On the Highest Order Moment Closure Problem

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Abstract

Macroscopic transport models based on the first six moments of Boltzmann's equation are a natural extension to the drift-diffusion model (two moments) and the various energy-transport models (three or four moments). To close the system of equations the sixth moment has to be expressed as a function of the lower order moments. We investigate the inuence of the applied closure relation on the numerical properties of the six moments model comparing three different methods and propose a new solution to the closure problem. We present results of numerical solutions of six moments models and compare them to self-consistent Monte Carlo data.

Keywords: moments method, closure problem, cumulant, maximum entropy

Introduction

Macroscopic transport models based on the first six moments of Boltzmann's equation [1] are a natural extension to the well known drift-diffusion model (two moments) and the various energy-transport models (three or four moments) [2]. In addition to the solution variables of the energy-transport (ET) model, which are the carrier concentration $n = \langle 1 \rangle$ and the average energy $w_1 = \langle \varepsilon \rangle$, the six moments (SM) model provides $w_2 = \langle \varepsilon^2 \rangle$, which contains additional information about the distribution function. The quantity $\beta = (3/5)\, w_2/w_1^2$ is the kurtosis of the distribution function and indicates the deviation from a heated Maxwellian distribution for which $\beta = 1$ holds (for parabolic bands). The knowledge of β allows us to model non-equilibrium processes like hot carrier tunneling [3] and impact ionization [4] with improved accuracy within macroscopic transport models.

Six Moments Model

A six moments model (SM) for the description of hot carrier phenomena within the diffusion approximation was introduced in [1]. In the diffusion limit [5] the stationary balance and flux equations of the six moments transport model are [6]:

$$\nabla nV_i - iF\,nV_{i-1} = -n\frac{w_i - w_{i,eq}}{\tau_i} \qquad (1)$$

$$qnV_i = -\mu_i\left(\frac{2}{3}\nabla(nw_{i+1}) + qnEw_i\left(1+\frac{2}{3}i\right)\right) \qquad (2)$$

with $V_i = \langle \varepsilon^i \mathbf{u} \rangle$, $i = 0; 1; 2$, where $\mathbf{u}$ is the group velocity. The mobilities μ_i and the relaxation times τ_1 and τ_2 were taken from tabulated bulk MC data and modeled as a function of the average energy w_1 only, in analogy to [7].

In addition to the SM model we consider the corresponding ET model, where the equation for w_2 is kept but the equation for the energy-ux V_1 is closed with $w_2 = (5/3)w_1^2$, corresponding to a heated Maxwellian distribution. This decouples the equation for w_2 from the lower order equations and provides an estimate for w_2 and thus β [1].

The Closure Problem

To close the system of equations the sixth moment has to be expressed as a function of the lower order moments. We investigate the inuence of the applied closure relation on the numerical properties of the six moments model comparing three methods from the literature.

First, the use of cumulants instead of moments for the description of the distribution function [8] leads to a generalized Gaussian closure. Second, the maximum entropy principle in the diffusion approximation was applied to solve the closure problem. Finally, the closure relations proposed in [1] are considered, where the sixth moment is modeled as a function of the variance and the kurtosis of the distribution function using a real number c as parameter. In the last case the closure problem is reduced to the choice of *c*. This indeterminacy can be eliminated by requiring consistency with bulk Monte Carlo data.

Cumulant Closure

From a theoretical point of view probability distributions are better described in terms of cumulants than in terms of moments. This motivated us to study the notion of cumulants and apply it to the closure problem. Previously, it was suggested in [8] to use cumulants in the formulation of semiconductor

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cumulants in the formulation of semiconductor equations.

In probability theory and statistics, the cumulants k_n of a probability distribution f are given by

$$E(e^{tX}) = \exp\left(\sum_{n=1}^{\infty} \frac{k_n t^n}{n!}\right) \quad (3)$$

where X is any random variable whose probability distribution is the one whose cumulants are taken. The first cumulant is equal to the logarithm of the total mass of the distribution function (hence zero for proper probability distribution functions). The second cumulant is the variance. Cumulants of order greater than 2 are measures of nonnormality. In particular, the third and fourth cumulants are related to the skewness and the kurtosis respectively.

