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On thermodynamic consistency of a Scharfetter-Gummel scheme based on a modified thermal voltage for drift-diffusion equations with diffusion enhancement

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Abstract. Driven by applications like organic semiconductors there is an increased interest in numerical simulations based on drift-diffusion models with arbitrary statistical distribution functions. This requires numerical schemes that preserve qualitative properties of the solutions, such as positivity of densities, dissipativity and consistency with thermodynamic equilibrium. An extension of the Scharfetter-Gummel scheme guaranteeing consistency with thermodynamic equilibrium is studied. It is derived by replacing the thermal voltage with an averaged diffusion enhancement for which we provide a new explicit formula. This approach avoids solving the costly local nonlinear equations defining the current for generalized Scharfetter-Gummel schemes.

1. Introduction

In the stationary case, thermodynamic consistency for discretized drift-diffusion equations means that the zero bias solution coincides with the thermodynamic equilibrium. In the transient case, it means that for boundary conditions compatible with the thermodynamic equilibrium the solutions converge to this equilibrium when time tends to infinity. This property is important because its violation causes non-physical dissipation in the steady state, see Bessemoulin-Chatard (2012). The consistent approximation of dissipative effects is crucial for the solution of electrothermal models describing heating effects.

For the Boltzmann distribution Scharfetter and Gummel (1969) presented such a consistent scheme. Strictly monotonically increasing non-Boltzmann distribution functions lead to *diffusion enhancement.* Various extensions of the Scharfetter-Gummel scheme are suggested to account for this effect, see Purbo et al (1989); Jüngel (1995); Stodtmann et al (2012). Unfortunately, they are not thermodynamically consistent. Koprucki and Gärtner (2013a,b) introduced a thermodynamically consistent generalization in the spirit of Scharfetter and Gummel (1969) by solving local Dirichlet problems. But it requires solving local nonlinear equations during assembly and the iterative solution of the coupled system. Bessemoulin-Chatard (2012) presented another extension of the Scharfetter-Gummel scheme using a proper average of the nonlinear diffusion guaranteeing thermodynamic consistency for a specific choice of the distribution function. We present an alternative interpretation of her approach based on diffusion enhancement and give an explicit formula for this average for a very general class of statistical distribution functions.

2. Drift-diffusion equations and diffusion enhancement

The dependence of the carrier densities n and p on the chemical potentials for electrons and holes η_n and η_p are described by a statistical distribution function $\mathcal{F}(\eta)$ as well as conduction and valence band densities of states N_c and N_v via state equations $n = N_c\mathcal{F}(\eta_n)$ and $p = N_v\mathcal{F}(\eta_p)$. Typical choices for the distribution function are $\mathcal{F}(\eta) = \exp(\eta)$ (Boltzmann approximation) or $\mathcal{F}(\eta) = F_{1/2}(\eta)$ (Fermi-Dirac integral of order 1/2 describing degenerate semiconductors). The chemical potentials are related to the quasi-Fermi potentials of electrons and holes φ_n and φ_p through $\eta_n = (q(\psi - \varphi_n) - E_c)/(k_BT)$ and $\eta_p = (q(\varphi_p - \psi) + E_v)/(k_BT)$. Here

q denotes the elementary charge, ψ the electrostatic potential, k_B the Boltzmann constant, T the temperature and E_c and E_v the conduction and valence band-edge energies. We model a semiconductor device as a domain $\Omega \subset \mathbb{R}^d$ where the carrier transport in a self-consistent electrical field is described by a system of partial differential equations. In the steady-state case this drift-diffusion system consists of Poisson's equation for ψ and continuity equations for electrons and holes:

$$\begin{aligned} &(1) \qquad & -\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla \psi) &= q(C + p - n), \quad \mathbf{x} \in \Omega, \\ &(2) \qquad & -\nabla \cdot \mathbf{j}_n = -qR, &\qquad \nabla \cdot \mathbf{j}_p = -qR, \quad \mathbf{x} \in \Omega. \end{aligned}$$

Here, ε_r is the relative permittivity, C is the net doping profile, and $R = R(n, p)$ describes the recombination. Electron and hole currents can be expressed in terms of quasi-Fermi potentials by $\mathbf{j}_n = -q\mu_n n \nabla \varphi_n$, $\mathbf{j}_p = -q\mu_p p \nabla \varphi_p$, or for any strictly monotonic Fermi-like distribution function $\mathcal{F}(\eta)$ in drift-diffusion form

$$(3) \qquad \mathbf{j}_n = q\mu_n \Big[U_T g\Big(\frac{n}{N_c}\Big) \nabla n - n \nabla \psi \Big], \quad \mathbf{j}_p = -q\mu_p \Big[U_T g\Big(\frac{p}{N_v}\Big) \nabla p + p \nabla \psi \Big],$$

where μ_n and μ_p denote the electron and hole mobilities, resp., and $U_T = k_B T / q$ is the thermal voltage. The factor g can be defined in terms of densities, $g(x) = x(\mathcal{F}^{-1})'(x)$, or in terms of the non-dimensionalized chemical potential

$$(4) \qquad g_\eta(\eta) = \frac{\mathcal{F}(\eta)}{\mathcal{F}'(\eta)} = \frac{1}{\big(\log \mathcal{F}(\eta)\big)'}.$$

