}+\mathbf{F}\cdot\nabla_{\mathbf{p}} f_{\mathrm{S}}=Q_{\mathrm{A}}[f_{\mathrm{A}}]\,. \tag{32}$$

So far no simplifications have been introduced and (31) and (32) are equivalent to (24). In the diffusion limit, however, we neglect terms of second-order in κ, resulting in a simpler equation system [27–29]. Recall that by this assumption the hydrodynamic equation system [2] can be transfered into the energy-transport system [4]. In the following, however, we will be concerned with the derivation of the full equation system to deepen our understanding of the influence of the second-order terms. Only in Section 6.2.1 such a simplified model will be presented and discussed.

When (31) and (32) are multiplied by the weight functions $\mathscr{E}^i$ and $\mathbf{p}\mathscr{E}^i$ and integrated over $\mathbf{k}$-space we obtain the characteristic equations for the moments $\langle\mathscr{E}^i\rangle$ and $\langle\mathbf{p}\mathscr{E}^i\rangle$. Due to the structure of Boltzmann's equation additional moments appear in these characteristic equations. It is a non-trivial task to express these additional moments by the moments $\langle\mathscr{E}^i\rangle$ and $\langle\mathbf{u}\mathscr{E}^i\rangle$ which are taken as the unknowns of the equation system. This is referred to as closure of the equation system. Since this is a complicated problem, mostly empirical relations are used [4]. The closure issue can be tackled in a systematic way by using an analytic distribution function model [7]. In such an approach the distribution function which is the original unknown of Boltzmann's equation, is reconstructed using the available moments, which are the unknowns of the moment system. This is done by assuming an analytical description of the distribution function

$$f_{\mathrm{Analytic}}(\mathbf{k},\mathbf{r},t)=f_{\mathrm{Analytic}}(\mathbf{k},a_0(\mathbf{r},t),\ldots,a_L(\mathbf{r},t))\,, \tag{33}$$

which depends on L position-dependent parameters a_i. The parameters a_i are then determined by requiring that the moments of (33) exactly reproduce the given set of moments $\langle 1\rangle,\ldots,\langle\mathscr{E}^{M_{\mathrm{S}}}\rangle,\langle\mathbf{u}\rangle,\ldots,\langle\mathbf{u}\mathscr{E}^{M_{\mathrm{A}}}\rangle$, and possibly some additional constraints [11]. Finally, the additional moments can be calculated from (33) in a more or less straightforward way. It is then hoped that (33) is an accurate model for the real distribution function and gives good results for the missing additional moments. We shall see in the sequel, that this is not necessarily the case. Naturally, the accuracy of this approach relies heavily on the quality of this distribution function model. The derivation of a suitable distribution function model is the subject of the next section.

3. Distribution function model

For the derivation of the closure relations we will make use of an analytic distribution function model. This model should have the following properties: For zero bias, it must reduce to the Maxwellian distribution function, which is the equilibrium solution of Boltzmann's equation for non-degenerate semiconductors. In addition and more importantly, when some bias is applied, several effects become visible in the distribution function. First, the shape of the distribution function changes to account for the heating of the carrier gas. This effect is assumed to be the most dominant one. Second, the distribution function is slightly displaced in the direction of the current flow. And finally, the distribution function will display some anisotropy around the displaced origin, i.e., it becomes elongated in the direction of the current flow.

All these effects can be accounted for by displacing the distribution function with a small energy-dependent displacement $\kappa\mathbf{K}(\mathscr{E},\mathbf{r},t)$. Note that in the frequently used approximation of a displaced and heated Maxwellian distribution the displacement is assumed to be energy-independent and proportional to the average velocity $\langle\mathbf{u}\rangle(\mathbf{r},t)$. In unscaled variables we have

$$\mathbf{K}(\mathscr{E},\mathbf{r},t)=\mathbf{K}_0(\mathbf{r},t)=\tfrac{m^*}{\hbar}\langle\mathbf{u}\rangle(\mathbf{r},t)\,. \tag{34}$$

Based on results obtained from Monte Carlo simulations we know that the energy distribution function begins to deviate from the equilibrium distribution before this displacement becomes visible. We therefore first model an isotropic and thus purely energy-dependent distribution function $f_{\mathrm{I}}(\mathbf{k},\mathbf{r},t)$ and assume that the final distribution function can be obtained by displacing $f_{\mathrm{I}}(\mathbf{k},\mathbf{r},t)$ by a small amount $\kappa\mathbf{K}(\mathscr{E},\mathbf{r},t)$ and expand the shifted distribution function up to second-order

$$f(\mathbf{k})=f_{\mathrm{I}}(\mathbf{k}-\kappa\mathbf{K})=f_{\mathrm{I}}(\mathscr{E})-\kappa\frac{\partial f_{\mathrm{I}}(\mathscr{E})}{\partial\mathbf{k}}\cdot\mathbf{K}+\frac{\kappa^2}{2}\mathbf{K}^{\mathrm{T}}\frac{\partial^2 f_{\mathrm{I}}(\mathscr{E})}{\partial\mathbf{k}^2}\mathbf{K}+O(\kappa^3)\,. \tag{35}$$

Since the following considerations will be concerned with the calculation of the moments, the explicit space and time dependence of the distribution function has been dropped and is understood. Expansion (35) defines the zero-, first-, and second-order term of the distribution function as

$$f(\mathbf{k})=f_{\mathrm{S}}^{(0)}(\mathscr{E})+\kappa f_{\mathrm{A}}^{(1)}(\mathbf{k})+\kappa^2 f_{\mathrm{S}}^{(2)}(\mathbf{k})+O(\kappa^3)\,. \tag{36}$$

Note that the zero- and second-order terms contribute to the symmetric part of the distribution function, whereas the first-order term constitutes the anti-symmetric part of the distribution function.

To bring $f_{\mathrm{A}}^{(1)}(\mathbf{k})$ and $f_{\mathrm{S}}^{(2)}(\mathbf{k})$ into the form $f_{\mathrm{I}}(\mathscr{E})h(\mathbf{k})$ we express the energy-derivatives of the distribution function as

$$\frac{\partial f_{\mathrm{I}}(\mathscr{E})}{\partial\mathscr{E}}=g_1(\mathscr{E})f_{\mathrm{I}}(\mathscr{E})\quad\text{and}\quad\frac{\partial^2 f_{\mathrm{I}}(\mathscr{E})}{\partial\mathscr{E}^2}=g_2(\mathscr{E})f_{\mathrm{I}}(\mathscr{E})\,. \tag{37}$$

Since the distribution function models normally depend exponentially on the energy, we obtain compact results of the form

$$f_{\mathrm{A}}^{(1)}(\mathbf{k}) = f_{\mathrm{I}}(\mathscr{E}) F_{\mathrm{A}}(\mathscr{E}) \mathbf{K}^{\mathrm{T}} \mathbf{k}\,, \tag{38}$$

$$f_{\mathrm{S}}^{(2)}(\mathbf{k}) = f_{\mathrm{I}}(\mathscr{E}) \tfrac{1}{2} \mathbf{K}^{\mathrm{T}} \hat{\mathrm{F}}(\mathbf{k}) \mathbf{K} \tag{39}$$

with the auxiliary functions in unscaled variables

$$F_{\mathrm{A}}(\mathscr{E}) = -\frac{\hbar^2 H_{\mathrm{u}}(\mathscr{E})}{m^*} g_1(\mathscr{E})\,, \tag{40}$$

$$\hat{\mathrm{F}}(\mathscr{E}) = \frac{1}{f_{\mathrm{I}}} \left\{ \frac{\partial^2 f_{\mathrm{I}}}{\partial k_i \partial k_j} \right\} = F_{\mathrm{AI}}(\mathscr{E}) \mathbf{k} \otimes \mathbf{k} + F_{\mathrm{I}}(\mathscr{E}) \hat{\mathrm{I}}\,, \tag{41}$$

$$F_{\mathrm{AI}}(\mathscr{E}) = \left(\frac{\hbar^2 H_{\mathrm{u}}(\mathscr{E})}{m^*} \right)^2 (g_2(\mathscr{E}) - 2\alpha g_1(\mathscr{E}) H_{\mathrm{u}}(\mathscr{E}))\,, \tag{42}$$

$$F_{\mathrm{I}}(\mathscr{E}) = \frac{\hbar^2 H_{\mathrm{u}}(\mathscr{E})}{m^*} g_1(\mathscr{E})\,. \tag{43}$$

The function $F_{\mathrm{AI}}(\mathscr{E})$ describes the second-order $\mathbf{k}$-dependence of the symmetric part of the distribution function, whereas $F_{\mathrm{I}}(\mathscr{E})$ gives the second-order isotropic contribution.

3.1. Superposition of two distribution functions

From Monte Carlo simulations we know that for instance in the drain region of MOS transistors a mixture of a hot and a cold carrier gas exists which is clearly visible in the distribution function [11,30,31]. To reconstruct such a distribution function it has been found advantageous [11,32] to model these contributions separately by describing the total carrier gas as a superposition of two isotropic distribution functions $f_{\mathrm{h}}(\mathscr{E})$ and $f_{\mathrm{c}}(\mathscr{E})$ as $f_{\mathrm{I}}(\mathbf{k}) = f_{\mathrm{h}}(\mathscr{E}) + f_{\mathrm{c}}(\mathscr{E})$. However, when such a distribution function is displaced we have to consider that the gases flow with different velocities. We therefore have to use two different displacements $\mathbf{K}_{\mathrm{h}}$ and $\mathbf{K}_{\mathrm{c}}$. Attempts have been made to describe such a mixture of two carrier gases by two coupled macroscopic transport models [33]. Unfortunately, the coupling of these transport models is very difficult to model, particularly from a numerical point of view. In previous investigations it has been observed, that a simple heuristic relationship between the two displacements is quite accurate [34] and we will restrict ourselves to such a description. For the total distribution function we thus obtain

$$f(\mathbf{k}) = f_{\mathrm{h}}(\mathbf{k} - \kappa \mathbf{K}_{\mathrm{h}}) + f_{\mathrm{c}}(\mathbf{k} - \kappa \mathbf{K}_{\mathrm{c}}) \tag{44}$$

which can be expanded in the same manner resulting in

$$f_{\mathrm{S}}(\mathbf{k}) = f_{\mathrm{h}}(\mathscr{E}) + f_{\mathrm{c}}(\mathscr{E}) + \tfrac{\kappa^2}{2} (f_{\mathrm{h}}(\mathscr{E}) \mathbf{K}_{\mathrm{h}}^{\mathrm{T}} \hat{\mathrm{F}}_{\mathrm{h}} \mathbf{K}_{\mathrm{h}} + f_{\mathrm{c}}(\mathscr{E}) \mathbf{K}_{\mathrm{c}}^{\mathrm{T}} \hat{\mathrm{F}}_{\mathrm{c}} \mathbf{K}_{\mathrm{c}}) \tag{45}$$

for the symmetric part and

$$f_{\mathrm{A}}(\mathbf{k}) = f_{\mathrm{h}}(\mathbf{k}) F_{\mathrm{A,h}} \mathbf{K}_{\mathrm{h}}^{\mathrm{T}} \mathbf{K} + f_{\mathrm{c}}(\mathbf{k}) F_{\mathrm{A,c}} \mathbf{K}_{\mathrm{c}}^{\mathrm{T}} \mathbf{k} \tag{46}$$

for the anti-symmetric part of the distribution function. With the approximation $\mathbf{K}_{\mathrm{c}} \approx c_{\mathrm{A}} \mathbf{K}_{\mathrm{h}}$, where c_{A} is assumed to depend only on the moments, we get

$$f_{\mathrm{S}}(\mathbf{k}) = f_{\mathrm{h}}(\mathscr{E}) + f_{\mathrm{c}}(\mathscr{E}) + \frac{\kappa^2}{2} \mathbf{K}_{\mathrm{h}}^{\mathrm{T}} (f_{\mathrm{h}}(\mathscr{E}) \hat{\mathrm{F}}_{\mathrm{h}}(\mathbf{k}) + c_{\mathrm{A}}^2 f_{\mathrm{c}}(\mathscr{E}) \hat{\mathrm{F}}_{\mathrm{c}}(\mathbf{k})) \mathbf{K}_{\mathrm{h}} \tag{47}$$

and

$$f_{\mathrm{A}}(\mathbf{k}) = (f_{\mathrm{h}}(\mathscr{E}) F_{\mathrm{A,h}}(\mathscr{E}) + c_{\mathrm{A}} f_{\mathrm{c}}(\mathscr{E}) F_{\mathrm{A,c}}(\mathscr{E})) \mathbf{K}_{\mathrm{h}}^{\mathrm{T}} \mathbf{k} \,. \tag{48}$$

In the following it will be assumed that the ratio of the displacements is roughly proportional to the ratio of the reference energies a as $c_{\mathrm{A}} = a_{\mathrm{c}}/a$. This empirical relation is motivated by the diffusion law for ideal gases and the Einstein relation, which predicts a diffusion velocity proportional to the temperature of the gas. It has been chosen due to its simplicity and delivered reasonable results [34]. Additional research on this topic might be in order.

