Reformulation of Macroscopic Transport Models Based on the Moments of the Scattering Integral

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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 other closure relations are directly calculated via analytical models of the distribution function. We compare models of order four and six to demonstrate the substantially improved accuracy of the six moments description over the conventional four moments energy-transport formalism.**

I. Introduction

Macroscopic transport models based on Boltzmann's transport equation (BTE) are of fundamental importance for the modeling of semiconductor devices. These models are derived from the BTE by applying the method of moments which transforms the BTE into an infinite set of equations. To obtain a tractable equation set, this hierarchy has to be truncated after N equations. Since the highest order equation contains the $(N+1)^{th}$ moment, a closure relation has to be invoked which basically models the $(N+1)^{th}$ moment by the N lower order moments. This is a critical step which determines the accuracy of the model. Another crucial step is the modeling of the mobilities, commonly done by employing the macroscopic relaxation time approximation. In the relaxation time approximation the mobilities are normally expressed as a function of the average carrier energy or temperature. A rigorous treatment reveals, however, that the mobilities depend on the fluxes such as the carrier current and the energy flux and therefore on the odd moments of the distribution function [1], [2]. By assuming that the ratio of the fluxes approximately behaves like the ratio observed under homogeneous conditions this flux dependence is commonly transformed into an energy dependence. This can impair the quality of the model and we present a different formulation which avoids this assumption. Finally, when non-parabolic dispersion relations are used, additional factors appear in front of the streaming terms in the flux relations [3].

All three issues can be rigorously dealt with by using an analytical description of the distribution function. Obviously, the quality of this distribution function model has a strong impact on the quality of the transport model. We compare the six moments description presented in [4] with a standard model based on a heated Maxwell distribution.

II. Band Structure Model

In the following we will shortly outline the derivation of our model. We use a single equivalent isotropic non-parabolic band, and Kane's dispersion relation

$$\frac{\hbar^2 k^2}{2\,m^*} = \mathcal{E}\,(1+\alpha\mathcal{E}) \doteq \mathcal{E} H_{\mathcal{E}}(\mathcal{E}) \tag{1}$$

which gives

$$g(\mathcal{E}) = g_0\sqrt{\mathcal{E}}\,\sqrt{1+\alpha\mathcal{E}}\,(1+2\alpha\mathcal{E}) \doteq g_0\sqrt{\mathcal{E}} H_{\mathrm{g}}(\mathcal{E}) \tag{2}$$

for the density of states and

$$\mathbf{u}(\mathbf{k},\mathbf{r}) = \frac{\hbar\mathbf{k}}{m^*}\,\frac{1}{1+2\alpha\mathcal{E}} \doteq \frac{\hbar\mathbf{k}}{m^*}\,H_{\mathrm{u}}(\mathcal{E}) \tag{3}$$

for the group velocity. The non-parabolicity correction functions H_{x} are defined to equal unity for parabolic bands ($\mathrm{x} = \mathcal{E}, \mathrm{g}, \mathrm{u}$). We are aware that Kane's relation is only roughly valid for energies smaller $2\,\mathrm{eV}$ [5]. However, not even this first-order approximation to the real non-parabolic band structure allows a simple analytical treatment. 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. To obtain closed form solutions in the final coefficients of the transport equations the non-parabolicity functions H_{x} will be grouped together for each moment and approximated by a fit expression of the form

$$H_{\mathrm{y}}(\mathcal{E}) \approx 1 + \gamma_{\mathrm{y}}(\alpha\mathcal{E})^{\lambda_{\mathrm{y}}}\ , \tag{4}$$

similar to the procedure followed in [4]. Note that (4) is written in a form that preserves the non-parabolicity factor α in the final result.

III. The Diffusion Approximation

In the following we will restrict our discussion to the diffusion dominated regime, formally introduced by the diffusion approximation of the BTE. This assumption basically eliminates the convective terms appearing in hydrodynamic models and thus provides the transition to the energy-transport models which are commonly used in device simulators [3].

