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On the Discretization of van Roosbroeck's Equations with Magnetic Field

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Abstract

We investigate qualitative properties of the drift–diffusion model of carrier transport in semiconductors when a magnetic field is present. At first the spatially continuous problem is studied. Essentially, global stability of the thermal equilibrium is shown using the *free energy* as a Lyapunov function. This result implies exponential decay of any perturbation of the thermal equilibrium. Next, we introduce a time discretization that preserves the dissipative properties of the continuous system and assumes no more than the naturally available smoothness of the solution. Finally, we present a space discretization scheme based on weak and consistent definitions of discrete gradients and currents. Starting with a fundamental result on global stability (dissipativity) of the classical Scharfetter–Gummel scheme (without magnetic field), we adapt this scheme with respect to magnetic fields and study the M-property of the associated matrix. For two dimensional applications we formulate sufficient conditions in terms of the grid geometry and the modulus of the magnetic field such that our scheme is dissipative and yields positive solutions. These conditions cover fields up to $|\mathbf{b}|\mu_\nu \approx 0.5$ for very fine grids. This means approximately 200 Tesla for Silicon. Sufficient for some typical semiconductor sensor applications. The grid requirements might become prohibitive for large magnetic fields and complex three dimensional structures. Our techniques of defining discrete currents can be applied to similar situations, especially if projections of currents are involved in model parameters.

1. Introduction

The main issue of this paper is to provide the community, concerned with device simulations, with some of the results published in [1]. Space restrictions allow for the main results only, proofs, details and comments have to be omitted. The paper is organized to state the results mentioned in the abstract.

2. The spatially continuous problem

Let $S = (0,T)$ be a bounded time interval and let $\Omega \subset I\!R^N$, $2 \le N \le 3$, be a bounded Lipschitzian domain. Set $Q = S \times \Omega$. Suppose that $\partial\Omega = \Gamma_D \cup \Gamma$, $\Gamma_D \cap \Gamma \neq 0$, where Γ_D is closed and has a positive surface measure. Let us consider the following system of equations

$$-\nabla \cdot \epsilon \nabla \Psi = f + u_2 - u_1 \text{ in } Q,$$

$$\frac{\partial u_\nu}{\partial t} + q_\nu \nabla \cdot \mathbf{J}_\nu = R \text{ in } Q,\ \nu = 1,2,\ q_1 = -1,\ q_2 = 1, \tag{1}$$

$$\mathbf{J}_\nu = \mathbf{j}_\nu - q_\nu \mathbf{b} \times \mathbf{J}_\nu,\ \mathbf{j}_\nu = -\mu_\nu u_\nu \nabla \Phi_\nu.$$

The physical meaning of the various quantities is the following: Ψ - electrostatic potential, u_ν - carrier densities, $\Phi_\nu = \Psi + q_\nu \log u_\nu$ - quasi-Fermi potentials, ϵ - dielectric permittivity, f - density of impurities, R - recombination / generation rate $R = r(x, u_1, u_2)(1 - u_1 u_2)$, $\mathbf{J}_\nu$, $\mathbf{j}_\nu$ - current densities with / without magnetic field, $\mathbf{b}$ - the magnetic field vector, μ_ν - carrier mobilities $\left(\frac{\mu_\nu}{1+|b|^2}\right)(x) \geq \mu_b > 0$. We assume: $|\mathbf{b}|$, ϵ, $\mu_\nu, f \in L_\infty(\Omega)$, $0 < \epsilon < \epsilon_0$, $r = r(x, u_1, u_2)$ is continuous with respect to u_ν and measurable with respect to x. The growth condition $0 \leq r(x, u_1, u_2) \leq r_1(1 + |u_1| + |u_2|)$, $r_1 = \text{const} < \infty$ holds.
Using the matrix $B_\nu = \frac{1}{1+|\mathbf{b}|^2}(I + \mathbf{b}\,\mathbf{b}^T - q_\nu \mathbf{b}\times)$, the last line in (1) yields

$$\mathbf{J}_\nu = B_\nu \mathbf{j}_\nu. \tag{2}$$

We complete the system (1) by the initial conditions $u_\nu(0, \cdot) = u_{\nu 0}(\cdot)$ in Ω and the thermal equilibrium boundary conditions

$$\Psi = \Psi_D, \; u_\nu = e^{-q_\nu \Psi_D} \text{ on } S \times \Gamma_D, \tag{3}$$

$\mathbf{n} \cdot \epsilon \nabla \Psi + \alpha(\Psi - \Psi_\Gamma) = 0$, $\alpha \geq 0$, $\mathbf{n} \cdot \mathbf{J}_\nu = 0$ on $S \times \Gamma$, where $u_{\nu 0} \in L_\infty(\Omega)$, $\Psi_D \in L_\infty(\Gamma_D)$, $\Psi_\Gamma\ inL_\infty(\Gamma)$ are given and $\mathbf{n}$ is the outer unit normal with respect to Gamma.