3.2. Definition of the moments

We define a general moment of the distribution function based on the weight function ϕ as

$$\langle\langle \phi \rangle\rangle = \langle\langle \phi \rangle\rangle^{(0)} + \kappa \langle\langle \phi \rangle\rangle^{(1)} + \kappa^2 \langle\langle \phi \rangle\rangle^{(2)} \tag{49}$$

where the jth-order partial moment is given by

$$\langle\langle \phi \rangle\rangle^{(j)} = \int \phi f^{(j)}(\mathbf{k}) \, \mathrm{d}^3\mathbf{k} \tag{50}$$

and the normalized moment by

$$\langle \phi \rangle = \frac{\langle\langle \phi \rangle\rangle}{\langle\langle 1 \rangle\rangle} \,. \tag{51}$$

Since the zero-order moment required for the normalization contains second-order terms itself

$$\langle\langle 1 \rangle\rangle = \langle\langle 1 \rangle\rangle^{(0)} + \kappa^2 \langle\langle 1 \rangle\rangle^{(2)} \tag{52}$$

we make use of the approximation

$$\frac{1}{\langle\langle 1 \rangle\rangle} = \frac{1}{\langle\langle 1 \rangle\rangle^{(0)} + \kappa^2 \langle\langle 1 \rangle\rangle^{(2)}} \approx \frac{1}{\langle\langle 1 \rangle\rangle^{(0)}} \left(1 - \kappa^2 \frac{\langle\langle 1 \rangle\rangle^{(2)}}{\langle\langle 1 \rangle\rangle^{(0)}} \right) \tag{53}$$

or, in terms of the carrier concentration $n = \langle\langle 1 \rangle\rangle$,

$$\frac{1}{n} = \frac{1}{n^{(0)}} \left(1 - \kappa^2 \frac{n^{(2)}}{n^{(0)}} \right) . \tag{54}$$

Keeping only terms up to second-order gives for the general normalized moment

$$\langle \phi \rangle = \frac{\langle\langle \phi \rangle\rangle^{(0)}}{n^{(0)}} + \kappa \frac{\langle\langle \phi \rangle\rangle^{(1)}}{n^{(0)}} + \kappa^2 \left(\frac{\langle\langle \phi \rangle\rangle^{(2)}}{n^{(0)}} - \frac{\langle\langle \phi \rangle\rangle^{(0)}}{n^{(0)}} \frac{n^{(2)}}{n^{(0)}} \right)$$
$$= \langle \phi \rangle^{(0)} + \kappa \langle \phi \rangle^{(1)} + \kappa^2 \langle \phi \rangle^{(2)} . \tag{55}$$

As examples we obtain for the even moments $w_i = \langle \mathscr{E}^i \rangle = w_i^{(0)} + \kappa^2 w_i^{(2)}$

$$w_i = \frac{\langle\langle \mathscr{E}^i \rangle\rangle^{(0)}}{n^{(0)}} + \kappa^2 \left(\frac{\langle\langle \mathscr{E}^i \rangle\rangle^{(2)}}{n^{(0)}} - \frac{\langle\langle \mathscr{E}^i \rangle\rangle^{(0)}}{n^{(0)}} \frac{n^{(2)}}{n^{(0)}} \right) \tag{56}$$

$$= w_i^{(0)} + \kappa^2 \left(\frac{\langle\langle \mathscr{E}^i \rangle\rangle^{(2)}}{n^{(0)}} - w_i^{(0)} \frac{n^{(2)}}{n^{(0)}} \right) \tag{57}$$

and for the odd moments, which represent the fluxes of the system

$$\kappa \mathbf{V}_i = \kappa \frac{\langle\langle \mathbf{u} \mathscr{E}^i \rangle\rangle^{(1)}}{n^{(0)}} = \kappa \langle \mathbf{u} \mathscr{E}^i \rangle^{(1)} . \tag{58}$$

Note how the second-order contribution to the normalized even moment is modified by the second-order contribution to the carrier concentration and therefore in general $w_i^{(2)} \neq \langle\langle \mathscr{E}^i \rangle\rangle^{(2)}/n^{(0)}$. The odd moments, on the other hand, depend in this approximation only on the zero-order term of the carrier concentration since the second-order term would result in a third-order contribution to the fluxes.

When two distribution functions are superposed we get for the moments of the weight function ϕ

$$\langle\langle \phi \rangle\rangle = \langle\langle \phi \rangle\rangle_{\mathrm{h}} + \langle\langle \phi \rangle\rangle_{\mathrm{c}} \tag{59}$$
$$= \langle\langle \phi \rangle\rangle_{\mathrm{h}}^{(0)} + \langle\langle \phi \rangle\rangle_{\mathrm{c}}^{(0)} + \kappa(\langle\langle \phi \rangle\rangle_{\mathrm{h}}^{(1)} + c_{\mathrm{A}} \langle\langle \phi \rangle\rangle_{\mathrm{c}}^{(1)})$$
$$+ \kappa^2(\langle\langle \phi \rangle\rangle_{\mathrm{h}}^{(2)} + c_{\mathrm{A}}^2 \langle\langle \phi \rangle\rangle_{\mathrm{c}}^{(2)}) . \tag{60}$$

This gives for the jth-order partial moment

$$\langle\langle \phi \rangle\rangle^{(j)} = \langle\langle \phi \rangle\rangle_{\mathrm{h}}^{(j)} + c_{\mathrm{A}}^j \langle\langle \phi \rangle\rangle_{\mathrm{c}}^{(j)} . \tag{61}$$

3.3. Isotropic model

To capture the non-Maxwellian shape of the distribution function, we model its isotropic part following our previous work [11] as

$$f_{\mathrm{h}}(\mathscr{E}) = A \exp\left[-\left(\frac{\mathscr{E}}{a} \right)^b \right] = A f_{\mathscr{E}}(\mathscr{E}, a, b) . \tag{62}$$

Evaluating the moments of the expansion (35), we obtain general expressions of the form

$$\int \mathscr{E}^{r+(1/2)} f_{\mathscr{E}}(\mathscr{E}, a, b) H_{\mathscr{E}}^x(\mathscr{E}) H_{\mathrm{u}}^y(\mathscr{E}) H_{\mathrm{g}}(\mathscr{E}) \, \mathrm{d}\mathscr{E} . \tag{63}$$

Some integer powers x and y of the non-parabolicity correction factors appear in (63), depending on the moment under consideration. We now define a combined non-parabolicity function

$$H_{x,y}(\mathscr{E}) \doteq H_{\mathscr{E}}^{x}(\mathscr{E}) H_{\mathrm{u}}^{y}(\mathscr{E}) H_{\mathrm{g}}(\mathscr{E}) \tag{64}$$

to capture the non-parabolicity effects for each moment. Since $H_{x,y}(\mathscr{E})$ contains terms of the form $(1+a\mathscr{E})^{z}$, where in general z is not an integer, the solution of (63) cannot be obtained analytically and we have to resort to some approximation. A Taylor expansion of $H_{x,y}(\mathscr{E})$ delivers an alternating series and thus requires a relatively large number of terms to deliver satisfactory results [11,35]. We therefore use polynomials with non-integer powers similarly to our previous work [11]. Two cases have to be considered: When $\partial_{\mathscr{E}} H_{x,y}(\mathscr{E})|_{\mathscr{E}=0} > 0$ the functions $H_{x,y}(\mathscr{E})$ are nearly linear and a two-parameter polynomial approximation

$$H_{x,y}(\mathscr{E}) \approx 1 + \gamma_{x,y} (\alpha\mathscr{E})^{\lambda_{x,y}} \tag{65}$$

can be used. When $\partial_{\mathscr{E}} H_{x,y}(\mathscr{E})|_{\mathscr{E}=0} < 0$, however, the functions $H_{x,y}(\mathscr{E})$ can only be roughly resolved by (65). We, therefore, use a second term in the polynomial approximation

$$H_{x,y}(\mathscr{E}) \approx 1 + \gamma_{x,y}^{(1)} (\alpha\mathscr{E})^{\lambda_{x,y}^{(1)}} + \gamma_{x,y}^{(2)} (\alpha\mathscr{E})^{\lambda_{x,y}^{(2)}} . \tag{66}$$

In an actual implementation, however, the simple expression (65) might be accurate enough for both cases. The parameters were determined by a least square fit in the interval $\alpha\mathscr{E} \in [0, 0.25]$. It is important to obtain an accurate fit in the low-energy region because the distribution function decays exponentially at higher energies. Note that the fit expressions are formulated in a way that preserves the non-parabolicity factor α in the final result. In particular, the parabolic result is retained by setting $\alpha = 0$.

Moments of the form (63) can now be expressed through gamma functions. With the auxiliary functions

$$\mathscr{G}(i,a,b) = \int \mathscr{E}^{i+(1/2)} \exp\left[-\left(\frac{\mathscr{E}}{a}\right)^{b}\right] \mathrm{d}\mathscr{E} = \frac{a^{i+(3/2)}}{b} \Gamma\left(\frac{i+\frac{3}{2}}{b}\right), \tag{67}$$

$$\mathscr{I}_{x,y}(i,a,b) = \int H_{x,y}(\mathscr{E}) \mathscr{E}^{i+(1/2)} \exp\left[-\left(\frac{\mathscr{E}}{a}\right)^{b}\right] \mathrm{d}\mathscr{E} \tag{68}$$

$$= \mathscr{G}(i,a,b) + \gamma_{x,y} \alpha^{\lambda_{x,y}} \mathscr{G}(i+\lambda_{x,y}, a, b) \tag{69}$$

we obtain for the moments of the distribution function (62)

$$\int \mathscr{E}^{r+(1/2)} f_{\mathscr{E}}(\mathscr{E}, a, b) H_{x,y}(\mathscr{E}) = \mathscr{I}_{x,y}(r,a,b) . \tag{70}$$

We model the superposition of a hot and a cold distribution function following our previous work [11] as

$$f_{\mathrm{I}}(\mathscr{E}) = f_{\mathrm{h}}(\mathscr{E}) + f_{\mathrm{c}}(\mathscr{E}) = A_{\mathrm{h}}(f_{\mathscr{E}}(\mathscr{E}, a, b) + c f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{c}}, 1)) , \tag{71}$$

where $c = A_c/A_h$. The jth-order partial moments of (71) are then obtained by expressions of the form

$$\mathscr{I}_{x,y}(r,a,b) + cc_A^j \mathscr{I}_{x,y}(r,a_c,1)\,. \tag{72}$$

4. Calculation of the moments

We will now calculate the moments of the combined distribution function (71). The parameters of the distribution function will then be determined by requiring the analytic moments to reproduce a given set of moments $\langle \mathscr{E}^i \rangle$ and $\langle \mathbf{u}\mathscr{E}^i \rangle$. The odd moments are determined by the fluxes $\mathbf{V}_i$ and thus the displacement $\mathbf{K}$. Through (39) the displacement influences the second-order contribution to the even moments. Therefore, the odd moments are calculated first.