We start with the scaled form of the BTE [6] and split the distribution function into its symmetric and anti-symmetric parts as $f(\mathbf{k}) = f_{\mathrm{S}}(\mathbf{k}) + \kappa f_{\mathrm{A}}(\mathbf{k})$. The scaling parameter of the BTE is the Knudsen number κ which represents the mean

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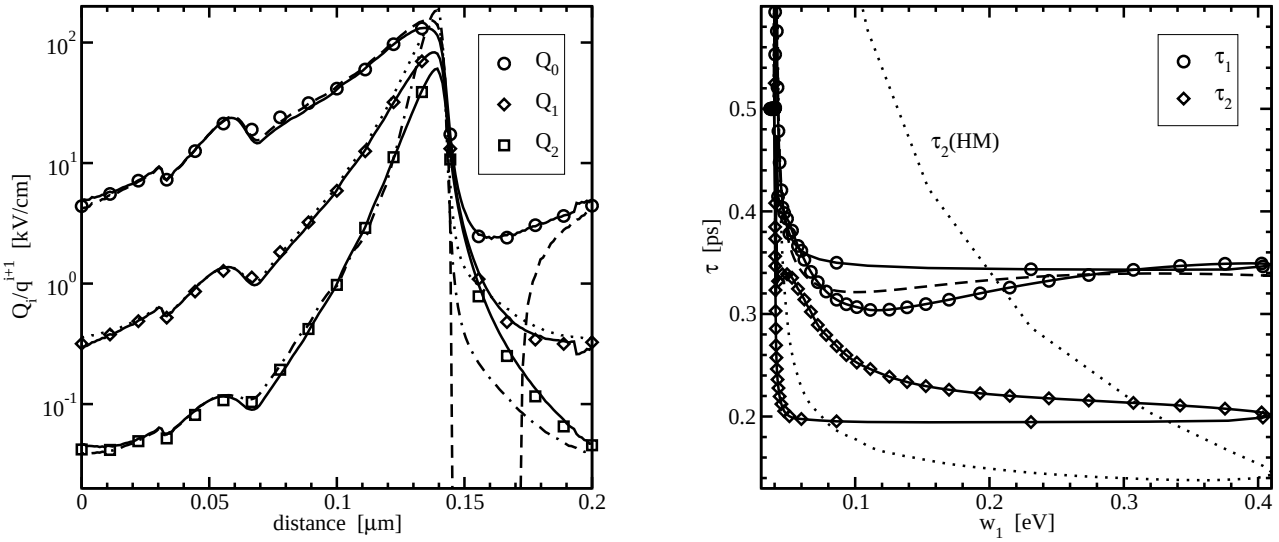

Fig. 1. Comparison of the moments $\mathbf{Q}_i$ (left) and the relaxation times τ_i (right) with Monte Carlo data. The Monte Carlo data is given by the symbols, the results based on the analytical distribution function model with $N = 6$ by the solid lines, and the heated Maxwellian distribution (HM) with $N = 4$ is represented by the other line styles.

free path relative to the device dimension [6]. In the diffusion approximation [6] it is assumed that κ is small, and all terms of order $O(\kappa^2)$ are neglected. We obtain

$$\partial_t f_\mathrm{S} + \mathbf{u}\cdot\nabla_\mathbf{r} f_\mathrm{A} + \mathbf{F}\cdot\nabla_\mathbf{p} f_\mathrm{A} = \frac{1}{\kappa^2} Q_\mathrm{S}[f_\mathrm{S}] \tag{5}$$

$$\mathbf{u}\cdot\nabla_\mathbf{r} f_\mathrm{S} + \mathbf{F}\cdot\nabla_\mathbf{p} f_\mathrm{S} = Q_\mathrm{A}[f_\mathrm{A}] \ . \tag{6}$$

