A. Glitzky (joint work with K. Gärtner)

Existence of bounded steady state solutions
to spin-polarized drift-diffusion systems
Switzerland

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Outline of the talk

- Spin-polarized drift-diffusion model
- Stationary model
  - Continuous system:
    Existence, boundedness, uniqueness for small applied voltages
  - Discretized system:
    Existence, boundedness, uniqueness for small applied voltages

Details:
A. G., K. Gärtner, *Existence of bounded steady state solutions to spin-
Spin-resolved drift-diffusion model

consider spin-resolved carriers \(e_\uparrow, e_\downarrow, h_\uparrow, h_\downarrow\)

spin-resolved densities for electrons and holes

\[
\begin{align*}
n_{\uparrow \downarrow} &= \frac{N_c}{2} \exp \left[ \frac{-E_{c0} \pm qg_c}{k_BT} \right] \exp \left[ \frac{\varphi n_{\uparrow \downarrow} + q\psi}{k_BT} \right] \\
p_{\uparrow \downarrow} &= \frac{N_v}{2} \exp \left[ \frac{E_{v0} \mp qg_v}{k_BT} \right] \exp \left[ -\frac{\varphi p_{\uparrow \downarrow} - q\psi}{k_BT} \right]
\end{align*}
\]

spin relaxation reactions

\(e_\uparrow \rightleftharpoons e_\downarrow, \quad h_\uparrow \rightleftharpoons h_\downarrow\)

recombination/generation of electrons and holes

\[
\begin{align*}
e_\uparrow + h_\uparrow &\rightleftharpoons 0, \quad e_\uparrow + h_\downarrow \rightleftharpoons 0 \\
e_\downarrow + h_\uparrow &\rightleftharpoons 0, \quad e_\downarrow + h_\downarrow \rightleftharpoons 0
\end{align*}
\]

effective densities of state

\(N_c, N_v\)

band edge energies

\(E_{c0}, E_{v0}\)

spin-resolved quasi-Fermi energies

\(\varphi n_{\uparrow \downarrow}, \varphi p_{\uparrow \downarrow}\)

elementary charge, electrostatic potential

\(q, \psi\)

splitting of carrier bands

\(g_c, g_v\)

due to magnetic impurities or an applied magnetic field

\(T, k_B\)

Temperature, Boltzmann constant
Spin-resolved drift-diffusion model

- system of 4 continuity equations containing spin-relaxation as well as generation-recombination terms
- coupled with a Poisson equation
- completed by boundary conditions from device simulation and initial conditions
- obtain a generalization of the classical van Roosbroeck system
- introduce scaled variables
Model equations in scaled variables

\( X_i \) species: \( e_\uparrow, e_\downarrow, h_\uparrow, h_\downarrow \)
\( \lambda_i \) charge numbers: \(-1, -1, 1, 1\)
\( \zeta_i = \ln \frac{u_i}{\bar{u}_i} + \lambda_i v_0 \) electrochemical potentials
\( a_i = e^{\zeta_i} \) electrochemical activities

Particle flux density for species \( X_i \)

\[
J_i = -D_i u_i \nabla \zeta_i = -D_i \bar{u}_i e^{-\lambda_i v_0} \nabla a_i
\]

\(-R_i\) net production rate of species \( X_i \)

\[
\begin{align*}
R_1 &= r_{13}(a_1 a_3 - 1) + r_{14}(a_1 a_4 - 1) + r_{12} e^{v_0} (a_1 - a_2), \\
R_2 &= r_{23}(a_2 a_3 - 1) + r_{24}(a_2 a_4 - 1) - r_{12} e^{v_0} (a_1 - a_2), \\
R_3 &= r_{13}(a_1 a_3 - 1) + r_{23}(a_2 a_3 - 1) + r_{34} e^{-v_0} (a_3 - a_4), \\
R_4 &= r_{14}(a_1 a_4 - 1) + r_{24}(a_2 a_4 - 1) - r_{34} e^{-v_0} (a_3 - a_4)
\end{align*}
\]
Model equations