4.1. Odd moments

For the calculation of the odd moments we expand the energy-dependent displacement vector $\mathbf{K}(\mathscr{E})$ into powers of the energy as

$$\mathbf{K}(\mathscr{E}) = \sum_{j=0}^{M_A} \mathscr{E}^j \mathbf{K}_j\,. \tag{73}$$

Note that in this way $M_A + 1$ vector-valued parameters $\mathbf{K}_i$ are introduced. To determine the coefficients $\mathbf{K}_i$ we calculate the moments of the anti-symmetric part of the distribution function using the weight functions

$$\mathbf{u}\mathscr{E}^i = \frac{\hbar\mathbf{k}}{m^*}\mathscr{E}^i H_u(\mathscr{E}) \quad i = 0,1,\ldots,M_A \tag{74}$$

and require that they exactly reproduce the $M_A + 1$ fluxes occurring in the N moments model. The fluxes $\mathbf{V}_i$ of the system are calculated from (58). For the analytic distribution function (62) we obtain

$$\langle \mathbf{u}\mathscr{E}^i \rangle_h^{(1)} = \frac{2\hbar}{3m^*}\frac{b}{a^b}\frac{g_0}{n^{(0)}}\sum_{j=0}^{2}\mathbf{K}_j \int H_{1,2}(\mathscr{E})\mathscr{E}^{i+j+b+(1/2)} f_I(\mathscr{E})\,\mathrm{d}\mathscr{E} \tag{75}$$

$$= \sum_{j=0}^{M} C_{ij,h}\mathbf{K}_j\,, \tag{76}$$

with

$$C_{ij,h} = C_M \tfrac{b}{a^b}\mathscr{I}_{1,2}(i+j+b)\,, \tag{77}$$

$$C_M = \frac{2\hbar}{3m^*}\frac{Ag_0}{n^{(0)}}\,. \tag{78}$$

The elements $C_{ij,\mathrm{h}}$ form a matrix $\hat{\mathrm{C}}_\mathrm{h}$. From the superposition (71) we obtain $\hat{\mathrm{C}} = \hat{\mathrm{C}}_\mathrm{h} + cc_\mathrm{A}\hat{\mathrm{C}}_\mathrm{c}$. Note that the quantity $n^{(0)}$ in (78) contains the contributions of both distribution functions since the normalization requires the total carrier concentration. As can be seen from (77), the components of the matrix $\hat{\mathrm{C}}$ have the property $C_{ij} = C_{kl}$ for $i+j = k+l$. Introducing the flux matrix $\hat{\mathrm{V}} = (\mathbf{V}_0, \mathbf{V}_1, \mathbf{V}_2)$ and the displacement matrix $\hat{\mathrm{K}} = (\mathbf{K}_0, \mathbf{K}_1, \mathbf{K}_2)$ we obtain the linear equation system

$$\hat{\mathrm{V}} = \hat{\mathrm{K}}\hat{\mathrm{C}}^\mathrm{T} \tag{79}$$

which has the solution

$$\hat{\mathrm{K}} = \hat{\mathrm{V}}\hat{\mathrm{D}}^\mathrm{T} \tag{80}$$

with $\hat{\mathrm{D}} = \hat{\mathrm{C}}^{-1}$. This linearity is of course a consequence of the expansion (35) and as such only a first-order approximation for the displaced distribution function. Note that the matrices and tensors given before are written explicitly for the case $M_\mathrm{A} = 2$. Simpler cases are obtained accordingly. Introducing the energy vector $\boldsymbol{\mathscr{E}} = (1, \mathscr{E}, \mathscr{E}^2)^\mathrm{T}$ we can express the displacement as $\mathbf{K}(\mathscr{E}) = \hat{\mathrm{K}}\boldsymbol{\mathscr{E}}$ and finally write the anti-symmetric part of the distribution function as

$$f_\mathrm{A}(\mathbf{k}) = (f_\mathrm{h}F_{\mathrm{A,h}} + c_\mathrm{A}f_\mathrm{c}F_{\mathrm{A,c}})\boldsymbol{\mathscr{E}}^\mathrm{T}\hat{\mathrm{D}}\hat{\mathrm{V}}^\mathrm{T}\mathbf{k}\,. \tag{81}$$

4.2. Even moments

We calculate the even moments of the distribution function using the weight functions $\mathscr{E}^i$ following (57) to obtain a zero- and second-order contribution as

$$w_i = w_i^{(0)} + \kappa^2\left(\frac{\langle\langle \mathscr{E}^i \rangle\rangle^{(2)}}{n^{(0)}} - w_i^{(0)}\frac{n^{(2)}}{n^{(0)}}\right). \tag{82}$$

The zero-order contribution to the carrier concentration $n^{(0)}$ is calculated as

$$n^{(0)} = g_0\int f_\mathrm{I}(\mathscr{E})\mathscr{E}^{1/2}H_\mathrm{g}(\mathscr{E})\,\mathrm{d}\mathscr{E} = C_\mathrm{m}m_{0,0}(0)\,, \tag{83}$$

$$m_{x,y}(i) = \mathscr{I}_{x,y}(i,a,b) + c\mathscr{I}_{x,y}(i,a_\mathrm{c},1) \tag{84}$$

with $C_\mathrm{m} = Ag_0$. The higher-order moments are obtained as

$$\langle \mathscr{E}^i \rangle^{(0)} = \frac{m_{0,0}(i)}{m_{0,0}(0)}\,. \tag{85}$$

The calculation of the second-order contribution is more involved. After some calculus we find

$$\langle\langle \mathscr{E}^i \rangle\rangle^{(2)} = \tfrac{1}{2}\mathrm{tr}(\hat{\mathrm{K}}\hat{\mathrm{W}}_i\hat{\mathrm{K}}^\mathrm{T})\,, \tag{86}$$

where the components of the tensors $\hat{\mathrm{W}}_i$ are given by

$$W_{i,lm} = W_{i,lm,\mathrm{h}} + cc_\mathrm{A}^2 W_{i,lm,\mathrm{c}}\,. \tag{87}$$

The individual contributions of the two distribution functions are obtained as

$$W_{i,lm,\mathrm{x}} = Ag_0 \frac{2\hbar^2}{3m^*}\frac{b}{a^b}\left(\frac{b}{a^b}\mathscr{I}_{1,2}(i+l+m+2b-1,a,b)\right.$$
$$+(1-b)\mathscr{I}_{1,2}(i+l+m+b-1,a,b)+2\alpha\mathscr{I}_{1,3}(i+l+m+b,a,b)$$
$$\left.-\tfrac{3}{2}\mathscr{I}_{1,1}(i+l+m+b-1,a,b)\right) \tag{88}$$

with x = h or c. The second term gives a non-Maxwellian correction, which is zero for the cold distribution ($b = 1$), and the third term gives a non-parabolicity contribution.

Substituting the previous result (80), $\hat{\mathrm{K}} = \hat{\mathrm{V}}\hat{\mathrm{D}}^{\mathrm{T}}$, into (86) gives

$$\langle\langle \mathscr{E}^i \rangle\rangle^{(2)} = \tfrac{1}{2}\mathrm{tr}(\hat{\mathrm{V}}\hat{\mathrm{R}}_i\hat{\mathrm{V}}^{\mathrm{T}})\,. \tag{89}$$

The tensor $\hat{\mathrm{R}}_i$ is given by $\hat{\mathrm{R}}_i = \hat{\mathrm{D}}^{\mathrm{T}}\hat{\mathrm{W}}_i\hat{\mathrm{D}}$. The carrier concentration thus results in

$$n = n^{(0)} + \kappa^2 n^{(2)} = C_{\mathrm{m}}m_{0,0}(0) + \kappa^2\tfrac{1}{2}\mathrm{tr}(\hat{\mathrm{V}}\hat{\mathrm{R}}_i\hat{\mathrm{V}}^{\mathrm{T}})\,, \tag{90}$$

whereas the normalized statistical averages of $\mathscr{E}^i$ equal

$$w_i = \frac{m_{0,0}(i)}{m_{0,0}(0)} + \kappa^2\tfrac{1}{2}\mathrm{tr}(\hat{\mathrm{V}}\hat{\mathrm{w}}_i\hat{\mathrm{V}}^{\mathrm{T}}) \tag{91}$$

with

$$\hat{\mathrm{w}}_i = \frac{\hat{\mathrm{R}}_i - \hat{\mathrm{R}}_0 w_i^{(0)}}{m_{0,0}(0)}\,. \tag{92}$$

Eq. (90) appears unusual at a first glance because the carrier concentration now depends on the fluxes of the system. Conventionally, with the displaced and heated Maxwellian distribution, the carrier concentration is independent of the fluxes. For this particular distribution function and parabolic bands it can be easily shown that the second-order term in (90) disappears. The reason why the fluxes appear in this generalized expression is that the displacement serves two purposes: First, the distribution function has to be displaced to reproduce the average velocity, and second, the shape of the anti-symmetric part of the distribution function has to be modified to make the higher-order fluxes independent of the average velocity. To obtain the latter effect the displacement has to be energy dependent. As a consequence the shape of the distribution function changes and thus the carrier concentration.

4.2.1. Calculation of the parameters

The solution of macroscopic transport models based on N moments, for instance the class of models derived in Section 6, determines the N unknowns, normally $n, w_1, \ldots, w_M, \mathbf{V}_0, \ldots, \mathbf{V}_M$. These values can then be used to determine N parameters of the distribution function model. In general we can use $N/2$ moments for the odd part to satisfy the linear equation system $\hat{\mathrm{K}} = \hat{\mathrm{V}}\hat{\mathrm{D}}^{\mathrm{T}}$. Determination of the parameters of the isotropic part is more complicated because (91) is non-linear in

the parameters A, a, b, c, and a_c, and a Newton algorithm has to be used. Since the highest order moments model we consider is of order six, we have two more parameters than moments provided by the transport model. Therefore, the additional conditions $a_c = k_B T_L$ and $\langle \mathscr{E}^2 \rangle_h = h(\langle \mathscr{E} \rangle_h)$ are assumed, where $h(\langle \mathscr{E} \rangle)$ is the relationship between $\langle \mathscr{E}^2 \rangle$ and $\langle \mathscr{E} \rangle$ in bulk, and $\langle \cdot \rangle_h$ is the moment of f_h only. Note that the cold population only exists inside the drain regions and that therefore c vanishes inside channel regions [11]. The issue of finding suitable additional relations is discussed in detail in [11]. Monte Carlo fits for these relations, which have been extracted from a set of $n^+ - n - n^+$ structures, have been published in [36]. Whether these expressions are valid for a broader range of devices and bias conditions, however, remains to be seen.