In the cumulant expansion method closure of the equations in the highest order can be achieved by setting all higher cumulants to zero. This translates to a condition on the moments and defines a generalized Gaussian closure:

$$w_3 = (35/6)w_1^3(3\beta - 2) \quad (4)$$

Unfortunately, in our numerical experiments the cumulant closure only worked for low bias values. For higher bias values and shorter devices we were not able to obtain a solution.

Maximum Entropy

The maximum entropy principle yields, for a given set of prior information, a density which contains least additional information in the sense of Shannon. It is obtained by maximizing the entropy

$$H(f) = -\langle f \ln f - f \rangle \quad (5)$$

under the constraint that a given set of moments of the distribution function f assumes prescribed values [9].

A maximum entropy approach to the closure problem was applied by Levermore [10]. A physical approach based on the maximum entropy principle was initiated by Anile [11] within the framework of extended thermodynamics.

The maximum entropy method has been criticized in [12]. For the semiconductor Boltzmann equation with parabolic bands the equilibrium states are located on the boundary of the domain of deffnition of the maximum entropy system. Arbitrarily close to equilibrium, the maximal characteristic velocity becomes arbitrarily large.

We combined the diffusion approximation with the maximum entropy closure which gives a linearized version of the maximum entropy closure.

However, in this case, the range of kurtosis for which the maximum entropy closure exists, is too limited and Monte Carlo results cannot be reproduced.

It can be shown, that

$$1 < \frac{w_0 w_4}{w_2^2} < \frac{5}{3} \quad (6)$$

holds, where the upper bound comes from a Maxwellian distribution. The lower bound is reached for a distribution function of the form $\exp(-ax^4 + x^2)$ in the limit $a \to 0$.

Bulk Data Approach

In [1] a family of closures parameterized by a real number c was introduced. We proposed to use a generalized Maxwellian closure $w_3 = (35/6)w^3{}_1\beta^c$, with c an integer in the range [0...3]. The sixth moment is thus modeled as a function of the variance and the kurtosis of the distribution function.

Stable implementations were only obtained for c=3, results for $c \leq 2$ showed pronounced oscillations in the solution. However, the results obtained from c=2, though often unstable, appeared to better reproduce the MC results. We now take a somewhat different approach: by requiring consistency with bulk MC simulations we obtain c from a best match of w_3 to $w^{MC}{}_3$, which gives c=2.7.

Simulation

The previously published results were mainly obtained by applying these models to Monte Carlo data in post-processing steps. Here we present results of numerical solutions of six moments models and compare them to self-consistent Monte Carlo data (SCMC). Relaxation times and mobilities are fitted to bulk Monte Carlo data as a function of the temperature and the doping.

To investigate the accuracy of the SM model and its corresponding ET model we consider a series of one-dimensional n^+-n-n^+ test-structures. Although these structures are not of practical relevance, they still display similar features as contemporary MOS and bipolar transistors like velocity overshoot and a

mixture of a hot and a cold distribution function in the 'drain' region.

The doping concentrations were taken to be $5x10^{19}$ and 10^{17}. The channel length was varied from 1000nm down to 50nm while maintaining a maximum electric field of 300 kV/cm.

In Fig. 1 we show the relative error of the closure for bulk and from the simulation result using the L_c=100nm device. It can be seen that for high electrical field the error from the cumulant closure increases, which also explains the observed bad convergence behaviour when a high bias is applied.

A comparison of the average velocity Vo and the kurtosis β obtained from the SM and ET models with the SCMC simulation is shown in Fig. 2 and Fig. 3 for the L_c = 100nm device. The spurious velocity overshoot is significantly reduced in the SM model, consistent with previous results [13], while the kurtosis produced by the ET model is only a poor approximation to the MC results.

Despite the fact that SM models provide the kurtosis of the distribution function, they do not require a heated Maxwellian closure in the energy ux relation. This has a significant impact on the resulting device currents for channel lengths smaller 100nm where the ET models show the well-known overestimation of the device currents (cf. Fig. 4). The results of the SM model, on the other hand, stay close to the SCMC results which makes the SM model a good choice for TCAD applications.

Conclusion

Closure relations derived from theoretical considerations based on analytical distribution function models ([4] or maximum entropy principle) and relations derived from the cumulants of the distribution function [8] do not deliver satisfactory results. In contrast the bulk data approach gives a numerically more robust closure and an accurate kurtosis, which is a prerequisite for modeling hot carrier effects.

