Closure Relations for Macroscopic Transport Models

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I. Introduction

To overcome some of the limitations of the classic drift-diffusion model [1], higher-order transport models have been proposed, including the energy-balance model [2], the hydrodynamic model [3] and a six moments model [4]. A vast number of these models exists and there is a considerable amount of confusion as to their relation to each other. The main differences between these models can be pinned down to the assumptions used for the closure relations.

II. Macroscopic Transport Models

Transport equations used in semiconductor device simulation are normally derived from Boltzmann's transport equation (BTE), a semiclassical kinetic equation, which reads for electrons

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{r}} f + \frac{\mathbf{F}}{\hbar} \cdot \nabla_{\mathbf{k}} f = Q[f] \ .$$

Here, $f(\mathbf{k}, \mathbf{r}, t)$ is the carrier distribution function, $Q[f]$ the scattering operator, $\mathbf{u}$ the group velocity, and $\mathbf{F}$ the external force, for instance $\mathbf{F}(\mathbf{r}) = -\mathrm{q}\mathbf{E}(\mathbf{r})$ for homogeneous band structures and neglected magnetic fields. The BTE represents an integro-differential equation in the seven-dimensional space $(\mathbf{k}, \mathbf{r}, t)$. To solve this equation numerically by discretization of the differential and integral operators is computationally very expensive. Widely used numerical methods for solving the BTE are the Monte Carlo method [5] and the spherical harmonics expansion method [6]. Both have been proven to give accurate results but are still computationally expensive.

A common simplification which will be the subject of this paper, is to investigate only some moments of the distribution function which are obtained by multiplying the distribution function with suitable weight functions $\phi = \phi(\mathbf{k})$ and integrating over $\mathbf{k}$-space as $n\langle\phi\rangle = \int \phi f \ \mathrm{d}^3\mathbf{k}$, with n being the carrier concentration. The equations which determine a given set of moments form a macroscopic transport model. Conventionally, the moment equations resulting from the weight functions $\mathbf{p}\mathcal{E}^i$ ($\mathbf{p} = \hbar\mathbf{k}$) give the flux relations whereas the weight functions $\mathcal{E}^i$ ($\mathcal{E}$ is the energy) deliver the balance equations as

$$
\begin{aligned}
\phi = 1 \quad &\Rightarrow \quad \partial_t n \ + \nabla \cdot n\mathbf{V}_0 &&= 0 \\
\phi = \mathbf{p} \quad &\Rightarrow \quad \partial_t n\mathbf{P}_0 + \nabla \cdot n\hat{\mathrm{U}}_1 - \ n\mathbf{F} &&= n\mathbf{Q}_0 \\
\phi = \mathcal{E} \quad &\Rightarrow \quad \partial_t nw_1 + \nabla \cdot n\mathbf{V}_1 - 1\,n\mathbf{F} \cdot \mathbf{V}_0 &&= nq_1 \\
\phi = \mathbf{p}\mathcal{E} \quad &\Rightarrow \quad \partial_t n\mathbf{P}_1 + \nabla \cdot n\hat{\mathrm{U}}_2 - \ n\mathbf{F} \cdot (w_1\hat{\mathrm{I}} + \hat{\mathrm{U}}_1) &&= n\mathbf{Q}_1 \\
\phi = \mathcal{E}^2 \quad &\Rightarrow \quad \partial_t nw_2 + \nabla \cdot n\mathbf{V}_2 - 2\,n\mathbf{F} \cdot \mathbf{V}_1 &&= nq_2 \\
\phi = \mathbf{p}\mathcal{E}^2 \quad &\Rightarrow \quad \partial_t n\mathbf{P}_2 + \nabla \cdot n\hat{\mathrm{U}}_3 - \ n\mathbf{F} \cdot (w_2\hat{\mathrm{I}} + 2\,\hat{\mathrm{U}}_2) &&= n\mathbf{Q}_2 \\
\vdots \quad && \vdots
\end{aligned}
$$