Stationary spin-polarized drift-diffusion model (SPDD model)

continuity equations

\[ \nabla \cdot J_i = -R_i \quad \text{in} \quad \Omega, \]
\[ \nu \cdot J_i = 0 \quad \text{on} \quad \Gamma_N, \]
\[ \zeta_i = \zeta_i^D \quad \text{on} \quad \Gamma_D, \quad i = 1, \ldots, 4. \]

Poisson equation

\[ -\nabla \cdot (\varepsilon \nabla v_0) = f + \sum_{i=1}^{4} \lambda_i \bar{u}_i e^{-\lambda_i v_0} a_i \quad \text{in} \quad \Omega, \]
\[ \nu \cdot (\varepsilon \nabla v_0) = 0 \quad \text{on} \quad \Gamma_N, \quad v_0 = v_0^D \quad \text{on} \quad \Gamma_D. \]
Continuous system: A-priori estimates

Theorem 1. If \((v_0, \zeta_1, \ldots, \zeta_4) \in (W^{1,2}(\Omega) \cap L^{\infty}(\Omega))^5\) is a weak solution to the stationary SPDD model then

\[ v_0 \in [\underline{L}, \overline{L}], \quad \zeta_i \in [-M, M], \quad a_i \in [e^{-M}, e^M], \quad i = 1, \ldots, 4, \text{ a.e. in } \Omega, \]

where \(M, \underline{L}, \overline{L}\) are constants given by the data such that

\[
|\zeta_i^D| \leq M, \quad \esssup_{\Gamma_D} v_0^D - \essinf_{\Gamma_D} v_0^D \leq M, \\
\underline{L} := \min \left( \essinf_{\Gamma_D} v_0^D, \ln \frac{c_f + \sqrt{c_f^2 + 16C_{\overline{u}}c_{\overline{u}}}}{4C_{\overline{u}}} - M \right), \\
\overline{L} := \max \left( \esssup_{\Gamma_D} v_0^D, \ln \frac{C_f + \sqrt{C_f^2 + 16C_{\overline{u}}c_{\overline{u}}}}{4c_{\overline{u}}} + M \right).
\]
Continuous system: A-priori estimates

Idea of the proof:

- test continuity equations by

\[(\zeta_1 - M)^+, (\zeta_2 - M)^+, -(\zeta_3 + M)^-, -(\zeta_4 + M)^-\]

and

\[(-(\zeta_1 + M)^-, -(\zeta_2 + M)^-, (\zeta_3 - M)^+, (\zeta_4 - M)^+)\]

- test Poisson equation by \((v_0 - L)^+, -(v_0 + L)^-\)

use strict monotonous decay of \(y \mapsto \sum_{i=1}^{4} \lambda_i \tilde{u}_i a_i e^{-\lambda_i y}\)
Continuous system: Existence

Theorem 2. There exists at least one solution \((v_0^\bullet, a^\bullet)\) to the stationary SPDD model.

Idea of the proof:

- use Slotboom variables: \((v_0, a_1, a_2, a_3, a_4)\), where \(a_i = e^{\zeta_i}\), Gummel map

- iterate \(a^n = Q_c(a^o)\), solve fixed point problem \(a^\bullet = Q_c(a^\bullet)\) for \(Q_c : \mathcal{M}_c \to L^2(\Omega)^4\),

\[
\mathcal{M}_c := \{ a \in L^2(\Omega)^4 : a_i \in [e^{-M}, e^M] \text{ a.e. in } \Omega, \quad i = 1, \ldots, 4 \}. 
\]

- \(Q_c\) is continuous, maps the bounded, closed, convex set \(\mathcal{M}_c \neq \emptyset\) into itself, \(Q_c[\mathcal{M}_c]\) is a precompact subset of \(L^2(\Omega)^4\)