2.1. Stability of the thermal equilibrium

Let $\Psi^* \in H^1(\Omega)$ be the (unique weak) solution of the boundary value problem $-\nabla \cdot \epsilon \nabla \Psi = f + e^{-\Psi} - e^{\Psi}$ in Ω, $\Psi = \Psi_D$ on Γ_D, $\mathbf{n} \cdot \nabla \Psi + \alpha(\Psi - \Psi_\Gamma) = 0$ on Γ.

Definition 1 The triple (Ψ^*, u_ν^*), $u_\nu^* = e^{-q_\nu \Psi^*}$, is called the thermal equilibrium solution; the functionals
$F(\Psi, u_\nu) = \int [\sum_\nu u_\nu (\log \frac{u_\nu}{u_\nu^*} - 1) + u_\nu^*]\, d\Omega + \frac{1}{2} \|\Psi - \Psi^*\|^2$,
with $\|h\|^2 = \int \epsilon |\nabla h|^2\, d\Omega + \int \alpha h^2\, d\Gamma$, and
$d_b(\Psi, u_\nu) = \int [\frac{1}{1+|\mathbf{b}|^2} \sum_\nu u_\nu \mu_\nu (|\nabla \Phi_\nu|^2 + (\mathbf{b} \cdot \nabla \Phi_\nu)^2) + r(x, u_1, u_2)(u_1 u_2 - 1) \log(u_1 u_2)]\, d\Omega$,
$d_b \geq 0$ are the *free energy* and the *dissipation rate*, respectively.

Proposition 1 *Let (Ψ, u_ν) be a solution of (1) - (3). Then the function $L(t) = F(\Psi(t), u_1(t), u_2(t))$ satisfies: $0 \leq L(t) = L(0) - \int_0^t d_b\, ds$.*

Remark 1 By proposition 1 the function L decreases strictly monotone as long as the dissipation rate is nonzero. Thus we can conclude that $L(u(t)) \to 0\ for\ t \to \infty$. Moreover, L turns out to be a Lyapunov function of the system and indicates global stability of the thermal equilibrium.

The decay rate towards the thermal equilibrium can be estimated:

Corollary 1 *Let (Ψ, u_ν) be a solution to (1) - (3) with $\|\Psi(t)\|_\infty \leq k < \infty\ \forall t > 0$. Then (Ψ, u_ν) tends to the thermal equilibrium solution (Ψ^*, u_ν^*). Moreover, it holds*

$$\sum_\nu \|\sqrt{u_\nu(t)} - \sqrt{u_\nu^*}\|^2 + \|\Psi(t) - \Psi^*\|^2 \leq 4e^{-\lambda t} L(0) \to 0, \; t \to \infty. \tag{4}$$

Proposition 2 *Suppose $r(x, u_1, u_2) \geq r_0 = \text{const} > 0$ and $\alpha = 0$. Then the function L decreases exponentially. In particular, we have $L(t) \leq e^{-\tilde{\lambda} t} L(0)$.*

The proposition shows, that the assumptions of the corollary can be cancelled in special situations even for $N = 3$, the constants λ, $\tilde{\lambda}$ are given in [1].

2.2. Time discretization

Let $S = \cup_j S_j$, $S_j = [t_{j-1}, t_j]$, $\tau_j := t_j - t_{j-1} > 0$, $t_0 = 0$. According to the backward Euler's scheme, we discretize the system as follows $-\nabla \cdot \epsilon \nabla \Psi^j = f + u_2^j - u_1^j$ in Ω, $j = 0, 1, 2, \ldots$, $\frac{u_\nu^j - u_\nu^{j-1}}{\tau_j} + q_\nu \nabla \cdot \mathbf{J}_\nu^j = R^j$ in Ω, $j = 0, 1, 2, \ldots$, $u_\nu^0 = u_{\nu 0}$.