4.2.2. Energy-like tensors

In the moment equations energy-like tensors $\hat{\mathrm{U}}_i$ will appear which are defined as

$$n\hat{\mathrm{U}}_i = \langle\langle \mathscr{E}^{i-1}\mathbf{u}\otimes\mathbf{p}\rangle\rangle . \tag{93}$$

We call them energy-like tensors since their unit is energy to the power i. They will be calculated in a similar manner as the statistical averages of the carrier energy. The zero-order contribution evaluates to

$$\langle\langle \mathscr{E}^{i-1}\mathbf{u}\otimes\mathbf{p}\rangle\rangle^{(0)} = \int f_I \mathscr{E}^{i-1}\frac{\hbar^2}{m^*} H_u \mathbf{k}\otimes\mathbf{k}\,\mathrm{d}^3\mathbf{k} \tag{94}$$

$$= \frac{2}{3} g_0 \int f_I(\mathscr{E})\mathscr{E}^{i+(1/2)} H_{1,1}(\mathscr{E})\hat{\mathrm{I}}\,\mathrm{d}\mathscr{E} \tag{95}$$

$$= \frac{2}{3} A g_0 m_{1,1}(i)\hat{\mathrm{I}} . \tag{96}$$

Following (55) we thus obtain for the zero-order component of the energy-like tensor

$$\hat{\mathrm{U}}_i^{(0)} = \frac{\langle\langle \mathscr{E}^{i-1}\mathbf{u}\otimes\mathbf{p}\rangle\rangle^{(0)}}{n^{(0)}} = \frac{2}{3}\frac{m_{1,1}(i)}{m_{0,0}(0)}\hat{\mathrm{I}} = U_i\hat{\mathrm{I}} . \tag{97}$$

It is convenient to introduce the zero-order parabolic contribution to the energy-like tensors as

$$\hat{\mathrm{U}}_i^{\mathrm{P}(0)} = \frac{2}{3}\langle \mathscr{E}^i\rangle^{(0)}\hat{\mathrm{I}} = \frac{2}{3}\frac{m_{0,0}(i)}{m_{0,0}(0)}\hat{\mathrm{I}} = U_i^{\mathrm{P}}\hat{\mathrm{I}} . \tag{98}$$

The term parabolic contribution was chosen because in standard parabolic models U_i is modeled as $U_i = 2w_i/3$. Actually, as can be seen from (98), U_i^{P} contains non-parabolicity information as well, but the relations between the average energies w_i and U_i^{P} do not depend on the band structure. The zero-order energy-like tensors can then be written as

$$\hat{\mathrm{U}}_i^{(0)} = \frac{2}{3}\frac{m_{0,0}(i)}{m_{0,0}(0)}\frac{m_{1,1}(i)}{m_{0,0}(i)}\hat{\mathrm{I}} = U_i^{\mathrm{P}} H_i \hat{\mathrm{I}} , \tag{99}$$

which introduces the non-parabolicity functions H_i as a generalization of the concept used in [9]. The functions H_i depend on the distribution function and are

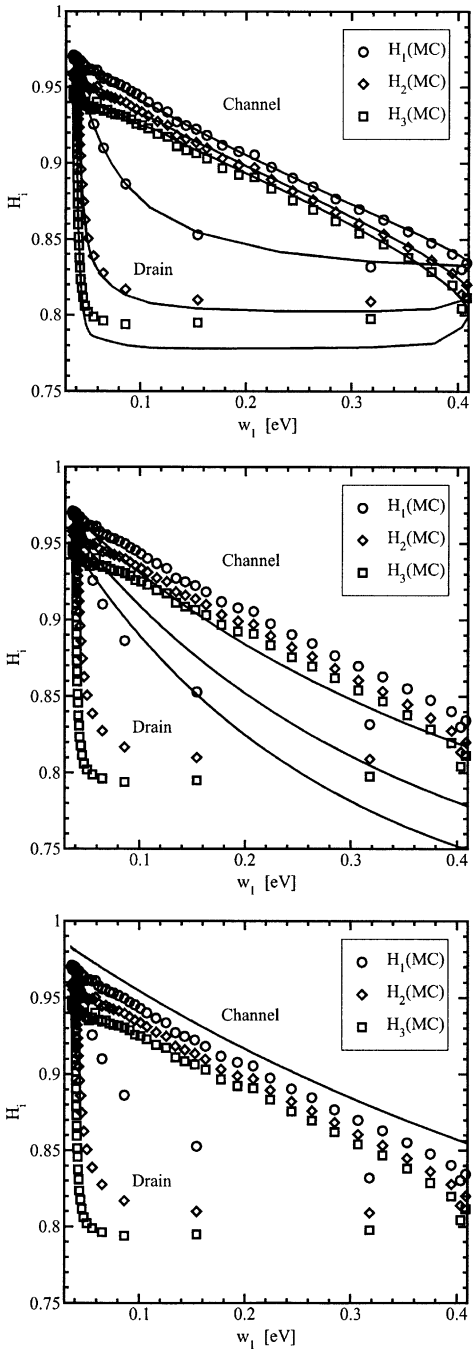

Fig. 1. The non-parabolicity factors H_i required for the zero-order contribution to the energy-like tensors $\hat{U}_i^{(0)}$. The top figure shows the results obtained by the six moments model ($M = 2$), the middle figure the results obtained by the four-moments model ($M = 1$), and the bottom figure the expression proposed by Bordelon et al. [9].

shown in Fig. 1 as a function of the average energy for the six moments model ($M = 2$), the four-moments model ($M = 1$), and for the expression proposed by Bordelon et al. [9]

$$H_1(w_1) = \frac{1 + \alpha w_1}{1 + 2\alpha w_1} \,. \tag{100}$$

Clearly, the coefficients H_i are not single valued functions of the average energy w_1 and only the six moments distribution function provides sufficient information to accurately model the coefficients H_i.

The calculation of the second-order contribution to the energy-like tensors is more involved due to the occurrence of tensors of the form $(\mathbf{k} \otimes \mathbf{k})(\mathbf{K}_l^{\mathrm{T}}(\mathbf{k} \otimes \mathbf{k})\mathbf{K}_m)$. Since only the even components of these tensors can contribute to the final result we can drop the odd components. By eliminating the angle dependency through integrating in polar-coordinates we finally arrive at

$$(\mathbf{k} \otimes \mathbf{k})(\mathbf{K}_l^{\mathrm{T}}(\mathbf{k} \otimes \mathbf{k})\mathbf{K}_m) = \tfrac{1}{15}\hat{\mathrm{K}}_{lm} k^4 \,, \tag{101}$$

where the auxiliary tensors $\hat{\mathrm{K}}_{lm}$ are given by

$$\hat{\mathrm{K}}_{lm} = \mathbf{K}_l \cdot \mathbf{K}_m \hat{\mathrm{I}} + \mathbf{K}_l \otimes \mathbf{K}_m + \mathbf{K}_m \otimes \mathbf{K}_l \,. \tag{102}$$

The second-order contribution is then obtained as

$$\langle\langle \mathscr{E}^{i-1}\mathbf{u} \otimes \mathbf{p} \rangle\rangle^{(2)} = \frac{\hbar^2}{2m^*} \hat{\mathrm{L}}_i \,, \tag{103}$$

where

$$\hat{\mathrm{L}}_i = \hat{\mathrm{L}}_{i,00} + \hat{\mathrm{L}}_{i,11} + \hat{\mathrm{L}}_{i,22} + 2(\hat{\mathrm{L}}_{i,01} + \hat{\mathrm{L}}_{i,02} + \hat{\mathrm{L}}_{i,12}) \tag{104}$$

with the tensors $\hat{\mathrm{L}}_{i,lm}$ consisting of a contribution due to the hot and the cold distribution function as

$$\hat{\mathrm{L}}_{i,lm} = \hat{\mathrm{L}}_{i,lm,\mathrm{h}} + cc_{\mathrm{A}}^2 \hat{\mathrm{L}}_{i,lm,\mathrm{c}} \,. \tag{105}$$

The individual contributions are obtained via

$$\begin{aligned} \hat{\mathrm{L}}_{i,lm,\mathrm{x}} = {} & \frac{4}{15}\hat{\mathrm{K}}_{lm} \frac{b}{a^b} A g_0 \left(\frac{b}{a^b} \mathscr{I}_{2,3}(i + l + m + 2b - 1, a, b) \right. \\ & + (1 - b)\mathscr{I}_{2,3}(i + l + m + b - 1, a, b) \\ & \left. + 2\alpha \mathscr{I}_{2,4}(i + l + m + b, a, b) \right) \\ & - \mathbf{K}_l \cdot \mathbf{K}_m \hat{\mathrm{I}} \frac{b}{a^b} A g_0 \frac{2}{3} \mathscr{I}_{1,2}(i + l + m + b - 1, a, b) \,. \end{aligned} \tag{106}$$

For the energy-like tensor we thus get

$$\hat{\mathrm{U}}_i = U_i \hat{\mathrm{I}} + \kappa^2 \left(\frac{\hbar^2}{2m^* n^{(0)}} \hat{\mathrm{L}}_i - U_i \frac{n^{(2)}}{n^{(0)}} \hat{\mathrm{I}} \right) . \tag{107}$$

4.3. Discussion

For the expansions of the distribution to be useful it is required that terms of order higher than two are negligible. This, however, cannot be guaranteed when the kinetic energy becomes large in quasi-ballistic religions. At a first glance, the non-expanded distribution function seems to be the ideal choice and the expansion is only introduced to facilitate closed form analytical expressions for the odd moments. We pay for this by obtaining a distribution function that may become negative. Looking at this issue more closely, however, reveals some surprising facts. As pointed out by Dreyer et al. [37] for moment equations based on the Fokker–Planck and Boltzmann equation, the non-expanded distribution functions based on the maximum entropy principle can develop a second peak, which is unphysical. This happens whenever the polynomial in the exponent has a minimum or equals zero. Dreyer et al. compared this to Grad's method [5,7,38], which they interpreted as linearization of the exponential term, and showed that this additional peak is absent there. As a conclusion they proposed that Grad's method is preferable over models based on the maximum entropy principle. Unfortunately, in the particular case of semiconductor devices, Grad's method does not properly resolve the exponential nature of the symmetric part and is as such unsuitable, unless a very large number of moments is used. The approach of Anile et al. [39] and the approach followed here, where only the anti-symmetric components are linearized, avoids this issue. For the maximum entropy models this issue of course re-arises when higher-order polynomials are required for the symmetric part. The model presented here, on the other hand, allows to use six moments without introducing additional peaks in the symmetric part.

This issue is demonstrated in Figs. 2 and 3 for a heated Maxwellian distribution which is displaced by polynomials of order $M_A = 0, 1$, and 2. The parameters of the expanded distribution function are determined to match Monte Carlo bulk simulation results, once for low bias and once for intermediate bias conditions, and then inserted into the non-expanded distribution function. As can be seen in Fig. 2, for the low bias condition the five moments model ($M_S = 1, M_A = 2$) shows a second peak at $5.2\,\mathrm{nm}^{-1}$ which is absent in the expanded distribution. For the intermediate bias region a second peak already begins to form for the four moments model ($M_S = 1, M_A = 1$) as shown in Fig. 3. This issue is even more crucial for the inhomogeneous situation in devices. In Figs. 4 and 5 the energy tensor $\hat{U}_1$ calculated by six different distribution functions is shown. For the six moments model, the first three terms of the expansion are not sufficient inside the channel for $M_A \geqslant 1$, whereas for the displaced heated Maxwellian distribution this occurs only for $M_A \geqslant 2$. For the two critical points (or regions) where this phenomenon is observed the displacement $\mathbf{K}$ is shown in Fig. 6 in comparison with corresponding (convergent) bulk results. The bulk values were selected from a Monte Carlo simulation with the same average energy and the same doping levels. In the inhomogeneous case the displacement has to vary much stronger to reproduce the correct fluxes.