- evaluate \(v_0^\bullet\) as the unique weak solution to

\[
- \nabla \cdot (\varepsilon \nabla v_0) = f + \sum_{i=1}^{4} \lambda_i \bar{u}_i e^{-\lambda_i v_0} a_i^\bullet \quad \text{on } \Omega \quad + \text{mixed BCs.}
\]
Theorem 3.
1. If the Dirichlet data is compatible with thermodynamic equilibrium, i.e.
\[ \zeta_i^{D*} = \text{const}, \quad i = 1, \ldots, 4, \quad \zeta_1^{D*} = \zeta_2^{D*} = -\zeta_3^{D*} = -\zeta_4^{D*} \]
then the thermodynamic equilibrium \((v^*_0, \zeta_1^{D*}, \ldots, \zeta_4^{D*})\) with
\[ -\nabla \cdot (\varepsilon \nabla v^*_0) = f + \sum_{i=1}^{4} \lambda_i \bar{u}_i e^{\zeta_i^{D*}} - \lambda_i v^*_0 \quad \text{on } \Omega \quad + \text{mixed BCs} \]
is the unique solution to the stationary SPDD model.

2. Let \(v_0^{D*} \in W^{1,2,\omega_D}(\Omega)\) for some \(\omega_D \in (N - 2, N)\). If the applied voltage is sufficiently small, then the stationary SPDD model possesses exactly one solution.
Ideas of the proof:

- formulation in a Sobolev-Campanato space setting, use results of Gröger, Recke’06

- write \((v_0, \zeta_1, \ldots, \zeta_4) = Z + z^D\), where \(z^D = (v_0^D, \zeta_1^D, \ldots, \zeta_4^D)\)

- Frechet derivative of the linearization w.r.t. \(Z\) at thermodynamic equilibrium \((Z^*, z^{D*})\) is an injective Fredholm operator of index zero

\[
W_{0}^{1,2,\omega}(\Omega \cup \Gamma_N)^5 \to W^{-1,2,\omega}(\Omega \cup \Gamma_N)^5
\]

for some \(\omega \in (N - 2, \omega_D]\)

- apply implicit function theorem
Discretization

use boundary conforming Delaunay grids with \( r \) grid points

matrix \( \tilde{G} \) maps from nodes to edges of a triangle (tetrahedron)

\[
\tilde{G}_2 = \begin{pmatrix}
1 & -1 & 0 \\
0 & 1 & -1 \\
-1 & 0 & 1
\end{pmatrix}, \quad \tilde{G}_3 = \begin{pmatrix}
1 & -1 & 0 & 0 \\
0 & 1 & -1 & 0 \\
-1 & 0 & 1 & 0 \\
-1 & 0 & 0 & 1 \\
0 & -1 & 0 & 1 \\
0 & 0 & -1 & 1
\end{pmatrix}
\]

\( G = \sqrt{[\gamma]} \tilde{G} \) discrete gradient matrix

\([\gamma]\) diagonal matrix of geometric weights per simplex, \( \gamma_{\sigma} = \frac{m_{\sigma}}{d_{\sigma}} \)

\( G^T[\cdot]Gw \) indicates the global function including boundary conditions

\( w \in \mathbb{R}^r \) vector of values in grid points

\([\cdot]\) diagonal matrix, \( [\cdot]_j \) its \( j \)th diagonal element
Discretized system: Scharfetter-Gummel scheme

\[ A_i^S(v_0) := G^T [D_i \bar{u}_i e^{-\lambda_i v_0} / \text{sh}(\tilde{G} \frac{v_0}{2})] G, \quad i = 1, \ldots, 4, \]

where

\[ \text{sh}(t) = \frac{\sinh t}{t}, \quad v_0 = \frac{v_{0,j} + v_{0,k}}{2}. \]

The ‘average’ \( D_i \bar{u}_i e^{-\lambda_i v_0} / \text{sh}(\tilde{G} \frac{v_0}{2}) \) is called Scharfetter-Gummel scheme and results from solving a two-point BVP along each edge, \((e^{-\lambda_i v_0 a_i'})' = 0\).

