Exact Method to Solve the Boltzmann Equation to any Order in the Driving Forces: Application to Transport Parameters

S. C. Brugger[*1], **V. Peikert**[1], and **A. Schenk**[1,2]

[1] Integrated Systems Laboratory, ETH Zurich, Gloriastrasse 35, CH-8092 Zürich, Switzerland
[2] Synopsys LLC., Affolternstrasse 52, CH-8050 Zürich, Switzerland

Received zzz, revised zzz, accepted zzz
Published online zzz

PACS 73.50.Dn, 73.50.Fq, 72.20.Dp

In this paper a method to compute transport parameters in semiconductor devices as a function of the driving forces is presented. The method is based on an exact expansion of the distribution function (solution of the Boltzmann transport equation) in a series in the electric field and the gradient of the quasi-Fermi potential. Eventhough this series probably diverges for high fields, it is still usable for low and moderate field intensities. Results for silicon clearly show that the usual parametrisation of the mobility in TCAD models is inaccurate in pn junctions. Furthermore, it gives new insights into the form of the correct parametrisation.

Introduction Solving the Boltzmann transport equation (BTE) in realistic semiconductor devices, taking all physically relevant effects into account, is still an open challenge for TCAD (Technology Computer Aided Design). Nowadays, two main methods exist to solve the BTE. The first mehtod consists in directly discretizing and solving the BTE using standard numerical methods for differential equations [**?**, **?**]. The second, called the Monte Carlo (MC) method, solves the BTE as being the stationary solution of a stochastic differential equation. Advantages of the first method are that the numerical error on the solution is mathematically assessable and that small signal and RF-noise analysis can be performed directly. The disadvantage is that it requires a lot of memory and can only be applied to small devices. The advantage of the MC method is that it requires less memory and hence can be used to solve the BTE in larger devices. Main disadvantages are that the error on the solution is difficult to estimate and that AC and RF-noise computations are laborious. Furthermore, the MC method is computationally very inefficient in highly doped regions where low to medium field intensities prevail, because of the very strong elastic scattering rate. To try to compensate this handicap, a current-based one-particle MC (CBOPMC) method has been proposed [**?**, **?**]. The main idea of the CBOPMC method is to use MC "only" to extract transport parameters (TPs). These TPs are then inserted in a generalised drift-diffusion (GDD) equation where the solution variables are the electrostatic potential and the quasi-Fermi potential. Therefore, the CBOPMC method theoretically allows to use MC only in regions where a semi-analytical solution of the BTE does not exist, i.e. typically outside the highly doped regions. Thus, if one could find a general way to localise regions where MC is not needed and where a semi-analytic solution exists, one could significantly improve the efficiency and applicability of the CBOPMC method.

In a previous work [**?**], a method to solve the space-homogeneous BTE in any order in the electric and magnetic field has been proposed. This method has been recently extended to the space-inhomogeneous BTE [**?**]. It allows to expand the distribution function to any order in the gradient of the quasi-Fermi potential, the electric field, and the magnetic field (i.e. to any order in the driving forces). In the following it will be shown that using this method one can easily find a semi-analytical formula for the TPs in second

* Corresponding author: e-mail: brugger@iis.ee.ethz.ch, Phone: +41 44 632 23 48, Fax: +41 44 632 11 94

order in the driving forces (DFs). This formula then enables to divide a device in regions where the MC method is needed and in regions where a semi-analytical expansion is sufficient.

Section 1 introduces the theory and the general formula for the expansion of the solution of the space-inhomogeneous BTE in a series in the DFs. In Section 2, the computation of TPs will be explained and explicit formulas for the mobility and the diffusivity will be given. Section 3 describes how mobility and diffusivity, developed up to second order, can be combined to produce a TCAD mobility model. The results will be briefly discussed in Section 4.

1 Theory In Ref. [**?**] the existence and uniqueness of an inverse of the scattering operator (ISO) of the BTE was proven and the concept of moments of the ISO (MISO) was introduced. Using the idea of MISO, the degenerate space-homogeneous BTE can be solved iteratively in all orders in the electric and magnetic field [**?**]. This idea has been recently generalised to the space-inhomogeneous BTE [**?**]. For the seek of simplicity, only the nondegenerate case without magnetic field will be considered here. In this case, the following recursion relation is found [**?**]:

$$f(k,r) = n(r)\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}|h_{l,m}\rangle = n(r)h_{eq}(k)(1+\sum_{l,m=1}^{\infty}\left[S^{-1}_{g_{l,m}}(k,r)+\alpha_{l,m}(r)\right]), \tag{1}$$

$$g_{l,m} := \frac{q}{h_{eq}}\left[\nabla_r\phi\left(\vec{v}(k)\beta h_{l-1,m}\left(r,k\right)+\frac{1}{\hbar}\nabla_k h_{l-1,m}\left(r,k\right)\right)-\vec{v}(k)\beta\nabla_r\psi h_{l,m-1}\left(r,k\right)\right], \tag{2}$$