What may seem slightly disconcerting at first is probably of little practical relevance since the expressions for the second-order contributions cause a

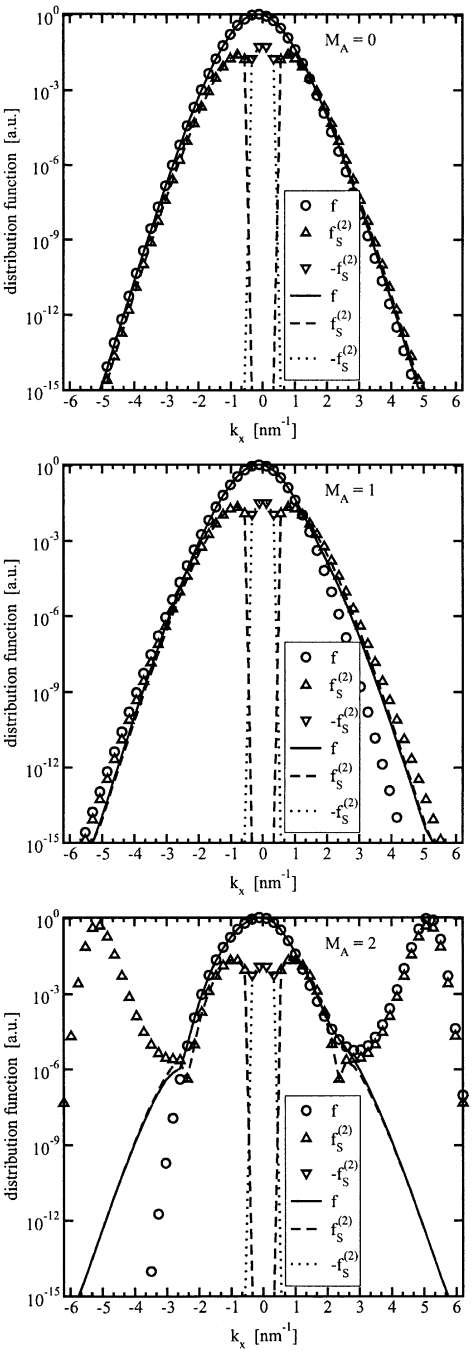

Fig. 2. Validity of the expansion (35) for higher-order energy-dependent displacements ($M_A = 0, 1, 2$) of a heated Maxwellian distribution. The results are from a bulk Monte Carlo simulation with $N_D = 10^{18}\,\mathrm{cm}^{-3}$ and $E = 22\,\mathrm{kV/cm}$ which resulted in an average carrier energy of 75 meV.

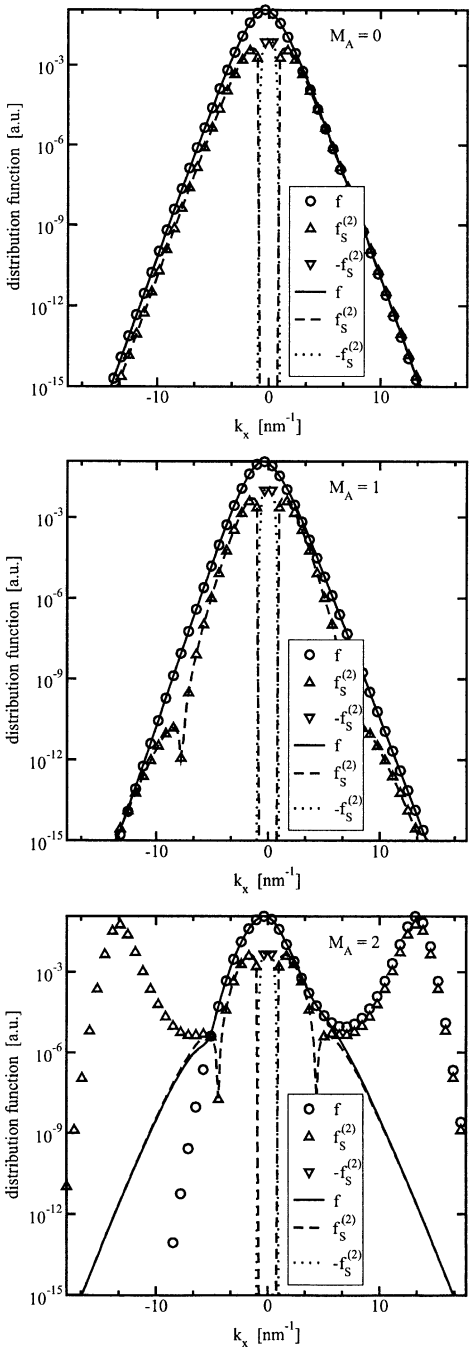

Fig. 3. Validity of expansion (35) for higher-order energy-dependent displacements ($M_A = 0, 1, 2$) of a heated Maxwellian distribution. The results are from a bulk Monte Carlo simulation with $N_D = 10^{18}\,\mathrm{cm}^{-3}$ and $E = 90\,\mathrm{kV/cm}$ which resulted in an average carrier energy of 323 meV.

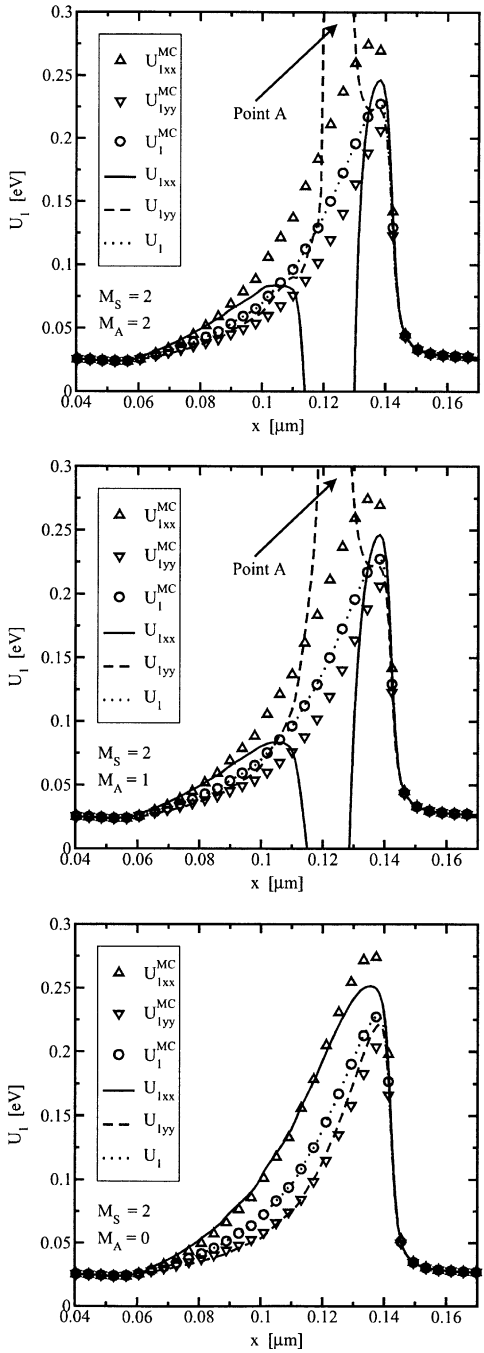

Fig. 4. Components of the energy tensor $\hat{U}_1$ for the example device for the six moments model ($M_S = 2, M_A = 0, 1, 2$). The critical point A around which the first three terms of expansion (35) are not sufficient is shown.

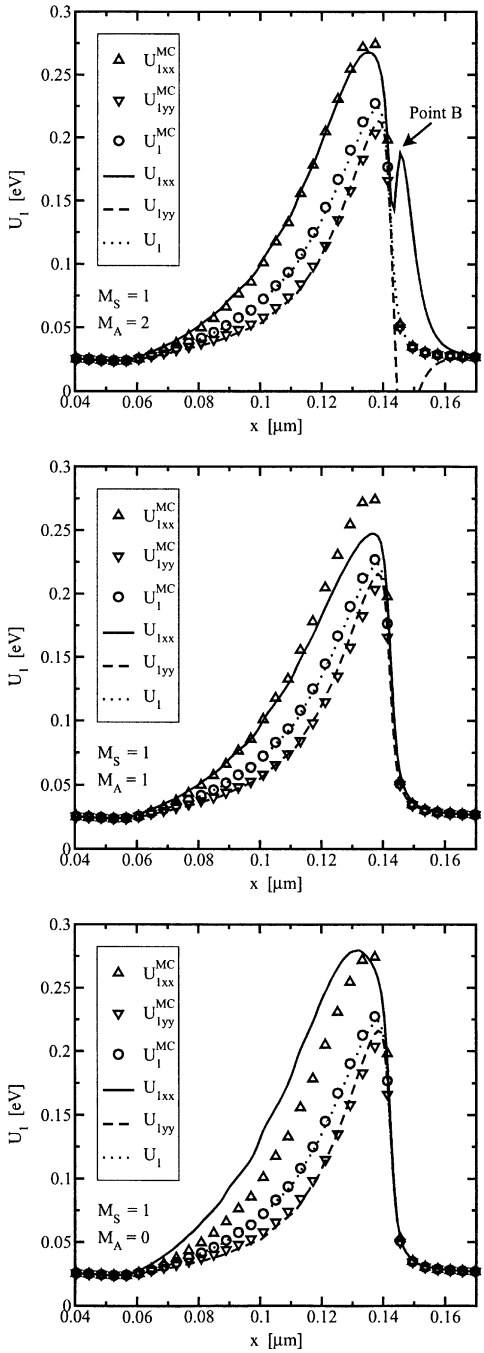

Fig. 5. Components of the energy tensor $\hat{U}_I$ for the example device for the heated Maxwellian distribution ($M_S = 1, M_A = 0, 1, 2$). The critical point B around which the first three terms of expansion (35) are not sufficient is shown.

