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Discretization scheme for drift-diffusion equations with a generalized Einstein relation

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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. Additionally the current modifies the argument of the Bernoulli functions.

1. Introduction

Any strictly monotone non-Boltzmann statistics based state-equation for the carrier density in a semiconductor results in a generalized Einstein relation describing the ratio of diffusion and drift current in thermodynamic equilibrium. Due to van Mensfoort and Coehoorn (2008) this can be interpreted as a *diffusion enhancement*. On the other hand looking at the problem from a variational formulation point of view, see Albinus et al (2002) and references therein, the drift term is the modified expression while the same generalized Einstein relation is fulfilled.

Following Scharfetter and Gummel (1969) one is interested in approximating the net electron current in order to discretize the drift-diffusion equation describing the carrier transport. 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 (non-dimensionalized) 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 $\eta < 1.3$ (Blakemore (1952)). 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 (Paasch and Scheinert (2010)), which is used to describe organic semiconductors (Coehoorn et al (2005)). The general situation is depicted in Figs. 1 and 2.

The aim of this paper is to present a generalization of the Scharfetter-Gummel scheme for the approximation of the net electron current governed by the carrier density expression (1).

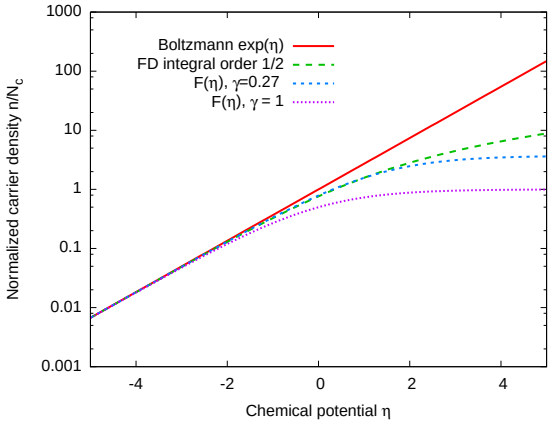

FIGURE 1. Plot of distribution function $\mathcal{F}(\eta) = 1/(\exp(-\eta) + \gamma)$ in dependence of the dimensionless chemical potential η for different values of the parameter γ. In the asymptotic limit $\eta << -2$ a Boltzmann behavior is observed. For $\gamma = 0.27$ a good approximation of the 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 (Paasch and Scheinert (2010)).

2. Carrier continuity equations and diffusion enhancement

The continuity equation for the electrons reads

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

with the current expression

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

and (non-dimensionalized) chemical potential

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

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, see van Mensfoort and Coehoorn (2008). 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

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

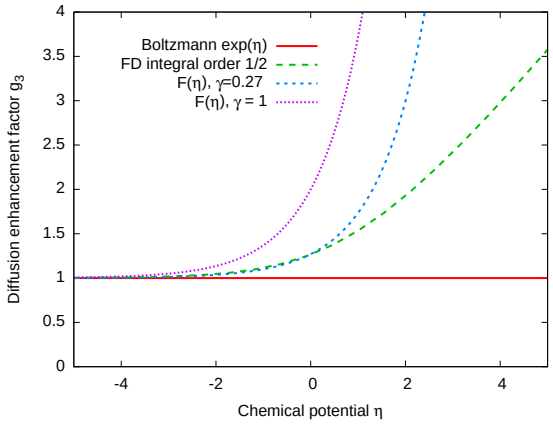

FIGURE 2. Plot of diffusion enhancement factor g_3 in dependence on the dimensionless chemical potential related to the distribution function $\mathcal{F}(\eta) = (\exp(-\eta)+\gamma)^{-1}$ for different values of the parameter γ. In the asymptotic limit $\eta << -2$ no diffusion enhancement is observed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

3. Generalized Scharfetter-Gummel scheme

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 equation

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

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 $-q\mu_n N_c \mathcal{F}\big(\eta(\varphi_n,\psi)\big)\varphi_n' = j = const.$ Replacing the quasi-Fermi potential φ_n by the chemical potential η using Eq. (3) the second integration results in an integral equation for the unknown current j:

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

The boundary values are

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

and potential difference $\delta\psi$ is given by $\delta\psi = \psi_b - \psi_a$. For details of this approach see Eymard et al (2006). For the distribution function (1) this integral equation leads to the following nonlinear, local equation for the edge current j:

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

where $B(x) = \frac{x}{e^x - 1}$ is the Bernoulli function. This is a fixed point equation for unkown the edge current j for fixed values of the chemical potentials η_a and η_b and

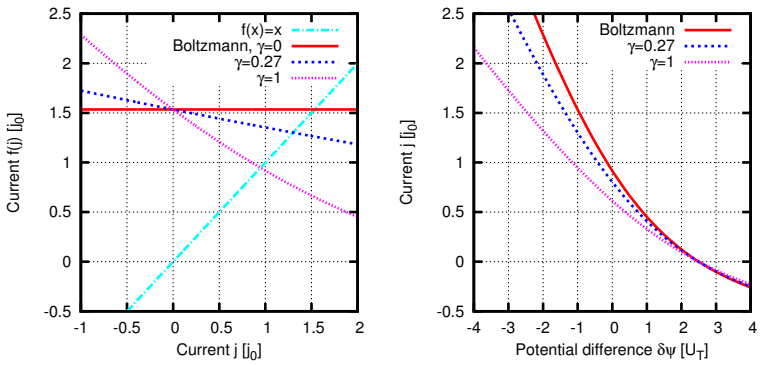

FIGURE 3. Solutions of fixed point equation (6) defining the current for different values of the parameter γ for fixed values of the chemical potentials $\eta_a = -2.5$, $\eta_b = 0$. Left: Graphical solution of the fixed point eq. by intersection of the function $f(j, \delta\psi)$ with j for $\delta\psi = -U_T$. Right: Variation of the self-consistent current $j(\delta\psi)$ on the potential difference $\delta\psi$.