Discrete stationary SPDD model:

\[ G^T \varepsilon G v_0 = [V](f + \sum_{i=1}^{4} \lambda_i [\bar{u}_i e^{-\lambda_i v_0}] a_i), \]

\[ A_1^S(v_0) a_1 = \sum_{i=3,4} [V][r_{1i}(u)](1 - [a_i] a_1) + [V][r_{12} e^{v_0}](a_2 - a_1), \]

\[ A_2^S(v_0) a_2 = \sum_{i=3,4} [V][r_{2i}(u)](1 - [a_i] a_2) - [V][r_{12} e^{v_0}](a_2 - a_1), \]

\[ A_3^S(v_0) a_3 = \sum_{i=1,2} [V][r_{3i}(u)](1 - [a_i] a_3) + [V][r_{34} e^{-v_0}](a_4 - a_3), \]

\[ A_4^S(v_0) a_4 = \sum_{i=1,2} [V][r_{4i}(u)](1 - [a_i] a_4) - [V][r_{34} e^{-v_0}](a_4 - a_3). \]
Theorem 4. There exists at least one solution \((v_0^*, a^*)\) to the discretized stationary SPDD model. Solutions fulfill the bounds

\[
a_{ij}^* \in [e^{-M}, e^M], \quad i = 1, \ldots, 4, \quad v_{0j}^* \in [L, L], \quad j = 1, \ldots, r.
\]

Idea of the proof:

- iterate \(a^n = Q(a^0)\), solve fixed point problem \(a^* = Q(a^*)\) for \(Q : \mathcal{M} \rightarrow \mathbb{R}^{4r}\),

\[
\mathcal{M} := \{a \in \mathbb{R}^{4r} : a_{ij} \in [e^{-M}, e^M], \quad j = 1, \ldots, r, \quad i = 1, \ldots, 4\}.
\]

- \(Q\) is continuous, maps the bounded, closed, non empty set \(\mathcal{M}\) into itself, apply Brouwer’s fixed point theorem

- evaluate \(v_0^*\) by

\[
G^T \varepsilon G v_0^* = [V] (f + \sum_{i=1}^{4} \lambda_i [\bar{u}_i e^{-\lambda_i v_0^*}] a_i^*).
\]
**Discretized system: Existence and bounds**

**Theorem 4.** There exists at least one solution \((\mathbf{v}^\bullet_0, \mathbf{a}^\bullet)\) to the discretized stationary SPDD model. Solutions fulfill the bounds

\[
a^\bullet_{ij} \in [e^{-M}, e^M], \quad i = 1, \ldots, 4, \quad \mathbf{v}^\bullet_{0j} \in [L, \bar{L}], \quad j = 1, \ldots, r.
\]

**Idea of the proof:**

- iterate \(\mathbf{a}^n = Q(\mathbf{a}^o)\), solve fixed point problem \(\mathbf{a}^\bullet = Q(\mathbf{a}^\bullet)\) for \(Q : \mathcal{M} \to \mathbb{R}^{4r}\),

\[
\mathcal{M} := \{\mathbf{a} \in \mathbb{R}^{4r} : a_{ij} \in [e^{-M}, e^M], \quad j = 1, \ldots, r, \quad i = 1, \ldots, 4\}.
\]

- \(Q\) is continuous, maps the bounded, closed, non empty set \(\mathcal{M}\) into itself, apply Brouwer’s fixed point theorem

- evaluate \(\mathbf{v}^\bullet_0\) by

\[
G^T \varepsilon G \mathbf{v}^\bullet_0 = [V](\mathbf{f} + \sum_{i=1}^{4} \lambda_i [\bar{u}_i e^{-\lambda_i v^\bullet_0}] \mathbf{a}^\bullet_i).
\]
Starting from \( \mathbf{a}^o = (a_1^o, a_2^o, a_3^o, a_4^o) \in \mathcal{M} \), we evaluate \( \mathbf{a}^n = Q(\mathbf{a}^o) \in \mathcal{M} \) by:

1. Determine \( \mathbf{v}_0^n \) as the unique solution to

\[
G^T \varepsilon G \mathbf{v}_0^n = [V](f + \sum_{i=1}^{4} \lambda_i \bar{u}_i e^{-\lambda_i v_0^n} a_i^o).
\]

2. Using this \( \mathbf{v}_0^n \) we solve the four decoupled discretized continuity equations

\[
A_1^S(\mathbf{v}_0^n) \mathbf{a}_1^n = \sum_{i=3,4} [V][r_{1i}(\mathbf{a}^o, \mathbf{v}_0^n)](1 - [a_i^o] \mathbf{a}_1^n) + [V][r_{12} e^{v_0^n}](\mathbf{a}_2^o - \mathbf{a}_1^n),
\]

\[\vdots\]

and evaluate \( \mathbf{a}^n = (\mathbf{a}_1^n, \ldots, \mathbf{a}_4^n) \).
Discretized system: Details