In addition, a relationship between the symmetric and anti-symmetric part can be derived when it is assumed that $f(\mathbf{k})$ is obtained by displacing a symmetric function $f_\mathrm{S}(\mathbf{k})$ by $\kappa\,\mathbf{k}_\mathrm{c}$. Under the assumption that $f_\mathrm{S}(\mathbf{k})$ is isotropic and thus depends only on the modulus of $\mathbf{k}$, and that κ is small we expand the distribution function

$$f(\mathbf{k}) = f_\mathrm{S}(\mathbf{k} - \kappa\,\mathbf{k}_\mathrm{c}) \approx f_\mathrm{S}(\mathbf{k}) - \nabla_\mathbf{k} f(\mathbf{k})\cdot\kappa\,\mathbf{k}_\mathrm{c} \ . \tag{7}$$

All terms of order $O(\kappa^2)$ are neglected, consistently with the diffusion approximation. The displacement of the anti-symmetric part $\kappa\,\mathbf{k}_\mathrm{c}$ is now assumed to depend only on the carrier energy as $\mathbf{k}_\mathrm{c} = \mathbf{k}_\mathrm{c}(\mathcal{E})$. The anti-symmetric part is thus obtained as

$$f_\mathrm{A}(\mathbf{k}) = -\nabla_\mathbf{k} f_\mathrm{S}(\mathbf{k})\cdot\mathbf{k}_\mathrm{c}(\mathcal{E}) = -\partial_\mathcal{E} f_\mathrm{S}(\mathcal{E})\,\hbar\mathbf{u}\cdot\mathbf{k}_\mathrm{c}(\mathcal{E}) \ . \tag{8}$$

We now assume that the symmetric part fulfills the ordinary differential equation

$$\partial_\mathcal{E} f_\mathrm{S}(\mathcal{E}) = -f_\mathrm{S}(\mathcal{E}) H_f(\mathcal{E}) \ . \tag{9}$$

The solutions of (9) include the Maxwellian distribution with $H_f = 1/(\mathrm{k_B}T)$. With (9) and (3) the anti-symmetric part can be written as $f_\mathrm{A}(\mathbf{k}) = \mathbf{B}(\mathcal{E})\cdot\mathbf{k}\,f_\mathrm{S}(\mathcal{E})$ where the vector $\mathbf{B}(\mathcal{E})$ is expanded in powers of the energy to finally give

$$f_\mathrm{A}(\mathbf{k}) = \sum_{j=0}^{M} \mathcal{E}^j \mathbf{B}_j\cdot\mathbf{k}\,f_\mathrm{S}(\mathcal{E}) \ . \tag{10}$$

Note that this definition implicitly defines $\mathbf{k}_\mathrm{c}(\mathcal{E})$. M denotes the number of fluxes and the number of even moments and equals $N/2 - 1$, where N is the order of the moments expansion. In the following we will use a heated Maxwellian distribution for $N = 4$ and the six moments description from [4] for $N = 6$.

IV. Transport Model

The macroscopic transport equations are obtained by multiplying the BTE with the weight functions $\mathcal{E}^i$ and $\mathbf{p}\mathcal{E}^i$ and integrating the product over $\mathbf{k}$ space. As solution variables of the final equation system we use $w_i = \langle\mathcal{E}^i\rangle$ and $\mathbf{V}_i = \langle\mathbf{u}\mathcal{E}^i\rangle$.