This factor is the so-called *diffusion enhancement* appearing as a density-dependent modification factor in the generalized Einstein relation, see van Mensfoort and Coehoorn (2008), leading in general to a non-linear diffusion coefficient. For the Boltzmann distribution, $\mathcal{F}(\eta) = \exp(\eta)$, we have $g \equiv 1$ and the current expressions (3) reduce to the usual ones with linear diffusion.

3. FINITE VOLUME SPACE DISCRETIZATION

We discretize the domain Ω using the Voronoï box based finite volume method introduced in Macneal (1953), also known as "box method" due to Bank and Rose (1987). It uses a simplical boundary conforming Delaunay grid (Si et al (2010)) which allows to obtain control volumes surrounding each given collocation point $\mathbf{x}_K$ by joining the circumcenters of the simplices containing it, see Fig. 1.

Let ∂K denote the boundary of the control volume K, and $|\xi|$ the measure of a geometrical object ξ. For each control volume K, we integrate the continuity equation (2) and apply Gauss's theorem to the integral of the flux divergence. Restricting our considerations to the electron transport equation, we obtain

$$(5) \qquad \begin{aligned} 0 &= \int\limits_{\partial K} \mathbf{j}_n \cdot \mathbf{n} + \int\limits_K R \, d\mathbf{x} = \sum_{L \text{ neighbor of } K} \int\limits_{\partial K \cap \partial L} \mathbf{j}_n \cdot \mathbf{n}_{KL} ds + \int\limits_K R \, d\mathbf{x} \\ &\approx \sum_{L \text{ neighbor of } K} \frac{|\partial K \cap \partial L|}{|\mathbf{x}_K - \mathbf{x}_L|} j_{n,KL} + |K| R(n_K, p_K), \end{aligned}$$

where $\mathbf{n}$ is the internal unit normal to ∂K and $\mathbf{n}_{KL}$ is the internal unit normal to the interface $\partial K \cap \partial L$ for each neighbor L of K. The values n_K, p_K are the densities n and p at the collocation points $\mathbf{x}_K$, and $j_{n,KL}$ are approximations of the (scaled by the edge length) normal currents through $\partial K \cap \partial L$, see Fig. 1. In the same manner the discretization of the Poisson equation can be obtained.

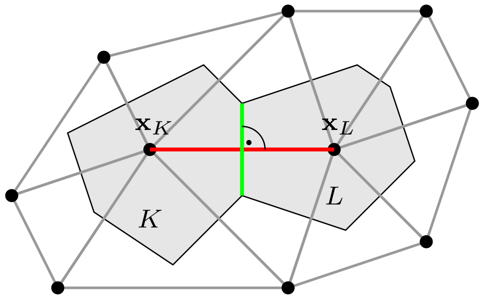

FIGURE 1. Collocation points (black), simplices (grey lines) and control volumes (filled) in two space dimensions. Note the right angle between the lines $\overline{\mathbf{x}_K\mathbf{x}_L}$ and $\partial K \cap \partial L$, which allows to approximate the normal current through the face boundary $\partial K \cap \partial L$ (green) by a finite difference expression along the edge $\overline{\mathbf{x}_K\mathbf{x}_L}$ (red).

4. Generalized Scharfetter-Gummel scheme

For the Boltzmann approximation the classical Scharfetter-Gummel scheme has been derived by solving a two-point boundary value problem resulting from a projection of the continuity equation (neglecting recombination) onto the discretization edge $\overline{\mathbf{x}_K\mathbf{x}_L}$ assuming constant current $j = \mathbf{j}_n \cdot \mathbf{n}_{KL}$ and constant electrical field with boundary values $n|_{\mathbf{x}_K} = n_K, n|_{\mathbf{x}_L} = n_L$, see Scharfetter and Gummel (1969). It approximates $j_{n,KL}$ by

$$j = q\mu_n U_T \Big[B\Big(-\frac{\delta\psi}{U_T} \Big) n_K - B\Big(\frac{\delta\psi}{U_T} \Big) n_L \Big], \tag{6}$$

where $B(x) = \frac{x}{\exp(x)-1}$ is the Bernoulli function and $\delta\psi = \psi_K - \psi_L$, $(\psi|_{\mathbf{x}_K} = \psi_K, \psi|_{\mathbf{x}_L} = \psi_L)$ is the electrostatic potential difference between neighboring cells, see Fig. 1. This scheme is not only dissipative but also consistent with thermodynamic equilibrium ($j = 0$ for $\varphi_n = const.$).