with $\mathbf{P}_i = \langle\mathbf{p}\mathcal{E}^i\rangle$, $\mathbf{V}_i = \langle\mathbf{u}\mathcal{E}^i\rangle$, $w_i = \langle\mathcal{E}^i\rangle$, $\hat{\mathrm{U}}_i = \langle\mathcal{E}^{i-1}\mathbf{u}\otimes\mathbf{p}\rangle$, and the moments of the scattering integral $nq_i = \int \mathcal{E}^i Q[f(\mathbf{k})] \ \mathrm{d}^3\mathbf{k}$ and $n\mathbf{Q}_i = \int \mathbf{p}\mathcal{E}^i Q[f(\mathbf{k})] \ \mathrm{d}^3\mathbf{k}$. This equation system contains more unknowns than equations and each equation is coupled to the next higher equation. To obtain a tractable equation set, this hierarchy has to be truncated after N equations. Since the current density is proportional to the average velocity $\mathbf{V}_0$ and many physical processes are modeled as a function of the average energy w_1, it is sensible to use the quantities $\mathbf{V}_i$ and w_i as solution variables. Now the additional moments $\mathbf{P}_i$, $\hat{\mathrm{U}}_i$, q_i, and $\mathbf{Q}_i$ have to be expressed as functions of the solution variables, which is not exactly possible and known as closure problem.

III. Closure Relations

For parabolic energy bands we obtain $\mathbf{P}_i = m\mathbf{V}_i$, with m being the effective mass. If we further assume that the distribution function can be reasonably described by a displaced and heated Maxwellian distribution, simple relationships can be derived for the energy-like tensors, for instance $\hat{\mathsf{U}}_1 = \frac{2}{3}w_1\hat{\mathsf{I}} - m\mathbf{V}_0^2/3 + m\mathbf{V}_0 \otimes \mathbf{V}_0$. However, even the simplest model of this type, the hydrodynamic model [3], is extremely difficult to solve for multidimensional devices due to the existence of hyperbolic modes. Thus, claiming that the system is diffusion dominated, the convective terms and the time derivatives in the flux relations are commonly neglected, resulting in parabolic partial differential equation systems [7] which are simpler to solve.

In the diffusion limit the energy-like tensors then evaluate to $\hat{\mathsf{U}}_i = \frac{2}{3}w_i H_i$, where H_i considers the influence of a non-parabolic band structure on the streaming terms ($H_i = 1$ for parabolic bands). H_i has been modeled as energy-dependent via a simple analytical expression [8] or by the incorporation of bulk Monte Carlo data [9]. Since it has been found that H_i is not a single-valued function of w_1, a more complex model has been proposed in [10] based on a six moments description. Since the equation system is truncated after N equations, the highest-order solution variable is $w_{N/2-1}$. However, in the highest-order equation the moment $\hat{\mathsf{U}}_{N/2}$ appears which has to be expressed as a function of the available moments. Conventionally, a heated Maxwellian distribution is used to derive such a relation [2, 3, 9] which is rather crude and better results have been obtained by a six moments description [10].

The closure relations for the even moments of the scattering integral q_i are in general not considered to be too critical. Conventionally, relaxation times of the form $\tau_i = -(w_i - w_{i,\mathrm{eq}})/q_i$ are introduced, with $w_{i,\mathrm{eq}}$ being the equilibrium value of w_i. The relaxation times are then modeled as either constant or energy-dependent [7]. The closure relations for $\mathbf{Q}_i$, on the other hand, are extremely critical. Rather simple expressions are obtained by introducing mobilities μ_i in analogy to the drift-diffusion model to express $\mathbf{Q}_i$ as $\mathbf{Q}_i = -\mathrm{q}\mathbf{V}_i/\mu_i$, where μ_i depends only on the average energy w_i. A rigorous treatment reveals, however, that these odd moments of the scattering integral $\mathbf{Q}_i$ depend on the odd moments of the distribution function [11, 12] as $\mathbf{Q}_i = \sum_{j=0}^{N/2-1} Z_{ij}\mathbf{V}_j$. This closure relation causes additional coupling between the equations [10].

IV. Conclusions

Despite the fact that higher-order transport models have been around for more than forty years and that they are commonly acknowledged as being a necessary extension of the classic drift-diffusion model, a considerable amount of uncertainty still prevails over how to properly close the equation system. Particularly critical seem to be the facts that in any practical implementation the convective terms in the energy-like tensors are neglected, that the equation system is closed with a heated Maxwellian distribution, and that the odd moments of the scattering integral are expressed via energy-dependent mobilities. Each of these assumptions can introduce considerable errors. Nevertheless, astonishingly accurate results have been reported with hydrodynamic models down to gate-lengths of 20 nm [13].

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