A. Moments of the Scattering Integral

We assume a linear scattering operator and consider phonon and impurity scattering based on the Golden Rule [5]. The moments of the scattering integral are calculated with the analytic distribution function model using the same standard scattering rates as in Monte Carlo calculations to obtain [9]

$$\mathbf{Q}_i = -\Big\langle\frac{\mathbf{p}\mathcal{E}^i}{\tau_p(\mathcal{E})}\Big\rangle = \sum_{j=0}^{M} Z_{ij}\mathbf{V}_j \ , \tag{11}$$

$$q_i = -\Big\langle\frac{\mathcal{E}^i}{\tau_{\mathcal{E}^i}(\mathcal{E})}\Big\rangle = -\frac{w_i - w_{i,\mathrm{eq}}}{\tau_i(w_1,\ldots,w_M)} \ , \tag{12}$$

where the coefficients Z_{ij} depend only on the even moments w_l. Note that each moment of the scattering integral $\mathbf{Q}_i$ depends on all fluxes $\mathbf{V}_j$ [1], [2]. The relaxation times τ_1 and τ_2 are the energy relaxation time and the kurtosis relaxation time, respectively [8].

A comparison of (11) to Monte Carlo results based on the same band structure and scattering models is shown in Fig. 1. As an example device we use a one-dimensional cut through

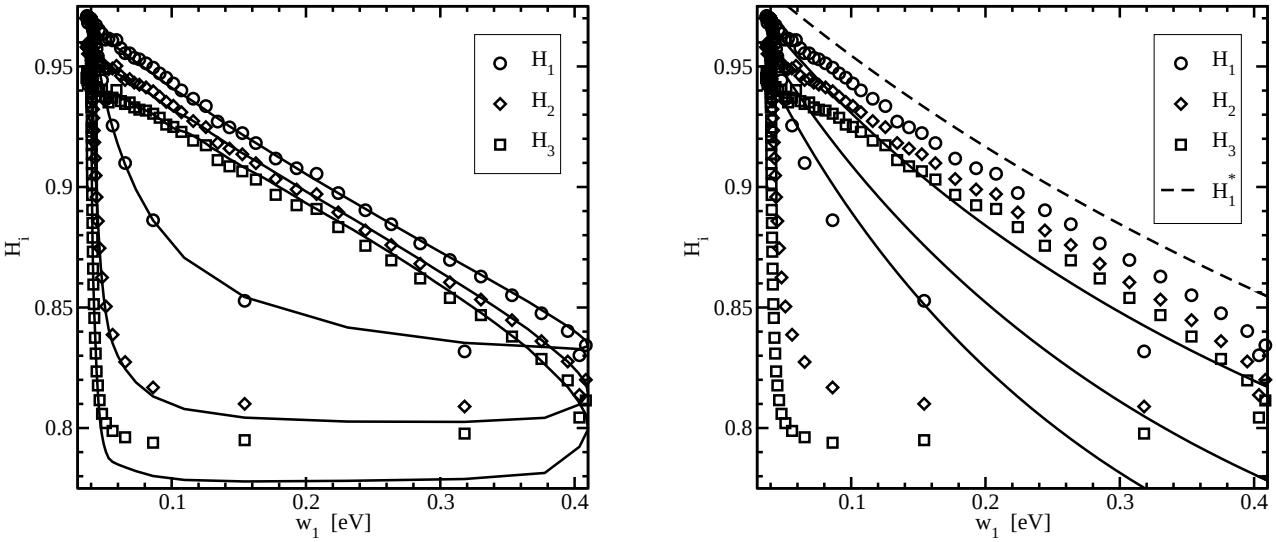

Fig. 2. Left: Comparison of the non-parabolicity factors H_i from Monte Carlo simulations (symbols) with the results obtained from the six moments model $N = 6$ (solid lines) Right: Comparison with the results obtained from the heated Maxwellian distribution $N = 4$ (solid lines). Also shown is H_1^* taken from [7].

the potential resulting from an energy-transport solution of the $90\,\mathrm{nm}$ well-tempered MOS [10] at $V_\mathrm{D} = V_\mathrm{G} = 1\,\mathrm{V}$. Inside the channel the heated Maxwellian approximation ($N = 4$) delivers fairly accurate results as long as $w_1 < 0.25\,\mathrm{eV}$. For higher energies the scattering rates are overestimated. Inside the drain region, the heated Maxwellian approximation fails completely. The six moments description ($N = 6$) delivers highly accurate results throughout the whole device. Similarly, the hysteresis in the relaxation times is only reproduced by the six moments description.