where $\beta := 1/(k_BT)$, $n(r) := \exp(q\beta(\phi(r)-\psi(r)))$ is the density, ϕ the electrostatic potential, ψ the quasi-Fermi potential, $h_{eq} := h_{0,0}$ is the equilibrium distribution function normalized by the density, and $h_{l,m}$ is the component of the normalized distribution function h proportional to $(\nabla_r\phi)^l(\nabla_r\psi)^m$. The $\alpha_{l,m}$s are normalisation constants, and the quantity $S^{-1}_{g_{l,m}}$ is the $g_{l,m}$-MISO. The method is recursive and the MISOs can be computed using a simple iterative algorithm. Developing h up to second order gives

$$\begin{aligned} f(k,r) = n(r)h_{eq}(k)&\left(1+q\beta\sum_{i=1}^{3}(\partial_{r_i}\psi S^{-1}_{v_i}(k))\right)\\ &+n(r)h_{eq}(k)q\beta\left(q\sum_{i,j=1}^{3}(\partial_{r_i}\phi\partial_{r_j}\psi\Pi_{i,j}(k,r))+q\beta\sum_{i,j=1}^{3}(\partial_{r_i}\psi\partial_{r_j}\psi\Omega_{i,j}(k,r))\right), \end{aligned} \tag{3}$$

where $\Pi_{i,j}(k,r)$ and $\Omega_{i,j}(k,r)$ are unequivocally defined by (1) and (2). Their explicit forms are given in Ref. [**?**]. Eq. (3) has three important properties. First, the expansion of f does not contain mere powers of the electric field (i.e. terms proportional to only $(\nabla_r\phi)^i$). Secondly, terms of the order $O((\nabla_r\phi)^l(\nabla_r\psi)^m)$ are proportional to the inverse of the total scattering rate to the power $l+m$. Therefore, the small parameters in the series are the gradients of the potentials divided by the total scattering rate. The higher the total scattering the faster the series (1) will converge. Thirdly, there is a mixed term containing products of electric field times gradient of quasi-Fermi potential. This will be of importance in Section 3.

2 Transport Parameters The theory exposed in the previous section can now be used to compute TPs as function of the DFs. In [**?**] the diffusivity tensor D and the mobility tensor μ are defined as:

$$D_{ij}(r) = -\frac{1}{n(r)}\int_{Bz}S^{-1}_{v_i}(k,r)v_j(k)f(k,r)d^3k = -\int_{Bz}S^{-1}_{v_i}(k,r)v_j(k)h(k,r)d^3k, \tag{4}$$

$$\mu_{ij}(r) = -\frac{q}{n(r)\hbar}\int_{Bz}\partial_{k_j}S_{v_i}^{-1}(k,r)f(k,r)d^3k = -\frac{q}{\hbar}\int_{Bz}\partial_{k_j}S_{v_i}^{-1}(k,r)h(k,r)d^3k, \tag{5}$$

where the integration domain Bz involves the first Brillouin zone and all bands. Inserting Eq. (3) into (5) and (4) gives

$$D_{ij}(r) = D_{ij}^{eq} + \sum_{m,l=1}^{3}(\partial_{r_m}\phi\partial_{r_l}\psi M_{m,l,i,j}^{1}(r)) + \sum_{m,l=1}^{3}(\partial_{r_m}\psi\partial_{r_l}\psi M_{m,l,i,j}^{2}(r)), \tag{6}$$

$$\mu_{ij}(r) = \mu_{ij}^{eq}(r) + \sum_{m,l=1}^{3}(\partial_{r_m}\phi\partial_{r_l}\psi M_{m,l,i,j}^{3}(r)) + \sum_{m,l=1}^{3}(\partial_{r_m}\psi\partial_{r_l}\psi M_{m,l,i,j}^{4}(r)) \tag{7}$$

with the definitions

$$\begin{aligned}
M_{m,l,i,j}^{1}(r) &:= -q^2\beta\int_{Bz}S_{v_i}^{-1}(k,r)v_j(k)h_{eq}(k)\Pi_{m,l}(k,r)d^3k,\\
M_{m,l,i,j}^{2}(r) &:= -q^2\beta^2\int_{Bz}S_{v_i}^{-1}(k,r)v_j(k)h_{eq}(k)\Omega_{m,l}(k,r)d^3k,\\
M_{m,l,i,j}^{3}(r) &:= -\frac{q^3\beta}{\hbar}\int_{Bz}\partial_{k_j}S_{v_i}^{-1}(k,r)h_{eq}(k)\Pi_{m,l}(k,r)d^3k,\\
M_{m,l,i,j}^{4}(r) &:= -\frac{q^3\beta^2}{\hbar}\int_{Bz}\partial_{k_j}S_{v_i}^{-1}(k,r)h_{eq}(k)\Omega_{m,l}(k,r)d^3k.
\end{aligned}$$

