Generalization of the Scharfetter-Gummel scheme to strictly monotonous carrier density state-equations

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Essential goals of the discretization

Models for the carrier density n in semiconductors $n = N_c\mathcal{F}(\eta)$, η chemical potential, include all strictly monotonous distribution functions $\mathcal{F}(\eta)$ in the range defined by Boltzmann-statistics (strongest increase of density) and the Fermi-Dirac-integral of order -1 (weakest increase of density), compare Fig. 1. The latter one appears as vanishing disorder limit of the Gauss-Fermi-integral [1] for hopping transport in organic semiconductors and in phase-separation models [2], where a 'discrete chain rule' was used to get stability for the discrete problem.

Looking at analytic results for Fermi-Dirac-statistics (e.g. [3]) and comparing them to those for the Boltzmann case suggests, that it should be possible to get all nice properties also for the discrete problem in the $\mathcal{F}(\eta)$-case: uniqueness for small applied voltages; bounded, positive steady states; existence of a unique transient solution; dissipativity. Such results are expected to hold for restricted classes of material models for all boundary conforming Delaunay grids and all time steps.

The goal here is to generalize the Scharfetter-Gummel-scheme for the above described range. Up to now degenerate semiconductors may be most precisely handled by a local, non-symmetric Boltzmann approximation and an outer iteration [4]. This outer iteration multiplies the total computation time, while a much more complex current relation may triple the assembly effort only, a small fraction of the total time.

A first approximation

In [5] the approximation introduced by Blakemore [6] of the distribution function $\mathcal{F}_{1/2}(\eta)$ for small arguments

$$\mathcal{F}_B(\eta) = \frac{1}{e^{-\eta} + \gamma}, \quad 0 \le n \le \frac{N_c}{\gamma} \tag{1}$$

was investigated for the governing equation

$$\frac{d}{dx}\Big(q\mu N_c\mathcal{F}(\eta(\varphi,\psi))\frac{d}{dx}\varphi(x)\Big) = 0, \tag{2}$$

describing a constant current j along an edge $[x_a, x_b]$ and the boundary values of the quasi-Fermi potential $\varphi(x_a) = \varphi_a$ and $\varphi(x_b) = \varphi_b$. This case is sufficiently simple to obtain explicit expressions and to study the essentials of the non-Boltzmann case, namely the generalized Einstein relation, describing the nonlinear ratio between diffusion coefficient and mobility $D/\mu \sim g_3(n)$, see Fig. 2.

Using Eq. (2), changing variables from quasi-Fermi potential to chemical potential together with a linearity assumption of the electrostatic potential ψ results in the following integral equation for j along the edge

$$\int_{\eta_a}^{\eta_b} \frac{1}{\frac{j}{\mathcal{F}(\eta)} + \delta\psi} d\eta = 1. \tag{3}$$

Inserting the approximation $\mathcal{F}_B(\eta)$ results in a fixed point problem for the current [5]:

$$j = B(\delta\psi + \gamma j)e^{\eta_b} - B(-(\delta\psi + \gamma j))e^{\eta_a}, \tag{4}$$

where $B(x) = \frac{x}{e^x - 1}$ is the Bernoulli function. Due to the properties of the Bernoulli function this fixed point problem has a unique solution for the current and for all finite arguments. Solutions of Eq. (3) for given potentials are shown in Fig. 3 together with their Boltzmann counterparts.

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THE GENERAL CASE

The approach is generalized to any strictly monotonous distribution function $\mathcal{F}(\eta)$, $-\infty < \eta < \infty$, by using a piecewise continuous approximation of the form

$$\mathcal{F}_i(\eta) = \frac{\sigma_i}{e^{-\eta} + \gamma_i}, \qquad \eta_i \le \eta \le \eta_{i+1},$$
$$\eta_a = \eta_0, \ \eta_b = \eta_{k+1}, \qquad \sigma_i > 0, \ \gamma_i > 0.$$

In this case the left hand side of equation (3) reads

$$\int_{\eta_a}^{\eta_b} \frac{d\eta}{\frac{j}{\mathcal{F}(\eta)} + \delta\psi} = \sum_{i=0}^{k} c_i, \ c_i = \int_{\eta_i}^{\eta_{i+1}} \frac{d\eta}{\frac{j}{\mathcal{F}_i(\eta)} + \delta\psi}.$$

Hence, a decomposition of unity $\sum_i c_i = 1$, $c_i > 0$, defines the current j. Simplifications for special choices of σ_i, γ_i and a detailed discussion of existence and uniqueness of a solution, which is supporting an implementation directly, will be in the focus of the talk.

CONCLUSION

The Scharfetter-Gummel scheme is extended to monotonous carrier density state equations in a unified way.

ACKNOWLEDGMENT

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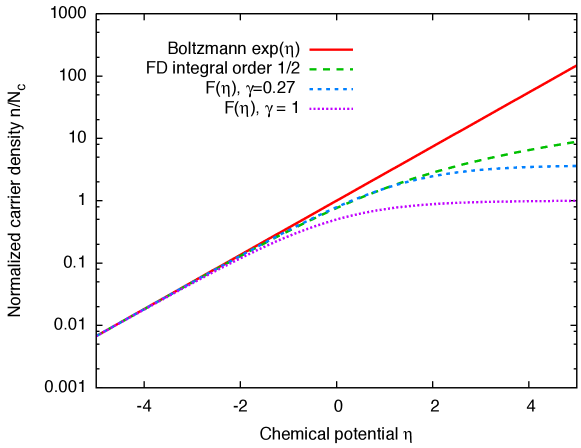

Fig. 1. Density in dependence of the chemical potential for different state equations.

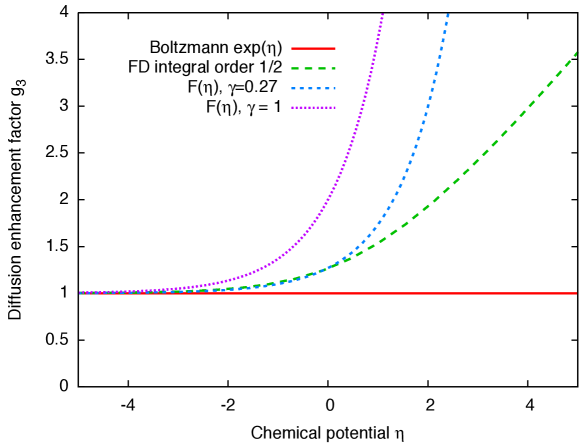

Fig. 2. Diffusion enhancement factor for different state equations, or: the generalized Einstein relation [7].

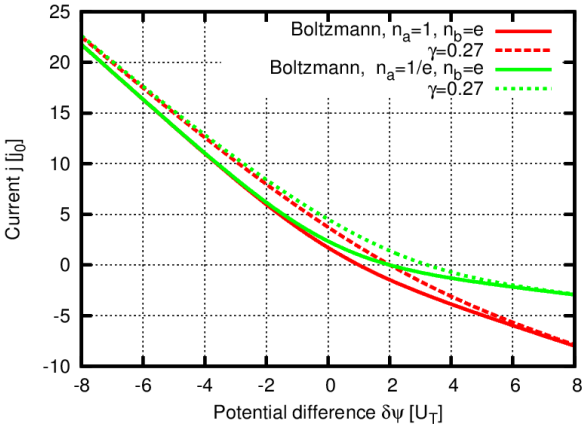

Fig. 3. Current comparison for different state equations.