B. Balance Equations

The balance equations of the six moments transport model are obtained by applying the weight function $\mathcal{E}^i$ and take the following general form

$$\partial_t n w_i + \nabla_\mathbf{r} \cdot n\mathbf{V}_i - i\mathbf{F} \cdot n\mathbf{V}_{i-1} = -n\frac{w_i - w_{i,\mathrm{eq}}}{\tau_i} \ . \quad (13)$$

Note that due to the choice of solution variables the balance equations are independent of the band structure model.

C. Flux Equations

By taking the moments of the BTE with the weight functions $\mathbf{p}\mathcal{E}^i$ we obtain general flux equations of the form $\mathbf{\Psi}_i = \mathbf{Q}_i$. The fluxes $\mathbf{\Psi}_i$ are given as

$$\mathbf{\Psi}_i = -\hat{\mathrm{U}}_{i+1} \nabla \log\frac{1}{n} + \nabla\hat{\mathrm{U}}_{i+1} - \mathbf{F}(w_i\hat{\mathrm{I}} + i\hat{\mathrm{U}}_i) \ , \quad (14)$$

with the tensors $\hat{\mathrm{U}}_i = \langle \mathbf{u} \otimes \mathbf{p}\,\mathcal{E}^{i-1} \rangle$. These tensors introduce the convective terms into hydrodynamic models [3] because they depend on the fluxes $\mathbf{V}_i$. In the diffusions approximation, however, the tensors $\hat{\mathrm{U}}_i$ reduce to scalars $\hat{\mathrm{U}}_i \approx U_i\hat{\mathrm{I}}$ which are calculated as follows

$$U_i = \tfrac{2}{3}\langle \mathcal{E}^i\, H_\mathrm{U}(\mathcal{E}) \rangle \doteq \tfrac{2}{3}\langle \mathcal{E}^i \rangle\, H_i \ . \quad (15)$$

The parameters of the analytic distribution functions are determined in such a way that the moments w_i are exactly reproduced for $i \leq M$ [4]. Consequently, the highest order moment w_{M+1} appearing in the flux equations is thus extrapolated and provides the closure of the equation system. In the same way, the coefficients H_i are interpolated via the distribution function for $i \leq M$ and extrapolated for H_{M+1}. The non-parabolicity corrections to the streaming terms, H_i, depend only on the even moments w_j and are shown in Fig. 2. Clearly, only the six moments representation correctly reproduces the hysteresis. In the extrapolated closure conditions for w_{M+1} a maximum error less than 10% is obtained with six moments model compared to an error of 150% to the case of a heated Maxwellian distribution.

Conventionally, inverse mobility tensors $\hat{\mu}_i^{-1}$ are introduced [3] to model $\mathbf{Q}_i$ analogously to the drift-diffusion model as

$$\mathbf{Q}_i = \sum_{j=0}^{M} Z_{ij}\mathbf{V}_j \doteq \mathrm{q}\,\hat{\mu}_i^{-1}\mathbf{V}_i \ . \quad (16)$$

Then it is assumed that $\mathbf{Q}_i$ and $\langle \mathbf{u}\mathcal{E}^i \rangle$ are co-linear, that is, that the mobility tensor can be approximated by a scalar to obtain the mobility as

$$\mu_i^* = \mathrm{q}\Big[\frac{\mathbf{V}_i}{|\mathbf{V}_i|^2} \cdot \sum_{j=0}^{M} Z_{ij}\mathbf{V}_j\Big]^{-1} \ . \quad (17)$$