1. Iterated Poisson equation

bounds for $v^n_0$: multiply equation by $(v^n_0 - \bar{L})^+ T$, $-(v^n_0 + L)^- T$

solvability: minimize $h : \mathbb{R}^r \rightarrow \mathbb{R}$,

$$h(y) = \frac{1}{2} y^T G^T \varepsilon G y - y^T [V] \left( f + \sum_{i=1}^{4} [\bar{u}_i e^{-\lambda_i y}] a_i^o \right).$$

uniqueness: suppose to have two solutions $v^n_0$, $\tilde{v}^n_0$, multiply equation by $(v^n_0 - \tilde{v}^n_0)^+ T$

continuous dependence on $a^o$

For $v^n_0$ with $|v^n_{0j}| \leq c$, $j = 1, \ldots, r$, for some $c > 0 \implies A_i^S (v^n_0)$ are weakly diagonally dominant M-matrices, $i = 1, \ldots, 4$, they have bounded positive inverses for homogeneous Dirichlet data.
Discretized system: Details

2. Iterated (1.) continuity equation

\[ A^S_1(v^n_0)a^n_1 = \sum_{i=3,4} [V][r_{1,i}(a^o, v^n_0)](1 - [a^o_i]a^n_1) + [V][r_{12} e^{v^n_0}](a^n_2 - a^n_1) \]

solvability:

\[ A^S_1(v^n_0) + \sum_{i=3,4} [V][r_{1,i}(a^o, v^n_0)][a^o_i] + [V][r_{12} e^{v^n_0}] \]

has a bounded inverse. Thus the problem is uniquely solvable.

boundedness: multiply by \((a^n_1 - e^M)^+ + T\), and \(-(a^n_1 + e^M)^- - T\)

continuous dependence on \(v^n_0\) and \(a^o\)
Lemma 1. If no voltage is applied to the device (the boundary conditions

\[ v_0|_{\Gamma_D} = v_0^{bi}, \quad a_i|_{\Gamma_D} = 1, \quad i = 1, \ldots, 4, \]

which are compatible with thermodynamic equilibrium) then there exists a unique solution \((v_0^*, a^*) = (v_0^*, 1, 1, 1, 1)\) to the discrete stationary SPDD model, here

\[ G^T \varepsilon G v_0^* = [V](f + \sum_{i=1}^{4} \lambda_i [\bar{u}_i e^{-\lambda_i v_0^*}] 1). \]

This solution is a thermodynamic equilibrium.
Discretized system: Uniqueness for small applied voltages

Theorem 5. If the applied voltage is sufficiently small, then the discrete stationary SPDD model possesses exactly one solution.

- Linearization of the discrete stationary SPDD system in the thermodynamic equilibrium \((v_0^*, a^*)\) (corresponding to no applied voltage, Lemma 1) has a bounded inverse.
- Due to the continuous dependence of the problem on \((v_0, a)\) the *implicit function theorem* gives the desired uniqueness result for small voltages.

Summary
The static SPDD system possesses very similar analytical and numerical properties compared to the stationary classical van Roosbroeck system.
References


Assumptions

(A1) \( \Omega \subset \mathbb{R}^N \) bounded Lipschitzian domain, \( N \leq 3 \),
\( \Gamma_N \) relative open subset of \( \partial \Omega \), \( \Gamma_D := \partial \Omega \setminus \Gamma_N \), \( \text{mes} \Gamma_D > 0 \).

(A1*) For all \( x \in \partial \Omega \) there exists an open neighborhood \( U \) of \( x \) in \( \mathbb{R}^N \) and a Lipschitz transformation \( \Phi : U \to \mathbb{R}^N \) such that \( \Phi(U \cap (\Omega \cup \Gamma_N)) \in \{E_1, E_2, E_3\} \).