Since all model parameters are obtained from bulk MC simulations the transport model is fit-parameter free and leaves us with 'no knobs to turn' [14]. The existence of many fit parameters is a particular inconvenience inherent in many energy-transport models [2]. This was found to be essential for higherorder models since the interplay between the various parameters is highly complex and the numerical stability of the whole transport model depends significantly on the choice of these parameters. In particular, the MC based model outperformed its counterparts based on analytical mobility models [1] significantly, both in terms of its numerical properties and in the quality of the simulation results.

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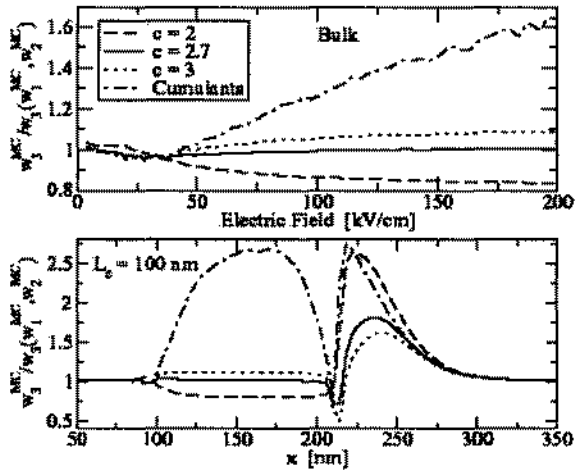

Figure 1: Relative error of the closure for bulk and for for the $L_c = 100\,\text{nm}$ device. Error from cumulant closure increases with high bias. Best fit for $c = 2.7$.

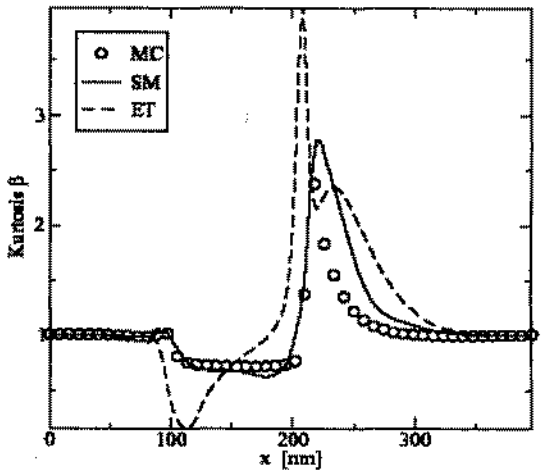

Figure 3: Comparison of the kurtosis obtained from the SM and ET models with the SCMC simulation for the $L_c = 100\,\text{nm}$ device.

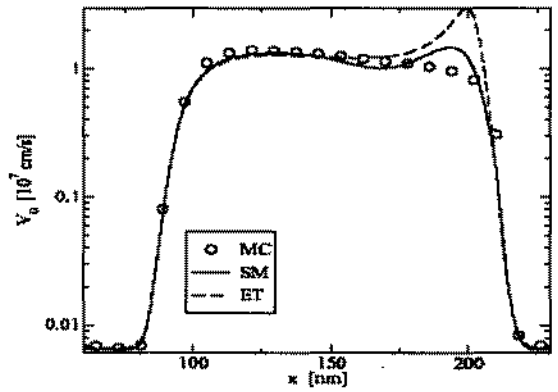

Figure 2: Comparison of the average velocity obtained from the SM and ET models with the SCMC simulation for the $L_c = 100\,\text{nm}$ device.

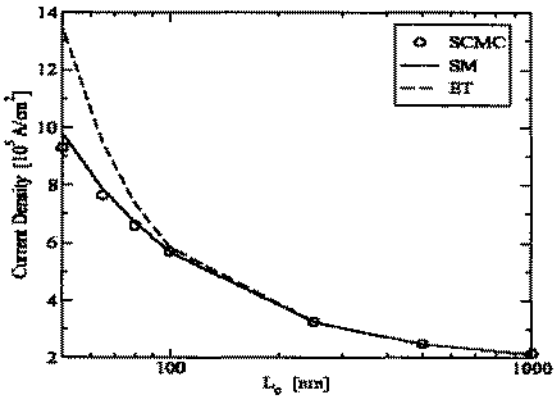

Figure 4: Comparison of the device currents obtained from the SM and ET models with the SCMC simulation for varying channel length.