The classic example of this type is the original form of the Hänsch mobility model [1]. Note that by this measure the implicit flux relations which are thought to represent $\mathbf{V}_i$ become artificially non-linear in $\mathbf{V}_i$. In addition, this flux-dependence is awkward to handle [11], particularly in two- and three-dimensional implementations. Therefore the ratio of

the fluxes is commonly replaced by bulk relations as

$$R_{ij}(w_1) = \frac{\mathbf{V}_i \cdot \mathbf{V}_j}{|\mathbf{V}_i|^2}\Big|_{\text{Bulk}} , \tag{18}$$

which can be given as a function of the average carrier energy w_1. Due to this simplification the model looses some of its accuracy because the mobility is actually a functional of the distribution function which is not accurately represented by the average carrier energy alone [12], [13]. Since the scattering matrix $\hat{\text{Z}}$ is conventionally modeled as a function of the average energy, this procedure results in a purely energy dependent mobility model of the form

$$\mu_i^*(w_1) = \text{q}\Big[\sum_{j=0}^{M} R_{ij}(w_1) Z_{ij}(w_1)\Big]^{-1} . \tag{19}$$

Note that in the most commonly used mobility model, the Hänsch model, the coefficients Z_{00} and Z_{01} are obtained by consistently reproducing measured bulk mobility values. Since this procedure is only possible for the carrier mobility μ_0^*, the energy flux mobility is commonly assumed to be of the form $\mu_1^* = r\,\mu_0^*$ with r being a constant ratio in the range $[0.8, 1]$, which is a rather crude approximation [3].

Another interesting consequence, which makes this approach questionable for higher-order transport models, can be noted when inspecting the flux relations (14) for the lowest order flux $\mathbf{V}_0$. The quantity $\mathbf{V}_0$ is the average carrier velocity which is directly proportional to the carrier current, the most important quantity. Since H_1 is normally modeled as either constant (e.g., $H_1 = 1$ for parabolic bands) or as energy dependent $H_1(w_1)$ [7], the electrical current depends only on w_1 and not on the higher order moments of the distribution function, which seams unreasonable.

In summary, the above outlined procedure, which is almost exclusively used in commercially available simulators, has several shortcomings. We therefore propose a different approach: By inverting the implicit flux relations $\mathbf{\Psi}_i = \mathbf{Q}_i(\mathbf{V}_0, \ldots, \mathbf{V}_M)$ we obtain explicit relations for the fluxes

$$\mathbf{V}_i = \mu_i \frac{\mathbf{F}}{\text{q}} + D_i^n \nabla \log \frac{1}{n} - \sum_{j=0}^{M} Y_{ij} \nabla U_{j+1} \tag{20}$$

$$\mu_i = -\text{q} \sum_{j=0}^{M} Y_{ij}\,(w_j + jU_j) \tag{21}$$

$$D_i^n = -\sum_{j=0}^{M} Y_{ij}\,U_{j+1} \tag{22}$$

where the coefficients Y_{ij} are the components of the inverted matrix $\hat{\text{Z}}^{-1}$ which are determined by the scattering models and depend only on the even moments w_l.

Formulation (20) has many interesting properties. First, the mobilities μ_i depend only on the even moments rather than on the fluxes. In addition, the fact that the mobilities are functions of the distribution function is well reproduced since the mobilities μ_i depend on all available even moments w_j rather than on w_1 alone. Second, as a result, the flux relations are linear in $\mathbf{V}_i$ as they should be. Furthermore, all fluxes depend on all even moments, most notably on the closure relation for w_{M+1}. Note that this is not the case with models based on the relaxation time approximation where the tensor $\hat{\text{Z}}$ is of diagonal form and thus only the highest order equation for the flux $\mathbf{V}_M$ depends directly on the closure relation.

V. Conclusion

We present a derivation of non-parabolic macroscopic transport models from Boltzmann's equation. The closure relations are derived from analytical distribution function models, most notably a 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. Thereby we avoid the awkward flux dependencies occurring in 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 models, which are based on a heated Maxwellian distribution function, a six moments description accurately models all closure relations. We therefore believe that this six moments model is a good choice for modeling hot-carrier effects in highly downscaled semiconductor devices.

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