Comparison of Consistent Flux Discretizations for Drift Diffusion beyond Boltzmann Statistics

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***Abstract*—We compare three thermodynamically consistent Scharfetter-Gummel schemes for non-Boltzmann statistics.**

I. Introduction

The classical Scharfetter-Gummel scheme in combination with a Voronoï finite volume method provides a discrete approximation to drift-diffusion currents for non-degenerate semiconductors which is consistent to the thermodynamic equilibrium in the sense that discrete solutions of the equilibrium nonlinear Poisson problem yield zero current.

Non-Boltzmann distribution functions $\mathcal{F}$ describing degenerate semiconductors are required for the simulation of single photon sources at cryogenic temperatures [1], [2] or organic semiconductors. Based on the analysis performed in [3], this paper compares several possible thermodynamically consistent generalizations of the Scharfetter-Gummel scheme to general strictly monotonously increasing distribution functions.

We consider the stationary van Roosbroeck system of charge transport in semiconductors using standard notation [3] (ψ: electrostatic potential, φ_n, φ_p: quasi-Fermi potentials, η_n, η_p: chemical potentials):

$$-\nabla\cdot(\varepsilon_0\varepsilon_r\nabla\psi) = q\,(p - n + C)\,, \tag{1a}$$

$$\nabla\cdot\mathbf{j}_n = qR, \qquad \mathbf{j}_n = -q\mu_n n\nabla\varphi_n, \tag{1b}$$

$$\nabla\cdot\mathbf{j}_p = -qR, \qquad \mathbf{j}_p = -q\mu_p p\nabla\varphi_p \tag{1c}$$

where the electron and hole densities are defined by

$$n = N_c\mathcal{F}(\eta_n), \qquad \eta_n = \frac{q(\psi-\varphi_n)-E_c}{k_BT}, \tag{2a}$$

$$p = N_v\mathcal{F}(\eta_p), \qquad \eta_p = \frac{q(\varphi_p-\psi)+E_v}{k_BT}. \tag{2b}$$

In the following we restrict our considerations to the continuity equation for the electrons, partially omitting the index n.

II. Discrete thermodynamic consistency

We require our numerical current approximation to satisfy a relationship which holds at the continuous level: constant quasi Fermi potentials lead to vanishing currents. Thus, setting any discrete numerical flux between two adjacent discretization nodes $\mathbf{x}_K$ and $\mathbf{x}_L$ corresponding to neighboring Voronoï cells (see [3] for more details) K and L to zero

$$j = j(\eta_L, \eta_K, \psi_L, \psi_K) = 0$$

shall imply

$$\frac{\psi_L - \psi_K}{U_T} =: \delta\psi_{KL} = \delta\eta_{KL} := \eta_L - \eta_K. \tag{3}$$

Thermodynamic consistency helps to avoid unphysical steady state dissipation [8]. Furthermore, the consistent discretization of dissipative effects is crucial when coupling the semiconductor equations to heat transport models.

III. Generalized Scharfetter-Gummel Schemes

If one assumes that the (unknown) flux j between two cells is constant, it fulfills the integral equation, see [4], [5],

$$\int_{\eta_K}^{\eta_L}\left(\frac{j_n/j_0}{\mathcal{F}(\eta)} + \frac{\psi_L-\psi_K}{U_T}\right)^{-1} d\eta = 1, \quad j_0 = q\mu_n N_c\frac{U_T}{h_{KL}} \tag{4}$$

where the integration limits are given by $\eta_K = \eta_n(\psi_K, \varphi_K)$ and $\eta_L = \eta_n(\psi_L, \varphi_L)$. For strictly monotonously increasing $\mathcal{F}(\eta)$ this equation has always a unique solution [6]. We will refer to it as the *generalized* Scharfetter-Gummel flux.

For the Boltzmann approximation, $\mathcal{F}(\eta) = e^\eta$, we obtain from (4) the classical Scharfetter-Gummel scheme [7],

$$j_{\mathrm{SG}} = B(\delta\psi_{KL})\,e^{\eta_L} - B(-\delta\psi_{KL})\,e^{\eta_K}, \tag{5}$$

for the non-dimensionalized edge current $j_{\mathrm{SG}} = j_n/j_0$ and the Bernoulli function $B(x) := x/(e^x - 1)$.

The Blakemore approximation $\mathcal{F}(\eta) = \frac{1}{e^{-\eta+\gamma}}$ yields for (4) a fixed point equation [5].

IV. Modified Scharfetter-Gummel Schemes

For general distribution functions, however, we cannot find closed expressions for the unknown current as a solution to (4). Since solving an integral equation for each pair of neighboring discretization points $\mathbf{x}_K, \mathbf{x}_L$ is too expensive in general, we introduce the following modified schemes as approximate solutions to (4). They keep the beneficial Scharfetter-Gummel structure and are all thermodynamically consistent.