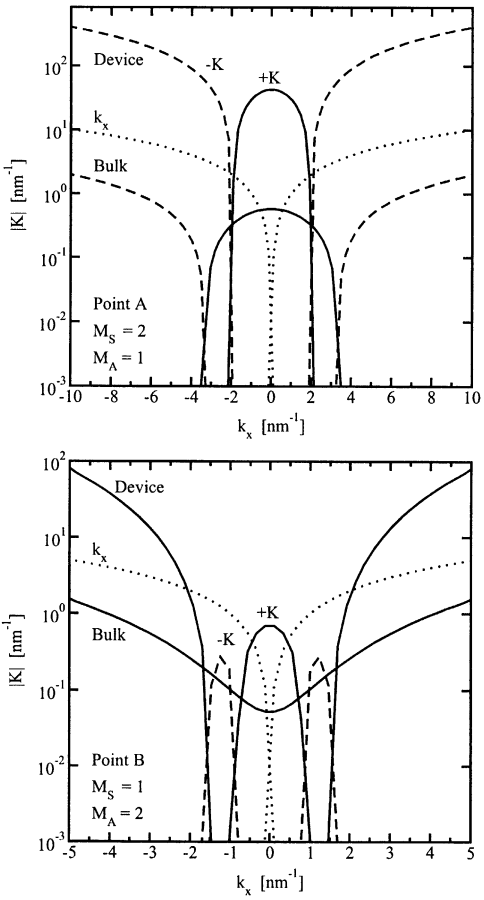

Fig. 6. Comparison of the displacement **K** for the two critical points A and B with a corresponding bulk result. The bulk values were selected from a Monte Carlo simulation with the same average energy and the same doping levels (Point A: $w_l = 9k_B T_L$, $N_D = 3 \times 10^{17}\,\mathrm{cm}^{-3}$, Point B: $w_l = 3k_B T_L$, $N_D = 10^{19}\,\mathrm{cm}^{-3}$). In the inhomogeneous case the displacement has to vary much stronger to reproduce the correct fluxes.

considerable complication compared to models of the form

$$\hat{\mathrm{U}}_i^{(2)} = \mathbf{V}_{i-1} \otimes \mathbf{P}\,. \tag{108}$$

These terms cause additional coupling between the individual flux relations (see Section 6). In addition, the second-order terms introduce hyperbolic modes into the equation system [40] which makes the transport model difficult to solve. Even though Baccarani and Wordeman [41] pointed out the importance of these convective terms in the 1980s, not even transport models based on the much simpler Eq. (108) have been used outside 'laboratory conditions'.

The new expressions are, however, very useful for studying the influence of the second-order contributions on the energy-like tensors. The highest-order moment

gives best results for small average carrier energies but cannot be used at higher energies. Even though the information about the kinetic energy is distributed over all fluxes in a higher-order expansion, Figs. 4 and 5, suggest that this is not that important for the calculation of the energy-like tensors. A feasible approximation might therefore be to calculate the second-order contributions to the energy-like tensors with the distribution function model $M_S = 2$ and $M_A = 0$, i.e., an energy-independently displaced six moments model. Expanded distribution functions based on an energy-independent displacement converge sufficiently throughout the whole device-structure.

It is important to realize that this issue is *not* a particular feature of this model, but rather common to all distribution function models employing exponential functions of polynomials. Other arguments of the exponential function may be found which do not exhibit these features but then the moments could probably not be calculated analytically anymore.

5. Modeling of the scattering integral

By introducing a microscopic relaxation time $\tau_\phi(\mathscr{E})$ for each weight function ϕ the scattering integral can be formally rearranged as [19]

$$\int \phi(\mathbf{k}) Q[f(\mathbf{k})]\,\mathrm{d}^3\mathbf{k} = -n\left\langle \frac{\phi(\mathbf{k})}{\tau_\phi(\mathscr{E})} \right\rangle . \tag{109}$$

For even weight functions the relaxation time is obtained as

$$\frac{1}{\tau_\phi(\mathscr{E})} = \int \left[1 - \frac{\phi(\mathbf{k}')}{\phi(\mathbf{k})}\right] S(\mathbf{k},\mathbf{k}')\,\mathrm{d}^3\mathbf{k}' . \tag{110}$$

Special care has to be taken if the weight function ϕ is a vector, since division as performed in (110) is not possible. Considering $\phi = \mathbf{k}$, the momentum relaxation time $\tau_{\mathbf{p}}(\mathbf{k})$ is obtained as [42]

$$\frac{1}{\tau_{\mathbf{p}}(\mathbf{k})} = \int \left[1 - \frac{k'}{k}\cos\vartheta\right] S(k, k'\cos\vartheta)\,\mathrm{d}^3\mathbf{k}' . \tag{111}$$

In the following we will evaluate the scattering integral considering acoustic deformation potential scattering (ADP), intravalley scattering (IVS), and impurity scattering (IMP) [42]. For IMP the Brooks–Herring model is used for simplicity, although more accurate models can be treated in the same manner. These scattering rates have in common that they are linear functionals of the distribution function. This property will be exploited in some of the following sections. Scattering processes such as short-range carrier–carrier scattering are non-linear in the distribution function and can be evaluated in the same manner. However, the resulting moments of the scattering operator will be of a more complicated form.

The momentum relaxation times for the three scattering processes considered read [42]

$$\text{ADP}: \frac{1}{\tau_{\mathbf{p}}(\mathscr{E})} = K_{\text{adp}} g(\mathscr{E}) \,, \tag{112}$$

$$\text{IVS}: \frac{1}{\tau^{\pm}_{\mathbf{p}}(\mathscr{E})} = K^{\pm}_{\text{ivs}} \sigma(\mathscr{E} \pm \mathscr{E}_0) g(\mathscr{E} \pm \mathscr{E}_0) \,, \tag{113}$$

$$\text{IMP}: \frac{1}{\tau_{\mathbf{p}}(\mathscr{E})} = K_{\text{imp}} T(t) H_{\text{imp}}(\mathscr{E}) \mathscr{E}^{-3/2} \,, \tag{114}$$

with the auxiliary definitions for IMP

$$T(t) = \left[\ln(1+t) - \frac{t}{1+t} \right] \quad \text{with} \quad t = \frac{4}{\mathscr{E}_\beta} \mathscr{E}(1+\alpha\mathscr{E}) \,, \tag{115}$$

$$H_{\text{imp}}(\mathscr{E}) = \frac{1+2\alpha\mathscr{E}}{(1+\alpha\mathscr{E})^{3/2}} \,. \tag{116}$$

The coefficients $K_{\text{adp}}, K^{\pm}_{\text{ivs}}, \mathscr{E}_0 = \hbar\omega_0, K_{\text{imp}}$, and $\mathscr{E}_\beta$ are energy-independent. Their definitions can be found, for example, in [19].

It is convenient to express the moments of the scattering operator in terms of the deviation of the associated moment $\langle \phi \rangle$ from its equilibrium value $\langle \phi \rangle_{\text{eq}}$, calculated with a cold Maxwellian distribution function. We then get [19]

$$\int \phi(\mathbf{k}) Q[f(\mathbf{k})] \, \mathrm{d}^3\mathbf{k} = -n \frac{\langle \phi \rangle - \langle \phi \rangle_{\text{eq}}}{\tau_\phi[f]} \,. \tag{117}$$

The macroscopic relaxation time $\tau_\phi[f]$ associated with the weight function ϕ is a functional of the distribution function and could be calculated if the distribution function was known. As such, (117) is exact and implies no approximation. Since the distribution function is in general not known, the so-called macroscopic relaxation time approximation is employed which assumes that the relaxation time depends only on the average energy $\tau_\phi[f] = \tau_\phi(w_1)$.

The relaxation time $\tau_\phi(w_1)$ is then frequently modeled in an ad hoc manner, either by fits to bulk Monte Carlo data or by empirical models. Particularly for the odd weight functions the influence of this assumption on observable quantities is not yet fully understood [4].

In the following we will calculate macroscopic relaxation times and mobilities by directly evaluating the scattering integral using the microscopic relaxation times and the analytic distribution function model.

5.1. Even moments of the scattering integral

For the balance equations we need the even moments of the scattering integral obtained from the weight functions $\mathscr{E}^i$. With neglected generation/recombination

processes the microscopic relaxation times evaluate to

$$\frac{1}{\tau_i(\mathbf{k})} = \int \left[1 - \left(\frac{\mathscr{E}(\mathbf{k}')}{\mathscr{E}(\mathbf{k})}\right)^i\right] S(\mathbf{k},\mathbf{k}')\,\mathrm{d}^3\mathbf{k}' \,. \tag{118}$$

Since the modeling of these relaxation times has never been considered too critical and mostly constant approximations have been employed we only consider the zero-order term of the distribution function. The moments of the scattering integral can then be written for the distribution function (62) as

$$q_{i,\mathrm{x}} = -\langle \frac{\mathscr{E}^i}{\tau_i(\mathscr{E})} \rangle = \frac{1}{m_{0,0}(0)} \int \mathscr{E}^{i+1/2} H_{\mathrm{g}}(\mathscr{E}) \frac{f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{x}}, b_{\mathrm{x}})}{\tau_i(\mathscr{E})}\,\mathrm{d}\mathscr{E} \,. \tag{119}$$

For the combined distribution function (71) we obtain $q_i = q_{i,\mathrm{h}} + cc_{\mathrm{A}} q_{i,\mathrm{c}}$. Finally we can express the relaxation times required in the macroscopic transport equations as

$$\tau_i = \frac{\langle \mathscr{E}^i \rangle - \langle \mathscr{E}^i \rangle_{\mathrm{eq}}}{q_i} \,. \tag{120}$$

Since ADP and IMP are assumed to be elastic, $\mathscr{E}(\mathbf{k}) = \mathscr{E}(\mathbf{k}')$, they do not contribute to these relaxation times. IVS is assumed to be isotropic with $\mathscr{E}(\mathbf{k}') = \mathscr{E} \pm \mathscr{E}_0$ which gives

$$\frac{1}{\tau_1(\mathscr{E})} = \pm \frac{\mathscr{E}_0}{\mathscr{E}} \int S(\mathbf{k},\mathbf{k}')\,\mathrm{d}^3\mathbf{k}' = \pm \frac{\mathscr{E}_0}{\mathscr{E}} \frac{1}{\tau_{\mathbf{p}}^{\pm}(\mathscr{E})} \,, \tag{121}$$

$$\frac{1}{\tau_2(\mathscr{E})} = \left[\pm \frac{2\mathscr{E}_0}{\mathscr{E}} - \frac{\mathscr{E}_0^2}{\mathscr{E}^2}\right] \int S(\mathbf{k},\mathbf{k}')\,\mathrm{d}^3\mathbf{k}' = \left[\pm \frac{2\mathscr{E}_0}{\mathscr{E}} - \frac{\mathscr{E}_0^2}{\mathscr{E}^2}\right] \frac{1}{\tau_{\mathbf{p}}^{\pm}(\mathscr{E})} \,. \tag{122}$$

The moments of the scattering integral are then obtained as

$$q_{1,\mathrm{x}} = \frac{\mathscr{E}_0}{m_{0,0}(0)} \int f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{x}}, b_{\mathrm{x}}) \mathscr{E}^{1/2} H_{\mathrm{g}}(\mathscr{E}) \left[\frac{1}{\tau_{\mathbf{p}}^{-}(\mathscr{E})} - \frac{1}{\tau_{\mathbf{p}}^{+}(\mathscr{E})}\right] \mathrm{d}\mathscr{E} \,, \tag{123}$$

$$q_{2,\mathrm{x}} = \frac{\mathscr{E}_0}{m_{0,0}(0)} \int f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{x}}, b_{\mathrm{x}}) \mathscr{E}^{1/2} H_{\mathrm{g}}(\mathscr{E}) \times \left[(2\mathscr{E} - \mathscr{E}_0) \frac{1}{\tau_{\mathbf{p}}^{-}(\mathscr{E})} - (2\mathscr{E} + \mathscr{E}_0) \frac{1}{\tau_{\mathbf{p}}^{+}(\mathscr{E})}\right] \mathrm{d}\mathscr{E} \,. \tag{124}$$

Because generation/recombination processes are neglected, q_0 evaluates to $q_0 = 0$.