The idea to solve a local two-point boundary value problem in order to derive current expressions has been generalized to nonlinear drift-diffusion problems by Eymard et al (2006). It has been applied by Koprucki and Gärtner (2013a) to the Blakemore distribution $\mathcal{F}(\eta) = \frac{1}{\exp(-\eta)+\gamma}$, which for $\gamma = 0.27$ provides a good approximation of $F_{1/2}$ up to $\eta \leq 1.3$, see Blakemore (1952). This approach leads to a nonlinear equation w.r.t. j having a unique solution. In Koprucki and Gärtner (2013b) this ansatz has been generalized to strictly monotonic distribution functions. The resulting schemes are dissipative and consistent with thermodynamic equilibrium. However, they require additional numerical effort for solving the local non-linear equations to determine the currents $j_{n,KL}$ in every single step of the iterative solution of the fully coupled van Roosbroeck system.

5. Scharfetter-Gummel scheme based on modified thermal voltage

As an alternative, we discuss a *modified Scharfetter-Gummel* scheme by replacing the thermal voltage U_T in the classical Scharfetter-Gummel expression with a modified value $U_T^* = U_T g(n/N_c)$ depending on the density. This idea is motivated by the structure of the diffusion term in current expressions (3). Assuming an averaged diffusion enhancement $\bar{g}_{KL} = \bar{g}_{KL}(n_K, n_L) \in [g(n_K), g(n_L)]$ on the edge $\overline{\mathbf{x}_K\mathbf{x}_L}$ this approach provides a current approximation of the form

$$j = q\mu_n U_T \bar{g}_{KL} \Big[B\Big(-\frac{\delta\psi}{U_T \bar{g}_{KL}} \Big) n_K - B\Big(\frac{\delta\psi}{U_T \bar{g}_{KL}} \Big) n_L \Big]. \tag{7}$$

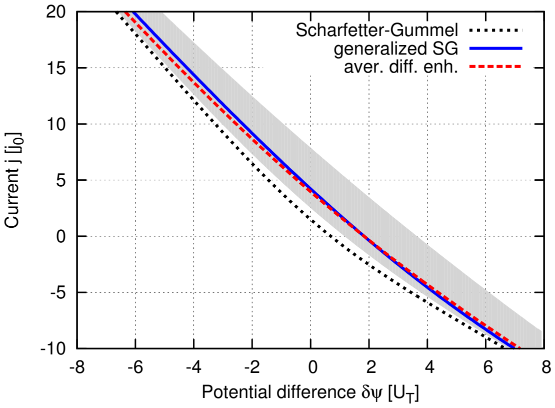

FIGURE 2. Comparison of the three different current approximations for the flux between neighboring cells for the Blakemore distribution $\mathcal{F}(\eta) = 1/(\exp(-\eta) + 0.27)$ and fixed densities $n_K = 1.5N_c$, $n_L = 3N_c$: generalized Scharfetter-Gummel scheme according to Koprucki and Gärtner (2013a) (solid line), Scharfetter-Gummel scheme with modified thermal voltage $U_T^* = U_T\bar{g}_{KL}$ with averaged diffusion enhancement $\bar{g}_{KL}$ according to (8) (dashed line), classical Scharfetter-Gummel (6) (dotted line). The minimal and maximal values $g(n_K)$ and $g(n_L)$ of the diffusion enhancement define the grey shaded area, within which generalized and modified Scharfetter-Gummel lies.

This kind of extension of the Scharfetter-Gummel scheme to Fermi-Dirac statistics has been suggested using arithmetic (Purbo et al (1989); Jüngel (1995)) or geometric (Stodtmann et al (2012)) averaging, leading in general to schemes which are not consistent with the thermodynamic equilibrium ($j = 0$ for $\varphi_n = const$). Bessemoulin-Chatard (2012) introduced for drift-diffusion equations with nonlinear diffusion a proper local average guaranteeing consistency with thermodynamic equilibrium. She provides an explicit formula for the special choice $\mathcal{F} = \eta^\nu$ describing the high density limit of the Fermi-Dirac distribution. Following her ideas, we obtain for any strictly monotonic statistical distribution function

$$\bar{g}_{KL} = \frac{\mathcal{F}^{-1}\left(\frac{n_L}{N_c}\right) - \mathcal{F}^{-1}\left(\frac{n_K}{N_c}\right)}{\log(n_L/N_c) - \log(n_K/N_c)} = \frac{\eta_L - \eta_K}{\log\mathcal{F}(\eta_L) - \log\mathcal{F}(\eta_K)}. \tag{8}$$

The definition in terms of the chemical potentials η_K, η_L on the right can be understood as an approximation of the diffusion enhancement (4) given as a logarithmic derivative by a differential quotient on the edge $\overline{\mathbf{x}_K\mathbf{x}_L}$. The resulting scheme is dissipative and consistent with thermodynamic equilibrium.

