Generalization of the Scharfetter-Gummel scheme

Thomas Koprucki and Klaus Gärtner
Weierstrass Institute (WIAS), Mohrenstr. 39, 10117 Berlin, Germany
Email: thomas.koprucki@wias-berlin.de

***Abstract*—For Blakemore-type distribution functions $\mathcal{F}(\eta) = 1/(\exp(-\eta)+\gamma)$ describing the carrier density in semiconductors a generalization of the classical Scharfetter-Gummel scheme can be derived resulting in a nonlinear equation per edge to calculate the edge current. This approach provides a good approximation of the carrier density in degenerate semiconductors for values of the chemical potential $\eta < 1.3k_BT$. We discuss an extension of this approach based on a piecewise approximation of the distribution function by functions of that type in order improve the approximation for larger values of the chemical potential.**

I. INTRODUCTION

The state equation for charge carriers in semiconductors has the form $n = N_c\mathcal{F}(\eta)$. It describes the dependence of the carrier density n on the chemical potential η by a statistical distribution function $\mathcal{F}(\eta)$ and the band-edge density of states N_c. Typical choices for the distribution function are $\mathcal{F}(\eta) = \exp\eta$ (Boltzmann approximation), $\mathcal{F}(\eta) = F_{1/2}(\eta)$ (Fermi-Dirac integral of order $1/2$ describing degenerate semiconductors), or the Gauss-Fermi integral [1], which is used for organic semiconductors [2].

The Scharfetter-Gummel scheme [3] is an established method for the discretization of the drift-diffusion equations describing the carrier transport in semiconductors. The resulting discretization of the fully coupled van Roosbroeck system on boundary conforming Delaunay meshes guarantees the following properties of the continuous problem, see [4], [5]: bounded and positive steady states with the same bounds as in the continuous case; uniqueness for small applied voltages; existence of a unique transient solution for the implicit Euler time discretization; dissipativity and exponential decay of the free energy along trajectories towards the unique thermodynamic equilibrium. The stability of the discretization is independent of the mesh size and the time step.

The classical Scharfetter-Gummel scheme exploits the special properties of the Boltzmann statistics, namely the exponential dependence on the chemical potential. Here we present a generalization to strictly monotonous distribution functions.

II. CONTINUITY EQUATION FOR CARRIER DENSITY

The carrier density fulfills the continuity equation given by

$$\frac{\partial n}{\partial t} - \frac{1}{q}\nabla\cdot J_n = 0, \tag{1}$$

with the current expression

$$J_n = -q\mu_n N_c\mathcal{F}(\eta)\nabla\varphi_n \tag{2}$$

and the (non-dimensionalized) chemical potential

$$\eta = \frac{q(\psi-\varphi_n)+E_{\mathrm{ref}}-E_c}{k_BT}, \tag{3}$$

where q denotes the elementary charge, μ_n the mobility, φ_n the quasi-Fermi potential, ψ the electrostatic potential, k_B Boltzmann's constant, T the temperature, E_{ref} a reference energy for the quasi-Fermi potential, E_c the (constant) band-edge energy.

III. GENERALIZED SCHARFETTER-GUMMEL APPROACH

In the current expression (2) the distribution function $\mathcal{F}(\eta)$ is a rapidly varying coefficient. The Scharfetter-Gummel discretization was already originally understood as a constant current approximation by solving the equation

$$\frac{d}{dx}\Big(q\mu_n N_c\mathcal{F}\big(\eta(\varphi_n,\psi)\big)\frac{d\varphi_n}{dx}\Big) = 0 \tag{4}$$

on the interval $[x_a, x_b]$ with the boundary conditions $\varphi_n(x_a) = \varphi_a$ and $\varphi_n(x_b) = \varphi_b$. The first integration results in $-q\mu_n N_c\mathcal{F}\big(\eta(\varphi_n,\psi)\big)\frac{d\varphi_n}{dx} = j_n = const.$

Replacing the quasi-Fermi potential φ_n by the chemical potential η via Eq. (3) and assuming a linear dependence of the electrostatic potential ψ on $x \in [x_a, x_b]$, the following integral equation for the unknown current j_n results:

$$\int_{\eta_a}^{\eta_b}\frac{1}{\frac{j_n/j_0}{\mathcal{F}(\eta)}+\delta\psi}\,d\eta = 1. \tag{5}$$

Here, the dimensionless potential difference is defined by $\delta\psi = (\psi_b-\psi_a)/U_T$, the thermal voltage by $U_T = \frac{k_BT}{q}$, and the reference current $j_0 = q\mu_n N_c\frac{U_T}{x_b-x_a}$. The bounds of the integral are $\eta_a = \mathcal{F}^{-1}(n_a/N_c), \eta_b = \mathcal{F}^{-1}(n_b/N_c)$.

IV. BLAKEMORE TYPE APPROXIMATION

In [6] the solution of Eq. (5) has been investigated for the special function $\mathcal{F}_B(\eta) = 1/(\exp(-\eta)+\gamma)$. As introduced by Blakemore [7] this provides good approximation of the Fermi-Dirac integral of order $1/2$ for $\eta < 1.3$, see Fig. 1. This choice of the distribution function leads to a fixed point equation for the unknown dimensionless current $j = j_n/j_0$:

$$j = f(j,\delta\psi) = B(\delta\psi+\gamma j)e^{\eta_b} - B(-(\delta\psi+\gamma j))e^{\eta_a}, \tag{6}$$

where $B(x) = \frac{x}{e^x-1}$ is the Bernoulli function. For $\gamma = 0$ the classical Scharfetter-Gummel expression is reproduced. A comparison of both currents is depicted in Fig. 2.

