Discretization scheme for drift-diffusion equations with strong diffusion enhancement

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***Abstract*—Inspired by organic semiconductor models based on hopping transport introducing Gauss-Fermi integrals a nonlinear generalization of the classical Scharfetter-Gummel scheme is derived for the distribution function $\mathcal{F}(\eta) = 1/(\exp(-\eta)+\gamma)$. This function provides an approximation of the Fermi-Dirac integrals of different order and restricted argument ranges. The scheme requires the solution of a nonlinear equation per edge and continuity equation to calculate the edge currents. In the current formula the density-dependent diffusion enhancement factor, resulting from the generalized Einstein relation, shows up as a weighting factor.**

I. Introduction

Any monotone non-Boltzmann statistics based state-equation for the carrier density of semiconductor results in a generalized Einstein relation describing the ratio of diffusion and drift current in thermodynamic equilibrium. This can be interpreted as a *diffusion enhancement* [1]. Following Scharfetter-Gummel one is interested in approximating the net electron current in order to discretize the drift-diffusion equation describing the carrier transport [2]. In the classical Scharfetter-Gummel scheme the exponential dependence of the carrier density on the chemical potential results in a current expression consisting of a weighted difference of the carrier densities. Here the usual state equation $n = N_c\mathcal{F}(\eta)$ for the carrier density in dependence on the chemical potential η, N_c denotes the density of states, is considered for the special distribution function

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

This approximation can be used for the Fermi-Dirac integral of order $1/2$ with $\gamma = 0.27$ and $\eta < 1.3$ [3]. For $\gamma = 1$ it coincides with Fermi-Dirac integral of order -1 describing zero-dimensional Fermi gases, namely hopping transport between individual sites. Furthermore, it is the limit for vanishing disorder σ of the Gauss-Fermi integral [4], which is used to describe organic semiconductors [5]. The general situation is depicted in Figs. 1 and 2.

Here we present a nonlinear generalization of the Scharfetter-Gummel scheme for the approximation of the net electron current governed by the carrier density expression (1).

II. Carrier continuity equations and diffusion enhancement

The continuity equation for the electrons reads

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

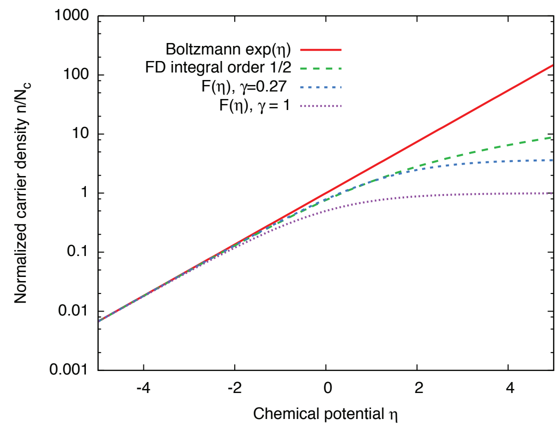

Fig. 1. Plot of distribution function $\mathcal{F}(\eta) = 1/(\exp(-\eta)+\gamma)$ in dependence of the dimensionless chemical potential η for different values of the parameter γ. In the asymptotic limit $\eta << -2$ a Boltzmann behavior is observed. For $\gamma = 0.27$ a good approximation of the Fermi-Dirac integral of order $1/2$ for $\eta < 1.3$ is provided, whereas the case $\gamma = 1$ corresponds to the limit of vanishing disorder of the Gauss-Fermi integral [4].

with the current expressions

$$J_n = -q\mu_n N_c \mathcal{F}(\eta)\nabla\varphi_n = -qn\mu_n\nabla\psi + qD_n\nabla n, \tag{2}$$

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

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 and E_c the band-edge energy. The mobility and the diffusion coefficient D_n fulfill the generalized Einstein relation

$$\frac{D_n}{\mu_n} = \frac{k_B T}{q}\frac{n}{N_c}(\mathcal{F}^{-1})'\left(\frac{n}{N_c}\right) =: \frac{k_B T}{q} g_3\left(\frac{n}{N_c}\right). \tag{4}$$

The factor g_3 in the generalized Einstein relation is describing a diffusion enhancement [1]. For our special choice of the distribution function (1) the relation becomes

$$g_3(x) = \frac{1}{1-\gamma x}, \tag{5}$$

while the current reads

$$J_n = -qn\mu_n\nabla\psi + \mu_n k_B T \frac{1}{1-\gamma\frac{n}{N_c}}\nabla n. \tag{6}$$