For the Blakemore distribution function different current approximations are depicted in Fig. 2. The scheme corresponding to the averaged diffusion enhancement (8) provides a very good approximation to the generalized Scharfetter-Gummel scheme, see Koprucki and Gärtner (2013a). Only this choice of the average $\bar{g}_{KL}$ guarantees consistency with thermodynamic equilibrium.

To study the influence of the discretization on the solution of the van Roosbroeck system (1) and (2), the classical Scharfetter-Gummel scheme and the approach based on modified thermal voltage have been applied to a GaAs-based n-doped/intrinsic/n-doped structure using a Blakemore distribution function, see Fig. 3. In the zero bias case the classical Scharfetter-Gummel scheme yields a numerical

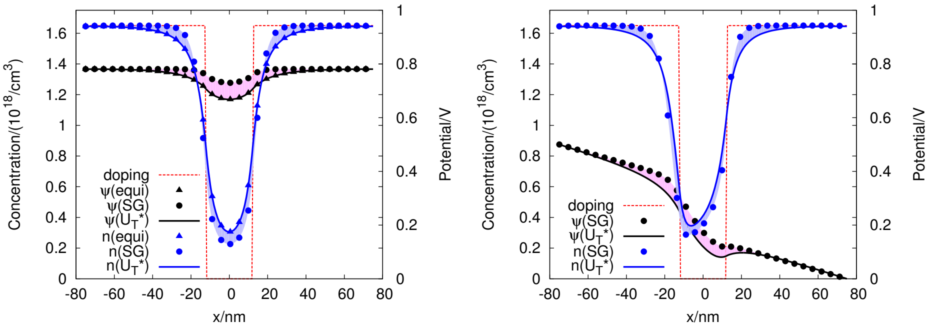

FIGURE 3. Comparison of numerical solutions for electrostatic potential and electron densities in an GaAs based n-doped/intrinsic/n-doped structure: classical Scharfetter-Gummel scheme (bullets) and the one based on modified thermal voltage $U_T^* = U_T \bar{g}_{KL}$ according to (7),(8) (solid lines). Left: zero bias. Right: applied voltage 0.5 V. The solutions for the modified scheme for zero bias are consistent with the thermodynamic equilibrium (triangles) only obtained by the nonlinear Poisson equation (1). Parameters: band gap $E_g = 1.424\,\mathrm{eV}$, density of states $N_c = 4.7 \times 10^{17}\,\mathrm{cm}^{-3}$, $N_v = 9 \times 10^{18}\,\mathrm{cm}^{-3}$, mobilities $\mu_n = 8500\,\mathrm{cm}^2/(\mathrm{Vs})$, $\mu_n = 400\,\mathrm{cm}^2/(\mathrm{Vs})$, relative permitivity $\varepsilon_r = 12.9$, n-doping $N_d = 1.65 \times 10^{18}\,\mathrm{cm}^{-3}$.

solution which is noticeably different from the thermodynamic equilibrium obtained by solving the discretized nonlinear Poisson equation. This difference is due to the inconsistent approximation of the diffusion enhancement in the classical Scharfetter-Gummel scheme in the case of nonlinear diffusion, see Fig. 2. The space charge region at the n-doped-intrinsic interface is influenced by the strong diffusion enhancement at high carrier densities which is missing in the classical, unmodified scheme. For an applied voltage the diffusion enhancement has a similar impact on the solution, see Fig. 3, resulting in a higher current. The diffusion related enhancement in current is roughly 9%.

6. CONCLUSION

The discretization of drift-diffusion equations with Fermi-like statistical distribution functions requires a proper treatment of the nonlinear diffusion. We studied an extension of the classical Scharfetter-Gummel scheme replacing the thermal voltage by an enhanced value. It is defined by a proper local average of diffusion enhancement that guarantees consistency with thermodynamic equilibrium which is important in order to obtain accurate results. This approach is an alternative to the costly generalized Scharfetter-Gummel schemes due to its simpler implementation for various distribution functions.

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