Weierstraß-Institut für Angewandte Analysis und Stochastik

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Analysis of Spin-Polarized Drift-Diffusion Models

Spin-resolved drift-diffusion model

consider spin-resolved carriers $e_\uparrow, e_\downarrow, h_\uparrow, h_\downarrow$

spin-resolved densities for electrons and holes

$$n_{\uparrow\downarrow} = \frac{N_c}{2} \exp\left[\frac{-E_{c0} \pm q g_c}{k_B T}\right] \exp\left[\frac{\varphi_{n\uparrow\downarrow} + q\psi}{k_B T}\right]$$

$$p_{\uparrow\downarrow} = \frac{N_v}{2} \exp\left[\frac{E_{v0} \mp q g_v}{k_B T}\right] \exp\left[\frac{-\varphi_{p\uparrow\downarrow} - q\psi}{k_B T}\right]$$

$N_c,\ N_v$	effective densities of state
$E_{c0},\ E_{v0}$	band edge energies
$\varphi_{n\uparrow\downarrow},\ \varphi_{p\uparrow\downarrow}$	spin-resolved quasi-Fermi energies
$q,\ \psi$	elementary charge, electrostatic potential
$g_c,\ g_v$	splitting of carrier bands due to magnetic impurities or an applied magnetic field
$T,\ k_B$	Temperature, Boltzmann constant

spin relaxation reactions

$$e_\uparrow \rightleftharpoons e_\downarrow, \quad h_\uparrow \rightleftharpoons h_\downarrow$$

recombination/generation of electrons and holes

$$e_\uparrow + h_\uparrow \rightleftharpoons 0, \quad e_\uparrow + h_\downarrow \rightleftharpoons 0$$

$$e_\downarrow + h_\uparrow \rightleftharpoons 0, \quad e_\downarrow + h_\downarrow \rightleftharpoons 0$$

Spin-resolved drift-diffusion model

charge current densities

$$j_{n\uparrow\downarrow} = \mu_{n\uparrow\downarrow} n_{\uparrow\downarrow} \nabla \varphi_{n\uparrow\downarrow},$$
$$j_{p\uparrow\downarrow} = \mu_{p\uparrow\downarrow} p_{\uparrow\downarrow} \nabla \varphi_{p\uparrow\downarrow},$$

- system of 4 continuity equations containing spin-relaxation as well as generation-recombination terms
- coupled with a Poisson equation
- completed by boundary 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: $e_\uparrow, e_\downarrow, h_\uparrow, h_\downarrow$	γ_i	charge numbers $\gamma = (-1, -1, 1, 1)$
u_i	densities	$\overline{u}_i$	reference densities
v_i	chemical potentials	v_0	electrostatic potential
		$\zeta_i = v_i + \gamma_i v_0$	electrochemical potentials

state equation for species X_i $\qquad u_i = \overline{u}_i \mathrm{e}^{v_i}$

particle flux densitiy for species X_i

$$J_i = -D_i u_i \nabla \zeta_i = -D_i \big(\overline{u}_i \nabla \frac{u_i}{\overline{u}_i} + u_i \gamma_i \nabla v_0 \big)$$

$-R_i$ net production rate of species X_i

$$R_1 = r_{13}(\mathrm{e}^{v_1+v_3} - 1) + r_{14}(\mathrm{e}^{v_1+v_4} - 1) + r_{12}(\mathrm{e}^{v_1} - \mathrm{e}^{v_2}),$$
$$R_2 = r_{23}(\mathrm{e}^{v_2+v_3} - 1) + r_{24}(\mathrm{e}^{v_2+v_4} - 1) - r_{12}(\mathrm{e}^{v_1} - \mathrm{e}^{v_2}),$$
$$R_3 = r_{13}(\mathrm{e}^{v_1+v_3} - 1) + r_{23}(\mathrm{e}^{v_2+v_3} - 1) + r_{34}(\mathrm{e}^{v_3} - \mathrm{e}^{v_4}),$$
$$R_4 = r_{14}(\mathrm{e}^{v_1+v_4} - 1) + r_{24}(\mathrm{e}^{v_2+v_4} - 1) - r_{34}(\mathrm{e}^{v_3} - \mathrm{e}^{v_4})$$

Model equations

continuity equations

$$\frac{\partial u_i}{\partial t} + \nabla \cdot J_i = -R_i \text{ in } \mathbb{R}_+ \times \Omega,$$

$$\nu \cdot J_i = 0 \text{ on } \mathbb{R}_+ \times \Gamma_N, \quad v_i = v_i^D \text{ on } \mathbb{R}_+ \times \Gamma_D,$$

$$u_i(0) = U_i \text{ in } \Omega, \quad i = 1, \ldots, 4.$$

Poisson equation

$$-\nabla \cdot (\varepsilon \nabla v_0) = f + \sum_{i=1}^{4} \gamma_i u_i \quad \text{in } \mathbb{R}_+ \times \Omega,$$

$$\nu \cdot (\varepsilon v_0) = 0 \quad \text{on } \mathbb{R}_+ \times \Gamma_N, \quad v_0 = v_0^D \text{ on } \mathbb{R}_+ \times \Gamma_D$$

use vectors $v = (v_0, \ldots, v_4), \quad u = (u_0, \ldots, u_4), \quad u_0 = \sum_{i=1}^{4} \gamma_i u_i$