Proposition 3 *Let (Ψ^j, u_ν^j) be a solution of the time discrete system. Then the discrete function $L^j = F(\Psi^j, u_\nu^j)$ satisfies $0 \leq L^{j+1} \leq L^j \leq L^0 - \sum_{l=1}^j \tau_l d_b^l$,
$d_b^l = d_b(\Psi^l, u_\nu^l) \geq 0$.*

3. Space discretization

For the space discretization we use N-dimensional simplices (elements) $\mathbf{E}_l^N$ such that $\Omega = \cup_l \mathbf{E}_l^N$. A simplex $E = E_l^N$ can be represented by the $N \times (N+1)$ matrix of its vertex coordinates.

$$P = \begin{pmatrix} x_{1,1} & . & . & . & x_{1,N+1} \\ . & . & . & . & . \\ x_{N,1} & . & . & . & x_{N,N+1} \end{pmatrix}, \quad \tilde{P} := \begin{pmatrix} \mathbf{1}^T \\ P \end{pmatrix}$$

where $\tilde{P}$ is an extension of P by elements of the null space of D^T (see below, $\tilde{P}$ is nonsingular for any nondegenerated simplex). $\mathbf{x}_i^T = (x_{1,i}, x_{2,i}, \ldots, x_{N,i})$ is the vector of the space coordinates of the vertex i of the simplex. The volume integral of a function is approximated by the corresponding sum over the Voronoi volume elements: $\int f \, d\Omega \approx \sum_m f_m |V_m|, \quad \sum_m |V_m| = |\Omega|$.
The contribution of the recombination R to the discrete dissipation rate is given by

$$d_{rec} := \sum_\nu \sum_m |V_m| (R\Phi_\nu)(\mathbf{x}_m) = \sum_m |V_m| r \; (u_1 u_2 - 1) \log(u_1 u_2)(\mathbf{x}_m) \geq 0. \tag{5}$$

3.1. Discrete Gradients

In order to discretize (1) - (3) we need projections of the currents onto the coordinate axes. Let D be a $(N+1) \times (N+1)$ matrix such that $\int \nabla u \cdot \nabla h \, dE \approx (D\mathbf{u}, \mathbf{h}) = \mathbf{h}^T D \mathbf{u}$, where $(.,.)$ is the scalar product in $I\!R^{N+1}$. By means of D we define the discrete version $\tilde{\nabla}$ of ∇ by $\tilde{\nabla} = \frac{1}{|\mathbf{E}|} PD$. Hence the projection of $\tilde{\nabla}\mathbf{u}$ onto the x-axis is given by $(\tilde{\nabla}\mathbf{u})_x = \frac{1}{|\mathbf{E}|}(D\mathbf{u}, \tilde{\mathbf{x}}), \quad \tilde{\mathbf{x}}^T = (x_{1,1}, \ldots, x_{1,N+1})$.
We suppose the matrix D to satisfy the following conditions:
(i) D is $(N+1) \times (N+1)$ matrix, (ii) rank $D = N$, $\mathbf{1}^T D = 0$, $\mathbf{1}^T = (1, \ldots, 1)$,
(iii) $(D\mathbf{u}, \mathbf{h}) = |\mathbf{E}| \, (\tilde{\nabla}\mathbf{u}, \tilde{\nabla}\mathbf{h}), \quad \forall \; \mathbf{u}, \; \mathbf{h}$.

Remark 2 The 'projection property' (iii) is the key for introducing consistent currents $\mathbf{j}$ on simpleces $\mathbf{E}$ in the next sections. (ii, iii) ensure the strict balance of discrete contact currents $\mathbf{j}_k$ defined by $\mathbf{j}_k = \sum_l |\mathbf{E}_l| \; (\mathbf{j}, \tilde{\nabla}\mathbf{h}_k)$. Where the $\mathbf{h}_k$ are suitable test functions: $h|_{\Gamma_k} = 1, \; h|_{\Gamma_j} = 0, \; j \neq k, \; h \in H^1(\Omega)$ and $\Gamma_D = \cup_i \Gamma_i$.