(A2) \( r_{ii'}' \in L^\infty(\Omega), ii' = 12, 34. r_{ii'} : \Omega \times (0, \infty)^4 \to \mathbb{R}_+, r_{ii'}(x, \cdot) \in C^1((0, \infty)^4) \) for a.a. \( x \in \Omega \). \( r_{ii'}(\cdot, u), \frac{\partial r_{ii'}'}{\partial u}(\cdot, u) \) are measurable for all \( u \in (0, \infty)^4 \).

(A2*) For every compact subset \( K \subset (0, \infty)^4 \) there exists a \( \Delta > 0 \) such that
\[ |r_{ii'}(x, u)|, \|\frac{\partial r_{ii'}'}{\partial u}(x, u)\| \leq \Delta \] for all \( u \in K \) and a.a. \( x \in \Omega \).
For every compact subset \( K \subset (0, \infty)^4 \) and \( \epsilon > 0 \) there exists a \( \delta > 0 \) such that
\[ |r_{ii'}(x, u) - r_{ii'}(x, \hat{u})| < \epsilon, \|\frac{\partial r_{ii'}'}{\partial u}(x, u) - \frac{\partial r_{ii'}'}{\partial u}(x, \hat{u})\| < \epsilon \] for all \( u, \hat{u} \in K \) with \( \|u - \hat{u}\| \leq \delta \) and a.a. \( x \in \Omega, ii' = 13, 14, 23, 24 \).

(A3) \( D_i, \varepsilon, f, \bar{u}_i \in L^\infty(\Omega), D_i, \varepsilon \geq c > 0, 0 < c_f \leq f \leq C_f, c_u \leq \bar{u}_i \leq C_u \)
a.e. on \( \Omega \), \( v_0^D, \zeta_i^D \in W^{1,2}(\Omega) \cap L^\infty(\Omega), i = 1, \ldots, 4 \).

(A4) \( \Omega \) is polyhedral with a finite polyhedral partition \( \Omega = \bigcup I \Omega^I \). On each \( \Omega^I \) the functions \( \varepsilon, \bar{u}_i, D_i, i = 1, \ldots, 4, r_{12}, r_{34}, r_{ii'}(\cdot, u), ii' = 13, 14, 23, 24 \), are constants. The discretization is boundary conforming Delaunay.
Definitions Sobolev-Campanato spaces

Campanato space

\[ \mathcal{L}^{2,\omega}(\Omega) := \{ v \in L^2(\Omega) : \|v\|_{L^2,\omega(\Omega)} < \infty \}, \]

\[ \|v\|_{2,\omega(\Omega)}^2 := \|v\|_{L^2}^2 + \sup_{x \in \Omega, \rho > 0} \left\{ \rho^{-\omega} \int_{B(x,\rho)} |v(y) - v_{B(x,\rho)}|^2 \, dy \right\}. \]

Sobolev-Campanato space

\[ W^{1,2,\omega}(\Omega) := \{ v \in W^{1,2}(\Omega) : \frac{\partial v}{\partial x_j} \in \mathcal{L}^{2,\omega}(\Omega), \; j = 1, \ldots, N \}, \]

\[ \|v\|_{W^{1,2},\omega(\Omega)}^2 := \|v\|_{L^2}^2 + \sum_{j=1}^N \left\| \frac{\partial v}{\partial x_j} \right\|_{2,\omega(\Omega)}^2. \]

\[ W^{1,2,\omega}_0(\Omega \cup \Gamma_N) := W^{1,2}_0(\Omega \cup \Gamma_N) \cap W^{1,2,\omega}(\Omega) \]

Sobolev-Campanato spaces of functionals

\[ W^{-1,2,\omega}(\Omega \cup \Gamma_N) := \{ F \in W^{-1,2}(\Omega \cup \Gamma_N) : \|F\|_{W^{-1,2,\omega}(\Omega \cup \Gamma_N)} < \infty \}, \]

\[ \|F\|_{W^{-1,2,\omega}(\Omega \cup \Gamma_N)} := \sup \left\{ \rho^{-\omega/2} |\langle F, v \rangle| : v \in W^{1,2}_0(\Omega \cup \Gamma_N), \|v\|_{W^{1,2}(\Omega)} \leq 1, \supp(v) \subset B(x,\rho), \; x \in \Omega, \; \rho > 0 \right\}. \]