A. Diffusion enhanced Scharfetter-Gummel scheme

In [8], [9], a logarithmic average of the nonlinear diffusion enhancement $g(\eta) = \frac{1}{(\ln\mathcal{F}(\eta))'} = \mathcal{F}(\eta)/\mathcal{F}'(\eta) \geq 1$ given by

$$g_{KL} = \frac{\eta_L - \eta_K}{\log\mathcal{F}(\eta_L) - \log\mathcal{F}(\eta_K)} \tag{6}$$

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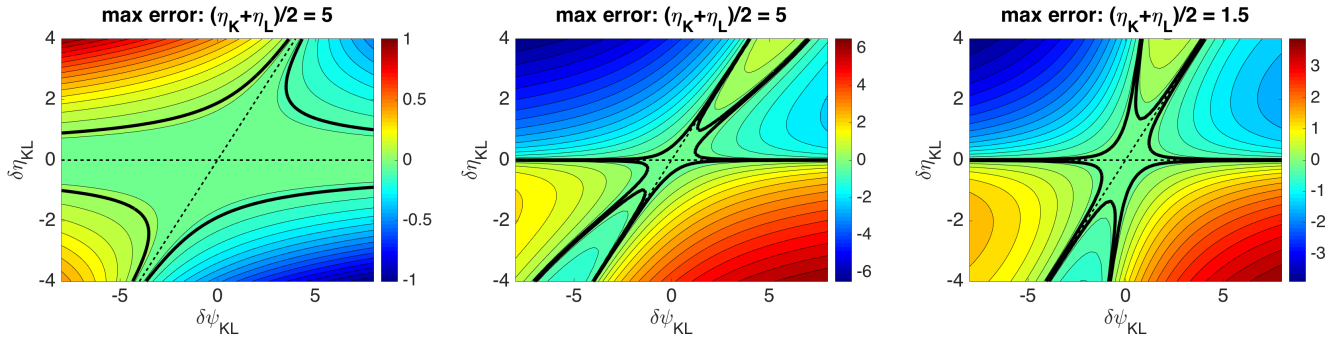

Fig. 1. Logarithmic absolute errors between the generalized Scharfetter-Gummel and the diffusion enhanced scheme (left), the arithmetically averaged inverse activity scheme (middle) and the geometrically averaged one (right) for $\bar{\eta}_{KL} = 5$, see [3].

was suggested, leading to the current approximation

$$j_{\text{DE}} = g_{KL}\left[B\left(\frac{\delta\psi_{KL}}{g_{KL}}\right)\mathcal{F}(\eta_L) - B\left(-\frac{\delta\psi_{KL}}{g_{KL}}\right)\mathcal{F}(\eta_K)\right]. \tag{7}$$

B. Inverse activity coefficients

Reformulation of (1b) in terms of activities e^{η_n} leads to a drift-diffusion flux of activities weighted by the inverse $\beta = \mathcal{F}(\eta)/e^{(\eta)}$ of the activity coefficient [10], leading to schemes

$$j_{\text{IA}} = -\bar{\beta}_{KL}\left(B\left(-\delta\psi_{KL}\right)e^{\eta_K} - B\left(\delta\psi_{KL}\right)e^{\eta_L}\right), \tag{8}$$

depending on the average $\bar{\beta}_{KL}$ of β_K and β_L. We consider arithmetic and geometric averages.

V. Error Estimates and Comparison

Neglecting third-order terms, setting $\bar{\eta}_{KL} = \frac{\eta_L+\eta_K}{2}$, the error between the modified fluxes and the generalized Scharfetter-Gummel flux j defined by the exact solution of (4) can be bounded by, see [3],

$$|j_{\text{IA}} - j| \le \frac{1}{2}\mathcal{F}(\bar{\eta}_{KL})|\delta\psi_{KL}\delta\eta_{KL}|, \tag{9}$$

$$|j_{\text{DE}} - j| \le \frac{1}{2}\frac{\mathcal{F}(\bar{\eta}_{KL})}{g(\bar{\eta}_{KL})}|\delta\psi_{KL}\delta\eta_{KL}|. \tag{10}$$

Fig. 1 shows the errors in terms of $\delta\eta_{KL}$ and $\delta\psi_{KL}$ for a fixed average $\bar{\eta}_{KL}$ and the Blakemore approximation. The errors vanish along the dashed lines indicating $\eta_K = \eta_L$ (pure drift current) as well as $\delta\psi_{KL} = \delta\eta_{KL}$ due to the consistency with the thermodynamic equilibrium. The diffusion enhancement $g(\bar{\eta}_{KL} = 5) = 41.07$ indicates that the Boltzmann approximation ($g \equiv 1$) is not valid. Such an high value of g can appear in devices operating at cryogenic temperatures [2]. Consistent with error estimates (9) and (10), the comparison in Fig. 1 reveals that the error of scheme (7) is considerably smaller than for scheme (8) for potential differences between neighboring cells larger than the thermal voltage U_T. This makes the diffusion enhanced scheme more accurate on coarser meshes. As the mesh becomes finer, we note that $\delta\psi_{KL}$ and $\delta\eta_{KL}$ tend to zero, and flux values close to the origin in Fig. 1 are attained where all schemes agree,

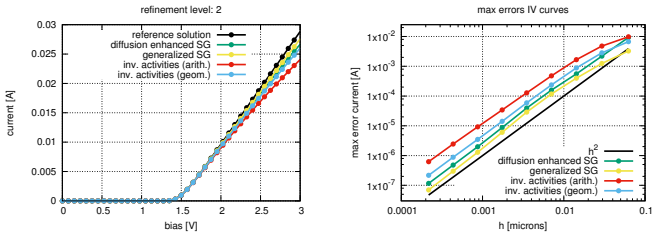

Fig. 2. Left: The IV curves computed with the different schemes for fixed mesh refinement. The reference solution (black) was computed using the generalized Scharfetter-Gummel scheme on refinement level 12. Right: Convergence studies for the absolute errors of the total current, see [3].

allowing to hypothesize that all schemes are convergent. Fig. 2 shows the influence of the flux discretizations to the solution of fully coupled van Roosbroeck system for a p-i-n benchmark.

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