5.2. Odd moments of the scattering integral

For the flux equations we need the odd moments of the scattering integral obtained from the weight functions $\mathbf{p}\mathscr{E}^i$. The relaxation times associated with the

weight function $\mathbf{p}\mathscr{E}^i$ are defined as

$$\frac{1}{\tau_{\mathbf{p}\mathscr{E}^i}(\mathbf{k})} = \int \mathrm{d}\cos\vartheta \int k'^2\,\mathrm{d}k' \left[1 - \frac{k'}{k}\cos\vartheta \frac{\mathscr{E}^i(\mathbf{k}')}{\mathscr{E}^i(\mathbf{k})}\right] S(k,k',\cos\vartheta)\,. \tag{125}$$

Since ADP and IMP are elastic, that is, $\mathscr{E}(\mathbf{k}) = \mathscr{E}(\mathbf{k}')$, (125) simplifies to

$$\frac{1}{\tau_{\mathbf{p}\mathscr{E}^i}(\mathbf{k})} = \int \left[1 - \frac{k'}{k}\cos\vartheta\right] S(k,k',\cos\vartheta)\,\mathrm{d}^3\mathbf{k}' = \frac{1}{\tau_{\mathbf{p}}(\mathbf{k})} \tag{126}$$

which is the definition of the momentum relaxation time $\tau_{\mathbf{p}}$. Since IVS is assumed to be isotropic, $S = S(k,k')$, the integration of $\cos\vartheta$ vanishes and we obtain

$$\frac{1}{\tau_{\mathbf{p}\mathscr{E}^i}(\mathbf{k})} = \int S(\mathbf{k},\mathbf{k}')\,\mathrm{d}^3\mathbf{k}' = \frac{1}{\tau(\mathbf{k})} = \frac{1}{\tau_{\mathbf{p}}(\mathbf{k})}\,. \tag{127}$$

We can now evaluate the scattering integral using the analytic distribution function to obtain

$$\mathbf{Q}_i = -\left\langle \frac{\mathbf{p}\mathscr{E}^i}{\tau_{\mathbf{p}}} \right\rangle = \frac{1}{n^{(0)}} \int \mathbf{p}\mathscr{E}^i \frac{f_{\mathrm{A}}}{\tau_{\mathbf{p}}}\,\mathrm{d}^3\mathbf{k} = \sum_{j=0}^{2} \mathbf{K}_j S_{ij} \tag{128}$$

with $S_{ij} = S_{ij,\mathrm{h}} + cc_{\mathrm{A}} S_{ij,\mathrm{c}}$ for the combined distribution function, where

$$S_{ij,\mathrm{x}} = C_{\mathrm{S}} \frac{b}{a^b} \int \mathscr{E}^{i+j+b+1/2} H_{1,1} \frac{f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{x}}, b_{\mathrm{x}})}{\tau_{\mathbf{p}}}\,\mathrm{d}\mathscr{E} \tag{129}$$

with the definition $C_{\mathrm{S}} = m^* C_{\mathrm{M}}$. Since the odd part of the distribution function is of first-order in κ, so are the odd moments of the scattering integral. Using the symbolic notation we can write

$$\hat{\mathrm{Q}} = \hat{\mathrm{K}}\hat{\mathrm{S}}^{\mathrm{T}} = \hat{\mathrm{V}}\hat{\mathrm{D}}^{\mathrm{T}}\hat{\mathrm{S}}^{\mathrm{T}} = \hat{\mathrm{V}}\hat{\mathrm{Z}}^{\mathrm{T}} \tag{130}$$

with the scattering matrix $\hat{\mathrm{Z}} = \hat{\mathrm{S}}\hat{\mathrm{D}}$. The scattering integral for the odd weight functions can thus be expressed as a linear combination of the fluxes with the coefficients Z_{ij} which only depend on the even moments. This is in accordance with the results obtained by Hänsch [6] and Anile [7]. The coefficients Z_{ij} contain the information about the scattering rates via the coefficients $S_{ij,\mathrm{x}}$ which are given as follows:

$$S^{\mathrm{adp}}_{ij,\mathrm{x}} = C_{\mathrm{S}} \frac{b}{a^b} K_{\mathrm{adp}} g_0 \int \mathscr{E}^{i+j+2} H_{\mathrm{adp}} f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{x}}, b_{\mathrm{x}})\,\mathrm{d}\mathscr{E}\,, \tag{131}$$

$$S^{\mathrm{ivs}}_{ij,\mathrm{x}} = C_{\mathrm{S}} \frac{b}{a^b} K^{\pm}_{\mathrm{ivs}} g_0 \int \mathscr{E}^{i+j+3/2} H^{\pm}_{\mathrm{ivs}} f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{x}}, b_{\mathrm{x}})\,\mathrm{d}\mathscr{E}\,, \tag{132}$$

$$S^{\mathrm{imp}}_{ij,\mathrm{x}} = C_{\mathrm{S}} \frac{b}{a^b} K_{\mathrm{imp}} \int \mathscr{E}^{i+j} H_{1,1} H_{\mathrm{imp}} f_{\mathscr{E}}(\mathscr{E}, a_{\mathrm{x}}, b_{\mathrm{x}})\,\mathrm{d}\mathscr{E} \tag{133}$$

with the auxiliary non-parabolicity functions

$$H_{\mathrm{adp}}(\mathscr{E}) = H_{1,1}(\mathscr{E})H_{\mathrm{g}}(\mathscr{E})\,, \tag{134}$$

$$H^{\pm}_{\mathrm{ivs}}(\mathscr{E}) = H_{1,1}(\mathscr{E})\sqrt{\mathscr{E} \pm \mathscr{E}_0}H_{\mathrm{g}}(\mathscr{E} \pm \mathscr{E}_0)\,. \tag{135}$$

Good approximations for the functions $H^{\pm}_{\mathrm{ivs}}(\mathscr{E})$ and $H_{\mathrm{imp}}(\gamma^2)$ are more difficult to obtain than for the non-parabolicity functions $H_{x,y}(\mathscr{E})$. For the evaluation of the examples, the scattering integrals (131)–(133) have been evaluated numerically. To obtain analytic approximations, the approach proposed in [43] can be transfered to the non-Maxwellian distribution functions used here.

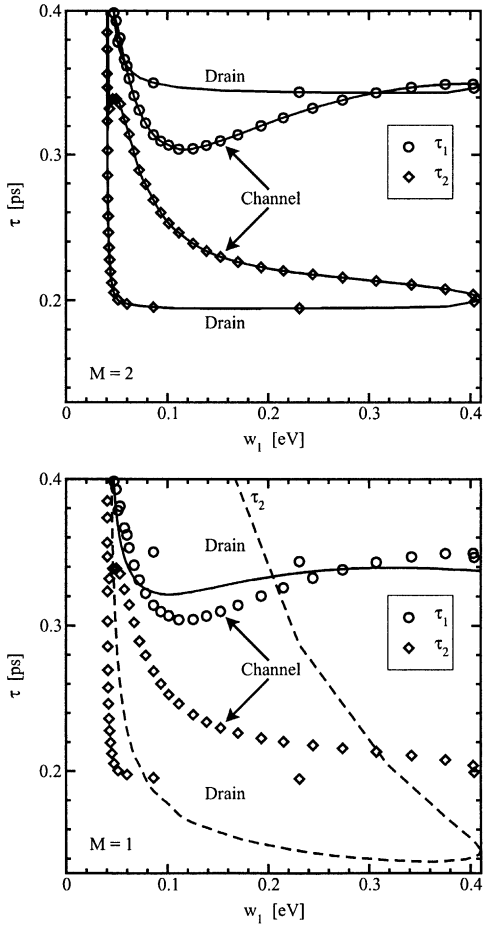

Fig. 7. Comparison of the relaxation times as a function of the average energy for two different models. At the top the non-Maxwellian six moments distribution function ($M = 2$) and at the bottom the heated Maxwellian model ($M = 1$).

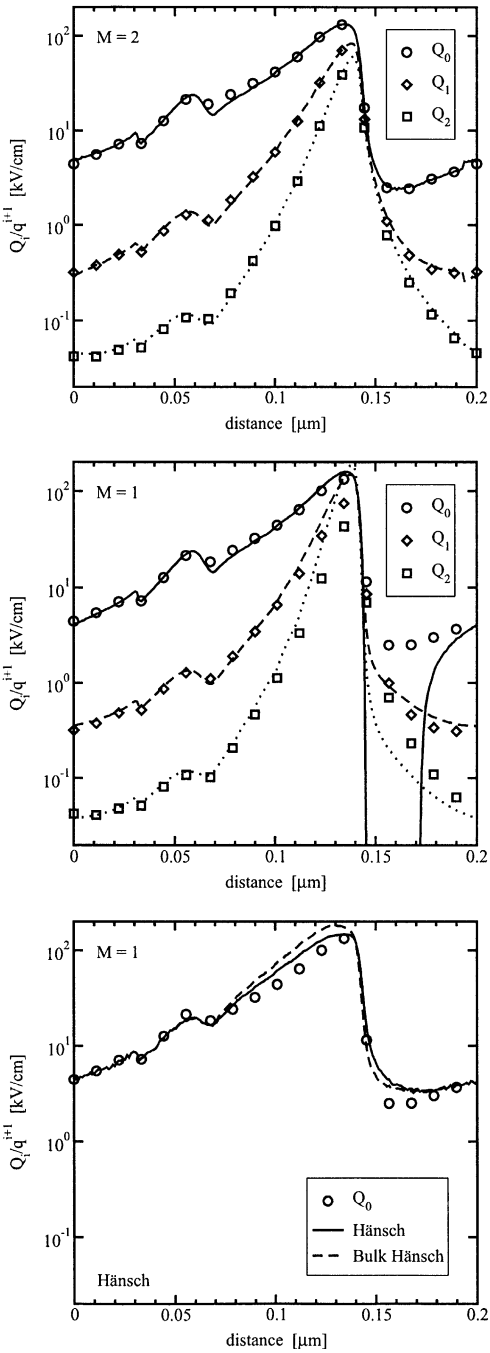

Fig. 8. Comparison of the first row of the scattering matrix $\hat{Z}$ for three different models. At the top the non-Maxwellian six moments model ($M = 2$), in the middle the heated Maxwellian model ($M = 1$), and at the bottom Hänsch's model.

5.3. Comparison

A comparison of the calculated relaxation times τ_i to Monte Carlo results based on the same band structure and scattering models is shown in Fig. 7. The relaxation times are plotted as a function of the average energy because they are commonly modeled as either constant or energy dependent [4]. As can be seen, this is only approximately true and we find two branches, one inside the channel region and the other for the drain region. This hysteresis in the relaxation times is only properly reproduced by the non-Maxwellian six moments distribution function model. The hysteresis in τ_2 obtained by the heated Maxwellian distribution is explained as follows: the moment of the scattering integral q_2 is of course a single valued function of w_1, because the parameters of the distribution function depend only on w_1. The relaxation time τ_2, on the other hand, is defined via (120) and thus depends on w_2 which *cannot* be expressed as a single valued function of w_1 and therefore introduces the hysteresis.

The moments of the scattering integral $\mathbf{Q}_i$ are compared to Monte Carlo results in Fig. 8. Inside the channel the heated Maxwellian approximation ($M = 1$) delivers fairly accurate results as long as the average carrier energy is not too high ($w_1 < 0.25\,\mathrm{eV}$). For higher energies the scattering rates are overestimated. Inside the drain region, the heated Maxwellian approximation fails completely and even delivers a different sign for $\mathbf{Q}_0$. This is a consequence of the linearization of the anti-symmetric part of the distribution function which is fatal in this case. The six moments description ($M = 2$), however, delivers highly accurate results throughout the whole device. Also shown in Fig. 8 is the scattering moment $\mathbf{Q}_0$ predicted by the popular Hänsch model [6] which overestimates scattering inside the channel.