Lemma 1 *The matrix D is uniquely defined by (i) - (iii). Moreover, D is the finite element matrix (for piecewise linear polynomials on the simplex) of the Laplacian.*

Hence the finite element discretization satisfies: $(D\mathbf{u}, \mathbf{h}) = |\mathbf{E}|(\tilde{\nabla}\mathbf{u}, \tilde{\nabla}\mathbf{h})$. Consistent currents can be defined via:

Lemma 2 *Let A be a $(N+1) \times (N+1)$ matrix such that $\mathbf{1}^T A = 0$ and* rank$A = N$. *Then* $\forall \; \mathbf{u}, \mathbf{h} \; \in I\!R^{N+1}$ $(A\mathbf{u}, \mathbf{h}) = |\mathbf{E}|(\mathbf{j}_u, \tilde{\nabla}\mathbf{h})$, *where* $\mathbf{j}_u = \frac{1}{|\mathbf{E}|} PA\mathbf{u}, \; \tilde{\nabla}\mathbf{h} = \frac{1}{|\mathbf{E}|} PD\mathbf{h}$.

3.2. Box discretization methods

The box discretization in principle approximates the Laplacian on the Voronoi volume V_m. Interpreting this with respect to the elements, one gets an discrete approximation of the Laplacian $\int \nabla u \cdot \nabla h \;\; dE_l \approx (A_{box}\mathbf{u}, \mathbf{h})$ on E_l, too. For $N = 2$ the matrices A_{box} and D coincide, in general we have for $N > 2$: $\frac{1}{|E|} A_{box} P \; P^T \; A_{box} \neq A_{box}$. However, because of Lemma 2 and $(A_{box}\mathbf{u}, \mathbf{1}) = 0$, we can define consistent currents and gradients on E by: $\mathbf{j}_u = \frac{1}{|\mathbf{E}|} PA_{box}\mathbf{u}, \; \tilde{\nabla}\mathbf{h} = \frac{1}{|\mathbf{E}|} PD\mathbf{h}$. Since time derivatives, recombination and right-hand sides can be discretized as stated above, it remains to look for discrete approximations of expressions as $\nabla e^\Psi \nabla v$, where $v = e^{-\Phi}$ is the Slotboom variable related to u_1. We have to preserve the Scharfetter–Gummel scheme - essentially an approximation of $\int (a(\Psi)\nabla v) \cdot (\nabla h) \; dE \approx (A_{SG}\mathbf{v}, \mathbf{h}), \; \mathbf{1}^T A_{SG} = 0, \; A_{SG} = A_{SG}^T$ for a strongly varying coefficient $a(\Psi)$. The index SG stands for Scharfetter–Gummel and Slotboom variables. This leads to the following representation of A_{SG} on the simplex:

$$A_{SG}\mathbf{v} = G_N^T Y G_N \mathbf{v}. \tag{6}$$

Here Y is a weight matrix, symmetric positive definite and diagonal, G_N is a $n_e \times n_v$ matrix (n_e the number of edges, n_v the number of vertices, for details see [1]). $y_k := y_{kk} = \frac{|\mathbf{s}_{ij}|}{|\mathbf{e}_{ij}|}$, $\beta_s(\log a(\psi_i), \log a(\psi_j))$, $k = 1, \ldots, n_e$, $\beta_s(x,y) = e^x \beta(x-y) = \frac{x-y}{e^{-y}-e^{-x}}$, $\beta_s(x,y) > 0, |x|, |y| < \infty$ is related to the Bernoulli function $\beta(x) = \frac{x}{e^x-1} \geq 0$. For $a = \text{const}$ holds $A_{SG} = A_{box}$. Consistent currents on $\mathbf{E}$ are defined as before: (we still write $\mathbf{j}_u$ because $\mathbf{u} = e^{\psi}\mathbf{v}$ introduces a diagonal transformation of the matrix and the variable only) $\mathbf{j}_u = \frac{1}{|\mathbf{E}|} P A_{SG} \mathbf{v}$, $\tilde{\nabla}\mathbf{h} = \frac{1}{|\mathbf{E}|} P D \mathbf{h}$.

Definition 2 The discrete dissipation rate (except recombination) on a simplex $\mathbf{E}$ for one carrier density (here the electrons) is (comp. definition 1)
$d_{0E} := -\mathbf{\Phi}^T A_{SG} \exp(-\mathbf{\Phi})$. (The recombination contribution $d_{recE} \geq 0$ is given by (5) with the sum restricted on $\mathbf{E}$.)