The term of Eq. (3) linear in the quasi-Fermi potential always disappears for symmetry reasons. Eqs. (6) and (7) are analytical expressions for the mobility and the diffusivity as function of the gradients of the quasi-Fermi potential and the electric field. The $M_{m,l,i,j}^{s}$ only depend on the scattering operator, the band structure, and the equilibrium distribution function h_{eq}. They can, therefore, be numerically computed using (3) together with the iterative method to obtain the MISOs presented in [**?**] and can then be stored in a table. Expressions (6) and (7) are good approximations for a given pair of driving forces as long as the terms of second order are larger than the terms of fourth order (the third order as well as all higher odd orders vanish because of symmetry reasons). For a given bias it is, therefore, possible to divide a device in regions, where (6) and (7) are valid, and regions where they fail, allowing to restrict the CBOPMC method to the latter ones.

3 TCAD Mobility and Drift-Diffusion Model The drift-diffusion transport model is a widely used tool in the TCAD and compact modelling community. In this model, the diffusivity is related to the mobility using the Einstein relation leading to the current equation: $\vec{J} = -qn(r)\mu^*\nabla_r\psi$. Inserting (6) and (7) into the drift-diffusion equation, using the Einstein relation between D_{eq} and μ_{eq} (which is exact in this case), and rearranging terms gives

$$\begin{aligned}
\mu_{ij}^{*} = \mu_{ij}^{eq} &- \sum_{a,b=1}^{3}\partial_{r_a}\phi\partial_{r_b}\phi(\beta M_{ajib}^{1} - M_{ajib}^{3})\\
&+ \sum_{a,b=1}^{3}\partial_{r_a}\psi\partial_{r_b}\phi(M_{ajib}^{4} + \beta M_{ajib}^{1} - \beta M_{ajib}^{2}) + \sum_{a,b=1}^{3}\partial_{r_a}\psi\partial_{r_b}\psi\beta M_{abij}^{2}.
\end{aligned} \tag{8}$$

Eq. (8) is fundamental for at least three reasons. First, it proves that as long as (6) and (7) are valid, the drift-diffusion model is valid too, provided that μ^*_{ij} is modelled based on Eq. (8). Secondly, it shows that in pn-junctions, μ^* cannot be parametrised using only one of the two DFs or using only the mixed term as was recommended in [**?**]. Thirdly, in pn-junctions the diagonal components of μ^* cannot be equal, in contrast to what is implicitly assumed when using a scalar mobility. To substantiate these claims, Fig. 1 gives the numerical values of the prefactors of the DFs for the three last terms on the rhs of (8) for silicon using the scattering model described in [**?**] (p.158–159). As one can see, all have the same order of magnitude.

4 Conclusion A method using the concept of MISO to solve the space-inhomogeneous BTE has been sketched. This method can be advantageously used in device regions of not too high DF intensities, which allows to replace the MC method there. Furthermore, the validity of the popular TCAD mobility model must be questioned for pn-junctions.

Acknowledgements The authors are grateful for the financial support by the Swiss National Science Foundation (project NEQUATTRO SNF 200021-109393/1) and by the European project PULLNANO (IST-4-026828).

References

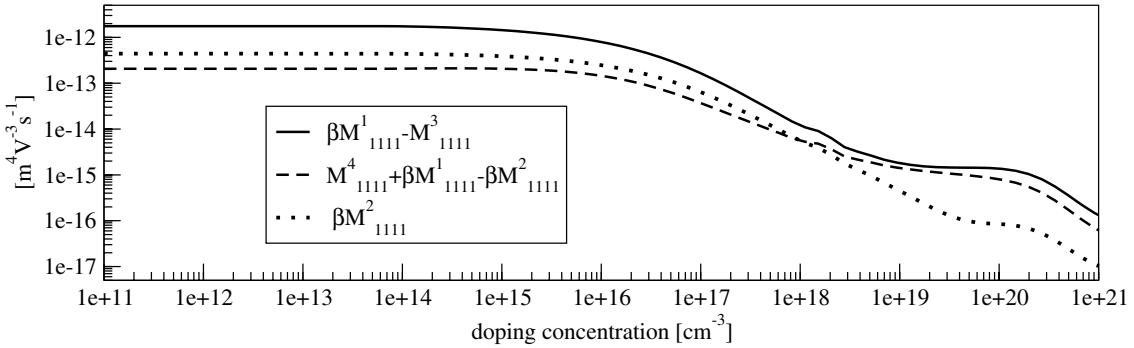

Fig. 1 Magnitude of the three coefficients contributing to μ^*_{11}.