6. General macroscopic moment models

In the following the transport equations determining the first six moments will be derived. The macroscopic transport equations are obtained by multiplying Boltzmann's equation with the appropriate weight functions and integrating the product over $\mathbf{k}$ space. As usual, we assume that the Brillouin zone extends towards infinity, which is justified because the distribution function declines exponentially [17]. We apply the weight functions $\mathscr{E}^i$ and $\mathbf{p}\mathscr{E}^i$ with $i = 0, 1, \ldots, M$ to the Boltzmann equation given by (31) and (32) to obtain $N = 2(M + 1)$ moment equations. The general transport model will be formulated in terms of the unknowns $w_i = \langle \mathscr{E}^i \rangle$ and $\mathbf{V}_i = \langle \mathbf{u}\mathscr{E}^i \rangle$. The required closure relations for the moments $\hat{\mathrm{U}}_i, q_i$, and $\mathbf{Q}_i$ have been calculated in the previous sections.

6.1. Balance equations

The balance equations are obtained as the moments of (31) with the even weight functions $\mathscr{E}^i$ as

$$\partial_t n \langle \mathscr{E}^i \rangle + \nabla_{\mathbf{r}} \cdot n \langle \mathbf{u}\mathscr{E}^i \rangle - n\mathbf{F} \cdot \langle \nabla_{\mathbf{p}} \mathscr{E}^i \rangle = \frac{1}{\kappa^2} \int \mathscr{E}^i Q_{\mathrm{S}}[f_{\mathrm{S}}]\, \mathrm{d}^3\mathbf{k}\,. \tag{136}$$

The calculation of the gradients of $\mathscr{E}^i$ is straightforward and gives

$$\nabla_{\mathbf{p}}\mathscr{E}^i = i\mathscr{E}^{i-1}\nabla_{\mathbf{p}}\mathscr{E} = i\mathscr{E}^{i-1}\mathbf{u}\,. \tag{137}$$

The balance equations can thus be rewritten as

$$\partial_t n w_i + \nabla_{\mathbf{r}}\cdot n\mathbf{V}_i - i\mathbf{F}\cdot n\mathbf{V}_{i-1} = -\frac{n}{\kappa^2}\frac{w_i - w_{i,\mathrm{eq}}}{\tau_i}\,, \tag{138}$$

where the definitions (120) of the relaxation times τ_i have been used. Note that due to the choice of solution variables the structure of the balance equations is independent of the band structure model.

6.2. Flux equations

To formulate the flux equations we apply the odd weight functions $\mathbf{p}\mathscr{E}^i$ to (32) and obtain

$$\kappa^2\partial_t n\langle\mathbf{p}\mathscr{E}^i\rangle^{(1)} + \nabla_{\mathbf{r}}\cdot n\langle\mathbf{u}\otimes\mathbf{p}\mathscr{E}^i\rangle - n\mathbf{F}\cdot\langle\nabla_{\mathbf{p}}\otimes\mathbf{p}\mathscr{E}^i\rangle = \int\mathbf{p}\mathscr{E}^i Q_A[f_A]\,\mathrm{d}^3\mathbf{k}\,, \tag{139}$$

or in compact form $\mathbf{\Psi}_i = \mathbf{Q}_i$. Eq. (139) contains gradients of several scalar and tensor-valued functions. The gradients of the weight functions $\mathbf{p}\mathscr{E}^i$ are

$$\nabla_{\mathbf{p}}\otimes\mathbf{p}\mathscr{E}^i = \mathscr{E}^i\nabla_{\mathbf{p}}\otimes\mathbf{p} + \mathbf{p}\otimes\nabla_{\mathbf{p}}\mathscr{E}^i = \mathscr{E}^i\hat{\mathrm{I}} + \mathbf{u}\otimes\mathbf{p}i\mathscr{E}^{i-1} \tag{140}$$

which gives for the averages

$$\langle\nabla_{\mathbf{p}}\otimes\mathbf{p}\mathscr{E}^i\rangle = w_i\hat{\mathrm{I}} + i\hat{\mathrm{U}}_i\,. \tag{141}$$

For the term $\partial_t\langle\mathbf{p}\mathscr{E}^i\rangle^{(1)}$ we get $\mathbf{P}_i = \langle\mathbf{p}\mathscr{E}^i\rangle^{(1)} = m^*(\mathbf{V}_i + 2\alpha\mathbf{V}_{i+1})$ and the fluxes $\mathbf{\Psi}_i$ can finally be written as

$$\mathbf{\Psi}_i = \kappa^2\partial_t n\mathbf{P}_i + \hat{\mathrm{U}}_{i+1}\nabla_{\mathbf{r}}\log n + \nabla_{\mathbf{r}}\cdot\hat{\mathrm{U}}_{i+1} - \mathbf{F}\cdot(w_i\hat{\mathrm{I}} + i\hat{\mathrm{U}}_i)\,. \tag{142}$$

Since there is no $\mathbf{k}$-space dependence in the macroscopic equations the subscript $\mathbf{r}$ of the nabla operator will be dropped for the remainder of this article.

Conventionally, inverse mobility tensors $\hat{\mu}_i^{-1}$ are introduced [4] to establish a relation between $\mathbf{Q}_i$ and $\mathbf{V}_i$ analogously to the drift-diffusion model. This procedure, which is almost exclusively used in today's available device simulators, has several shortcomings. We therefore propose a different approach: In matrix form we have the linear equation system $\hat{\Psi} = \hat{\mathrm{V}}\hat{\mathrm{Z}}^{\mathrm{T}}$ which has the solution $\hat{\mathrm{V}} = \hat{\Psi}\hat{\mathrm{Y}}^{\mathrm{T}}$ with $\hat{\mathrm{Y}} = \hat{\mathrm{Z}}^{-1}$. We can thus obtain explicit relations for the fluxes $\mathbf{V}_i$ as

$$\mathbf{V}_i = \sum_{j=0}^{M} Y_{ij}\mathbf{\Psi}_j = \kappa^2\sum_{j=0}^{M}\partial_t n\mathbf{P}_i + \hat{\mu}_i\frac{\mathbf{F}}{q} - \hat{\mathscr{D}}_i\nabla\log n - \sum_{j=0}^{M} Y_{ij}\nabla\cdot\hat{\mathrm{U}}_{j+1}\,, \tag{143}$$

where we introduced the mobility tensors $\hat{\mu}_i$ and the diffusion tensors $\hat{\mathscr{D}}_i$ as

$$\hat{\mu}_i = -q\sum_{j=0}^{M} Y_{ij}(w_j\hat{\mathrm{I}} + j\hat{\mathrm{U}}_j), \quad \text{and} \quad \hat{\mathscr{D}}_i = -\sum_{j=0}^{M} Y_{ij}\hat{\mathrm{U}}_{j+1}\,. \tag{144}$$

By defining $\mathbf{V}_i = \mathbf{V}_i^{(0)} + \kappa^2\mathbf{V}_i^{(2)}$, $\hat{\mu}_i = \mu_i\hat{\mathrm{I}} + \kappa^2\hat{\mu}_i^{(2)}$, and $\hat{\mathscr{D}}_i = D_i\hat{\mathrm{I}} + \kappa^2\hat{\mathscr{D}}_i^{(2)}$ we can split (143) into a zero- and second-order term

$$\mathbf{V}_i^{(0)} = \mu_i\frac{\mathbf{F}}{q} - D_i\nabla\log n - \sum_{j=0}^{M} Y_{ij}\nabla U_{j+1}\,, \tag{145}$$

$$\mathbf{V}_i^{(2)} = \sum_{j=0}^{M} \partial_t n\mathbf{P}_i + \hat{\mu}_i^{(2)}\frac{\mathbf{F}}{q} - \hat{\mathscr{D}}_i^{(2)}\nabla\log n - \sum_{j=0}^{M} Y_{ij}\nabla\cdot\hat{\mathrm{U}}_{j+1}^{(2)}\,, \tag{146}$$

where the zero-order contribution to the mobility and diffusion tensors reduce to scalars

$$\mu_i = -q\sum_{j=0}^{M} Y_{ij}(w_j + jU_j), \quad \hat{\mu}_i^{(2)} = -q\sum_{j=0}^{M} jY_{ij}\hat{\mathrm{U}}_j^{(2)}\,, \tag{147}$$

$$D_i = -\sum_{j=0}^{M} Y_{ij}U_{j+1}, \quad \hat{\mathscr{D}}_i^{(2)} = -\sum_{j=0}^{M} Y_{ij}\hat{\mathrm{U}}_{j+1}^{(2)}\,. \tag{148}$$

Formulation (145)–(146) has several interesting properties. First, the zero-order contributions to the mobilities $\hat{\mu}_i$ depend only on the even moments rather than on the fluxes. In addition, the fact that the mobilities are functionals of the distribution function is well reproduced since the mobilities depend on all available even moments w_j rather than on w_1 alone. Second, as a result, the zero-order contribution to the explicit flux relations (145) are linear in $\mathbf{V}_i$. Furthermore, all fluxes depend on all even moments, most notably on the closure relation for $\hat{\mathrm{U}}_{M+1}$. Note that this is not the case with models based on the relaxation time approximation, where the matrix $\hat{\mathbf{Z}}$ is of diagonal form and thus only the highest order equation for the flux $\mathbf{V}_M$ depends directly on the closure relation.

6.2.1. Diffusion approximation

Although the flux relations given by (143) are straightforward to evaluate with a given set n, w_i, and $\mathbf{V}_i$, the solution of the transport model is challenging. This is because the second-order terms introduce hyperbolic modes into the equation system which require discretization techniques known from computational fluid-dynamics [40,44–47]. The diffusion approximation can be applied when the Knudsen number κ is small. As a consequence the second-order terms (146) are neglected. The remaining

relation (145) results in a parabolic partial differential equation system which is simpler to solve.

Preliminary results indicate, however, that such an approach, as was for instance followed in [7] is problematic. For the simple bulk case with $\mathbf{E} = E\mathrm{e}_x$ we find from the full representation (143) that the current is proportional to E and $\mu_{0,00}$. The mobility tensor component $\mu_{0,00}$ depends on the second-order contribution to the energy-like tensors which can be substantial. In particular, we observed a deviation from the zero-order value U_1 of 7–25% in the bulk case, depending on the doping and bias conditions, and more than 40% inside the example device. This can lead to a considerable error even in the bulk mobility. We might therefore *not* even be able to reproduce the correct bulk mobility when applying the diffusion approximation, regardless of the fact that the moments of the scattering integral are modeled with a high accuracy. Note that this issue is not that severe for models based on the relaxation time approximation.

7. Conclusions

We present a rigorous derivation of non-parabolic macroscopic transport models of different order from Boltzmann's equation. The closure relations are derived from analytical distribution function models, most notably a non-Maxwellian six moments description. Instead of applying the relaxation time approximation we reformulate the moments of the scattering integral in terms of the fluxes of the equation system. In the diffusion limit, where only the zero- and first-order terms are kept, we thereby avoid any flux dependence of the mobilities and thus the non-linearities resulting therefrom. As a result, all fluxes occurring in the final equation system depend on all even moments and in particular on the closure relation. We show that in contrast to standard energy-transport and hydrodynamic models, which are based on a heated Maxwellian distribution function, a non-Maxwellian six moments description accurately models all closure relations. However, for the particular case when the scattering integral is systematically evaluated with an analytic distribution function model, the second-order convective terms seem to be too important to be neglected.

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