the potential difference $\delta\psi$. The function $f(j, \delta\psi)$ can be rewritten in the following way:

$$f(j, \delta\psi) = B(\delta\psi + \gamma j)e^{\eta_b}\Big(1 - e^{\delta\psi + \gamma j - (\eta_b - \eta_a)}\Big).$$

The unique thermodynamic equilibrium ($j = 0$) is obtained for $\varphi_a = \varphi_b$. The derivative

$$\frac{\partial f}{\partial j} = \gamma\Big(B'(\delta\psi + \gamma j)e^{\eta_b} + B'(-(\delta\psi + \gamma j))e^{\eta_a}\Big) < 0$$

is strictly negative. Hence, the implicit function theorem applied to $F(\delta\psi, j) = j - f(j, \delta\psi) = 0$ guarantees a unique and continuous solution $j(\delta\psi)$ by continuation from the thermodynamic equilibrium. In particular this holds also for the dependence on all parameters of the two-point boundary value problem, namely for the chemical potentials η_a, η_b and for $\gamma \geq 0$ describing the deviation from the Boltzmann case. In Fig. 3 the graphical solution of the fixed point equation (6) is illustrated for different values of γ for fixed chemical potentials $\eta_a = -2.5$, $\eta_b = 0$ and a potential difference $\delta\psi = -U_T$. The dependence of the current on the potential difference $j(\delta\psi)$ is also shown in Fig. 3.

Using the relation $\mathcal{F}^{-1}(x) = -\ln\left(\frac{1}{x} - \gamma\right)$ the current expression in terms of densities is given by

$$j = g_3\left(\frac{n_b}{N_c}\right)B(\delta\psi + \gamma j)\frac{n_b}{N_c} - g_3\left(\frac{n_a}{N_c}\right)B(-\delta\psi - \gamma j)\frac{n_a}{N_c}. \tag{7}$$

Here, the density-dependent factor g_3 related to the generalized Einstein relation (4) shows up explicitly. For $\gamma = 0$ the well-known Scharfetter-Gummel expression is reproduced. The expression (7) is indeed a modification of the Scharfetter-Gummel current in two respects: on the one hand a non-symmetric rescaling by g_3 and on the other hand a shift of the potential difference $\delta\psi = \psi_b - \psi_a$ entering the Bernoulli function by γj. For small deviations in the densities n_a, n_b and close to the thermodynamic equilibrium, Eq. (7) can be interpreted by rescaling the Boltzmann current by a common factor $g_3(\bar{n})$, where $\bar{n}$ has the meaning of averaged rescaled density related either to a modified temperature or a self-consistent adapted density of states N_c used in an outer fixed point iteration, see Bandelow et al (2005).

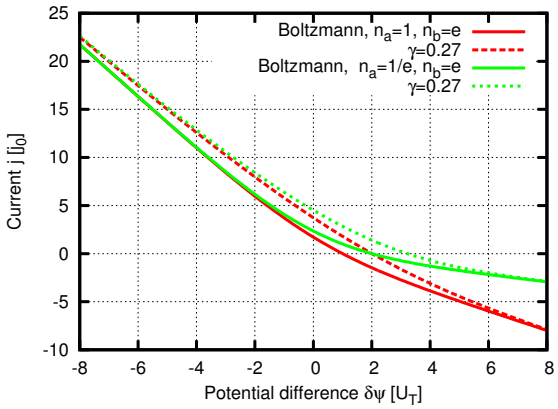

FIGURE 4. Comparison of 'Boltzmann' ($\gamma = 0$) and 'Fermi' ($\gamma = 0.27$) currents in dependence on the potential difference $\delta\psi = \psi_b - \psi_a$ for two choices of fixed densities $n_a = N_c$, $n_b = e\,N_c$ and $n_a = N_c/e$, $n_b = e\,N_c$ as given by the solution of equation (7). The corresponding values of the quasi-Fermi potentials change accordingly. For pure diffusion ($\delta\psi = 0$) the 'Fermi' current is roughly by a factor of two larger than the 'Boltzmann' current. The asymptotic behavior is dominated by the drift current.

To illustrate the influence of the statical distribution on the current again, in Fig. 4 the dependence of the current on the potential difference $\delta\psi = \psi_b - \psi_a$ is shown for the Boltzmann case ($\gamma = 0$) and for the distribution function (1) for $\gamma = 0.27$ with two different ratios of the densities n_a/n_b. The corresponding chemical potentials are in the range where Eq. (1) provides a good approximation of the Fermi-Dirac integral of order 1/2, see Fig. 1. Here, the Fermi statistics results in an increased current. Please note, that both cases (Figs. 3 and 4) are not a result of a self-consistent solution of the complete model equations used for device simulation (van Roosbroeck equations).

From the implementation point of view, the essential change compared to the classical scheme is now the solution of the nonlinear equation (7) for every edge of the spatial discretization during the assembly of each continuity equation.

4. Conclusion

For a restricted range of arguments of the Fermi-Dirac integral of order 1/2 a simple to implement, generalized 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.

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