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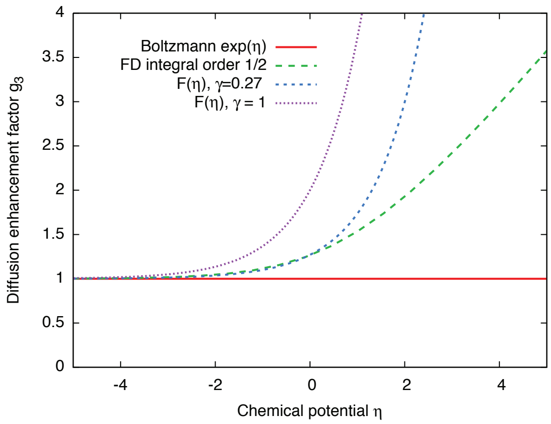

Fig. 2. Plot of diffusion enhancement factor g_3 in dependence on the dimensionless chemical potential related to the distribution function $\mathcal{F}(\eta) = (\exp(-\eta)+\gamma)^{-1}$ for different values of the parameter γ. In the asymptotic limit $\eta << -2$ no diffusion enhancement is observed (Boltzmann limit). Additionally, the diffusion enhancement factor g_3 related to the Fermi-Dirac integral of order 1/2 is depicted.

III. Current Approximation

In the following we consider the one-dimensional case on the spatial interval $[x_a, x_b]$ and the following scaling of the equation: the potentials are given in units of the thermal voltage $U_T = \frac{k_B T}{q}$ and the current is given in units of $j_0 = q\mu_n N_c \frac{U_T}{x_b - x_a}$. The Scharfetter-Gummel discretization is derived by solving the following equation

$$\Big(q\mu_n N_c \mathcal{F}\big(\eta(\varphi_n, \psi)\big)\varphi_n'\Big)' = 0, \tag{7}$$

on the interval $[x_a, x_b]$ with the boundary values $\varphi_n(x_a) = \varphi_a$ and $\varphi_n(x_b) = \varphi_b$. The electrostatic potential ψ is assumed to be linearly dependent on x, the mobility μ_n is taken to be an average value on the interval $[x_a, x_b]$. First integration yields $-q\mu_n N_c \mathcal{F}\big(\eta(\varphi_n, \psi)\big)\varphi_n' = j = const$. Second integration results in an integral equation for the unknown current j

$$\int_{\eta_a}^{\eta_b} \frac{1}{\frac{j}{\mathcal{F}(\eta)} + \delta\psi} d\eta = 1. \tag{8}$$

The boundary values are

$$\eta_a = \mathcal{F}^{-1}(n_a/N_c), \eta_b = \mathcal{F}^{-1}(n_b/N_c), \tag{9}$$

and potential difference $\delta\psi$ is given by $\delta\psi = \psi_b - \psi_a$. For details of this approach see [6]. For the distribution under consideration this integral equations leads to the following nonlinear, local equation for the edge current j:

$$j = f(j) = B(\delta\psi + \gamma j)e^{\eta_b} - B(-(\delta\psi + \gamma j))e^{\eta_a}. \tag{10}$$

where $B(x) = \frac{x}{e^x - 1}$ is the Bernoulli function. This equation has a unique solution $j = j(\psi_a, \psi_b, \eta_a, \eta_b)$ due to the monotonicity of the Bernoulli function. Using the relation $\mathcal{F}^{-1}(x) = -\ln\left(\frac{1}{x} - \gamma\right)$ the current expression in terms of densities is given by

$$j = g_3\left(\frac{n_b}{N_c}\right)B(\delta\psi + \gamma j)n_b - g_3\left(\frac{n_a}{N_c}\right)B(-\delta\psi - \gamma j)n_a. \tag{11}$$

Here, in this particular case the density-dependent diffusion enhancement factor g_3 shows up explicitly. With $\gamma = 0$ the well-known Scharfetter-Gummel expression is reproduced, while Eq. (11) is nonlinear with respect to the density and the potential difference $\delta\psi = \psi_b - \psi_a$ is modified by the local edge current and the parameter γ describing the deviation of the state-equation for the density with respect to the Boltzmann case.

The essential change compared with the classical scheme is now the solution of the nonlinear equation (11) on every edge of the spatial discretization during the assembly of each continuity equation.

IV. Conclusion

For a restricted range of arguments of the Fermi-Dirac integral of order $1/2$ a generalized, simple to implement, nonlinear Scharfetter-Gummel scheme has been derived. The effort is small compared with the introduction of an additional outer iteration. The local nonlinear equations for calculation of the edge currents can be solved due to the monotonicity properties of the Bernoulli function. The necessary conditions [7] for proving the existence of bounded steady state solutions, uniqueness of the equilibrium solution, and dissipativity are preserved, too.

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