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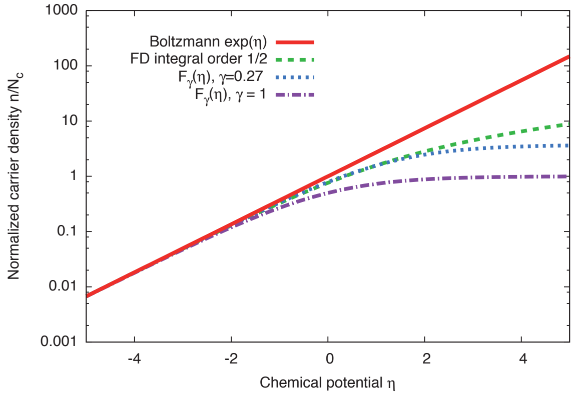

Fig. 1. Plot of distribution function $\mathcal{F}(\eta) = 1/(\exp(-\eta)+\gamma)$ in dependence on the dimensionless chemical potential η for different values of the parameter γ. For $\gamma = 0.27$ a good approximation of the Fermi-Dirac integral of order $1/2$ in the range $\eta < 1.3$ is provided.

V. EXTENSION TO LARGER ARGUMENTS

In order to improve the approximation (6) for larger arguments we propose a piecewise approximation of $\mathcal{F}(\eta)$ on N subintervals $[\eta_i, \eta_{i+1}]$, $i = 1, \dots, N$, $\eta_0 = \eta_a$, $\eta_{N+1} = \eta_b$, by Blakemore type functions

$$\mathcal{F}_i(\eta) = \frac{\sigma_i}{\exp(-\eta)+\gamma_i}, \; \eta_i \le \eta \le \eta_{i+1}, \sigma_i > 0, \gamma_i > 0. \quad (7)$$

See Fig. 3 for an example with asymptotic branches for small and large arguments.

This ansatz solves the integral equation for the current (5) if the following equations for are fulfilled simultaneously

$$\int_{\eta_i}^{\eta_{i+1}} \frac{1}{\frac{j}{\mathcal{F}_i(\eta)} + \delta\psi} d\eta = c_i \text{ for } i = 1, \dots, N, \quad (8)$$

$$\sum_{i=0}^{N} c_i = 1, \quad c_i > 0. \quad (9)$$

This results in a system of $N+1$ coupled nonlinear equations for the N weights c_i and the determination of the current j.

VI. CONCLUSION

A generalization of the Scharfetter-Gummel scheme based on a piecewise approximation by Blakemore type distributions functions has been presented. It is suitable for strictly monotonous distribution functions. Hence, the scheme can be applied to the Fermi-Dirac integral of order $1/2$ for typical ranges of the chemical potential occurring in high doping regions or active zones in semiconductor lasers as well as for the approximation of the distribution function $F_0(\eta)$, describing carriers in quantum wells, and to the Gauss-Fermi integral used in organic electronics. The solution of the local current equations (8), (9) requires local modifications of the typical algorithm based on solving linear systems inside Newton's method for the fully coupled van Roosbroeck system.

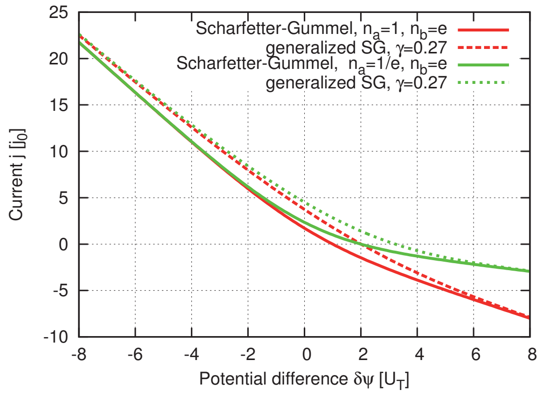

Fig. 2. Comparison of currents for classical Scharfetter-Gummel scheme ($\gamma = 0$) and the generalized one for the case $\mathcal{F}(\eta) = 1/(\exp(-\eta)+\gamma)$ with $\gamma = 0.27$ in dependence on the potential difference $\delta\psi$ for two choices of fixed densities as given by the solution of Eq. (6), compare [6].

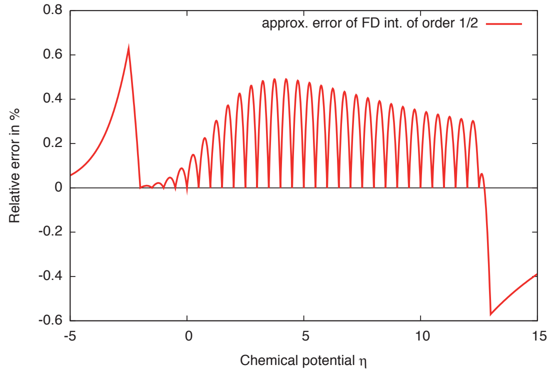

Fig. 3. Plot of the relative error $\big(\mathcal{F}_i(\eta) - F_{1/2}(\eta)\big)/F_{1/2}(\eta)$ for the approximation of the Fermi-Dirac integral of order $1/2$ by piecewise functions of the form $\mathcal{F}_i(\eta) = \sigma_i/(\exp(-\eta)+\gamma_i)$ with $\sigma_i > 0$, $\gamma_i > 0$ in dependence on the dimensionless chemical potential η. With 30 subintervals the relative approximation error is below 1% for $\eta < 12$.

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