Proposition 4 *The Scharfetter-Gummel scheme (6) is dissipative, i. e. , $d_{0E} \geq 0$, for any state of the system without magnetic field.*

3.3. Magnetic field

We are looking for a matrix A_{mag} approximating $\int J \cdot \nabla h \, dE \approx (A_{mag}\mathbf{v}, \mathbf{h})$, $\mathbf{1}^T A_{mag} = 0$, $A_{mag} \neq A_{mag}^T$. Here $J = J(\mathbf{b})$ denotes the continuous current with magnetic field. $J(\mathbf{b})$ is related to $j = J(\mathbf{0})$ by (see (2), the subscript $\nu = 1$ is deleted again) $J_u = B\ j_u$. We defined the discrete version of $\mathbf{j}_u$ by $\mathbf{j}_u = \frac{1}{|\mathbf{E}|} P A_{SG} \mathbf{v}$, $\mathbf{1}^T A_{SG} = \mathbf{0}$. In view of Lemma 2 we make an analogous ansatz for the discrete version of $\mathbf{J}_u$ $\mathbf{J}_u = \frac{1}{|\mathbf{E}|} P A_{mag} \mathbf{v}$, $\mathbf{1}^T A_{mag} = \mathbf{0}$. This yields $\tilde{P} A_{mag} = \tilde{B} \tilde{P} A_{SG}$, $\tilde{B} := \begin{pmatrix} 0 & 0 \\ 0 & B \end{pmatrix}$. Hence $A_{mag} = \tilde{P}^{-1} \tilde{B} \tilde{P} A_{SG}$. Since $\tilde{P}^{-1}$ is known, this is the desired expression for A_{mag}.

Remark 3 $\mathbf{J}_u$ has to fulfil the same boundary conditions as $\mathbf{j}_u$. The scheme is current conservative by construction.

Introducing for $N = 2$ $c_i := \cot \alpha_i$, α_i inner angles, some algebra yields: $A_{mag} = \frac{1}{1+b_z^2} A_{SG} + \delta A_{mag}$, $\delta A_{mag} = \frac{b_z}{1+b_z^2} G^T \operatorname{diag}[\cot(\alpha_{i-1})] S_{\downarrow} A_{SG}$, ($S_{\downarrow}$ is the shift matrix). In components this reads

$$A_{SG} = \begin{pmatrix} y_1 + y_3 & -y_1 & -y_3 \\ -y_1 & y_2 + y_1 & -y_2 \\ -y_3 & -y_2 & y_3 + y_2 \end{pmatrix},$$

$$(1+b_z^2)\delta A_{mag} = b_z \begin{pmatrix} -y_3 c_3 + y_1 c_2 & -y_2(c_2+c_3) - y_1 c_2 & y_3 c_3 + y_2(c_2+c_3) \\ y_3(c_1+c_3) + y_1 c_1 & y_2 c_3 - y_1 c_1 & -y_3(c_1+c_3) - y_2 c_3 \\ -y_1(c_1+c_2) - y_3 c_1 & y_1(c_1+c_2) + y_2 c_2 & y_3 c_1 - y_2 c_2 \end{pmatrix}.$$

Proposition 5 *Assume $y_i > 0$ and* (i) $|b_z||\cot \alpha_i| < 1$, (ii) $-y_i(1 + b_z c_{i+1}) - y_{i+1}(c_{i+1} + c_{i+2}) b_z < 0$, (iii) $-y_i(1 - b_z c_i) + y_{i+2}(c_i + c_{i+2}) b_z < 0$.
Then A_{mag} is a weak M-matrix.

Proposition 6 *The change in the dissipation rate due to the magnetic field on a triangle $\mathbf{E}$ can be estimated by $|\delta d_{b\,E}| \leq \max_{i,j} \cot(\alpha_{j-1}) \sqrt{\frac{y_i}{y_j}}\, \sqrt{3}\, |b_z|\, d_{0\,E}$.*

Remark 4 Because of $(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{a} = 0$, the dissipation part δd_b of the magnetic field vanishes exactly for $N = 2$ in the continuous case. Thus $\delta d_{b\mathbf{E}} \neq 0$ has to be considered as discretization error - for the equilateral triangle $\delta d_{b\mathbf{E}}$ is of the order $\delta \Psi^k \delta \Phi^{k'}$, $k + k' = 3$.

References

[1] H. Gajewski, K. Gärtner, On the discretization of van Roosbroeck's equations with magnetic field , Technical Report 94/14 Integrated Systems Laboratory, ETH Zurich, to appear in ZAMM.

and literature cited in [1].