Assumptions

(A1) $\Omega \subset \mathbb{R}^2$ bounded Lipschitzian domain, Γ_D, Γ_N are disjoint open subsets of $\partial\Omega$, $\partial\Omega = \Gamma_D \cup \Gamma_N \cup (\overline{\Gamma_D} \cap \overline{\Gamma_N})$, mes $\Gamma_D > 0$, $\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points ($\Omega \cup \Gamma_N$ is regular in the sense of Gröger);

(A2) $D_i \in L^\infty(\Omega)$, $D_i \geq c > 0$ a.e. on Ω, $i = 1, \dots, 4$;

(A3) $r_{ij} : \Omega \times \mathbb{R} \times \mathbb{R}^4_+ \to \mathbb{R}_+$, $r_{ij}(x, \cdot)$ Lipschitzian uniformly w.r.t. $x \in \Omega$, $r_{ij}(\cdot, y)$ measurable for all $y \in \mathbb{R} \times \mathbb{R}^4_+$, $r_{ij}(\cdot, 0) \in L^\infty(\Omega)$, $ij = 13, 14, 23, 24$, $r_{ij} \in L^\infty_+(\Omega)$, $ij = 12, 34$;

(A4) ε, $\overline{u}_i \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$, $\overline{u}_i \geq \underline{c} > 0$ a.e. on Ω, $i = 1, \dots, 4$, $f \in L^2(\Omega)$, $v_i^D \in W^{1,\infty}(\Omega)$, $i = 0, \dots, 4$, $\gamma = (-1, -1, 1, 1)$;

(A5) $u_i^0 \in L^\infty(\Omega)$, $u_i^0 \geq c > 0$ a.e. on Ω, $i = 1, \dots, 4$, $u_0^0 = \sum_{i=1}^4 \gamma_i u_i^0$.

Weak formulation

$$V = H_0^1(\Omega \cup \Gamma_N)^5,\ U = \{u \in V^* : u_i \in L^2(\Omega),\ \ln u_i \in L^\infty(\Omega),\ i = 1, ..., 4\}$$

define operators $E : V + v^D \to V^*$, $A : U \times (V + v^D) \longrightarrow V^*$

$$\langle Ev, \overline{v} \rangle = \langle E_0 v_0, \overline{v}_0 \rangle + \int_\Omega \sum_{i=1}^{4} \overline{u}_i \mathrm{e}^{v_i} \overline{v}_i \, \mathrm{d}x, \quad \overline{v} \in V,$$

$$\langle E_0 v_0, \overline{v}_0 \rangle = \int_\Omega \left\{ \varepsilon \nabla v_0 \cdot \nabla \overline{v}_0 - f \overline{v}_0 \right\} \mathrm{d}x, \quad \overline{v}_0 \in H_0^1(\Omega \cup \Gamma_N),$$

$$\langle A(u,v), \overline{v} \rangle = \int_\Omega \Big\{ \sum_{i=1}^{4} D_i u_i \nabla \zeta_i \cdot \nabla \overline{\zeta}_i + \sum_{ij=12,34} r_{ij} (\mathrm{e}^{v_i} - \mathrm{e}^{v_j})(\overline{v}_i - \overline{v}_j) + \sum_{ij=13,14,23,24} r_{ij}(\cdot, u)(\mathrm{e}^{v_i + v_j} - 1)(\overline{v}_i + \overline{v}_j) \Big\} \mathrm{d}x, \quad \overline{\zeta}_i = \overline{v}_i + \gamma_i \overline{v}_0.$$

Problem (P):

$$u' + A(u,v) = 0, \quad u = Ev \text{ a.e. on } \mathbb{R}_+, \quad u(0) = u^0,$$
$$u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, V^*), \quad v - v^D \in L^2_{\mathrm{loc}}(\mathbb{R}_+, V) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^5)).$$

Energy functionals

E is a strict monotone potential operator with potential $G : V + v^D \to \mathbb{R}$,

$$G(v) = \int_\Omega \Big\{ \frac{\varepsilon}{2} |\nabla v_0|^2 - \frac{\varepsilon}{2} |\nabla v_0^D|^2 - f(v_0 - v_0^D) + \sum_{i=1}^{4} \overline{u}_i (\mathrm{e}^{v_i} - \mathrm{e}^{v_i^D}) \Big\} \mathrm{d}x.$$

- $\Omega \subset \mathbb{R}^2$, Trudingers imbedding result $\Longrightarrow$ dom $G = V + v^D$
- G is continuous, strictly convex, Gateaux differentiable, subdifferentiable, $\partial G = E$

free energy $F : V^* \to \overline{\mathbb{R}}$,

$$F(u) = G^*(u) = \sup_{w \in V} \Big\{ \langle u, w \rangle - G(w + v^D) \Big\}.$$

- F is proper, lower semicontinuous, convex
- if $u = Ev \Longrightarrow F(u) = \langle u, v - v^D \rangle - G(v),\ v - v^D \in \partial F(u)$
- if $u \in V^*$ and $u_i \in L^2(\Omega)$, $u_i \geq 0$, $i = 1, \dots, 4$, $E_0 v_0 = u_0 \Longrightarrow$

$$F(u) = \int_\Omega \Big\{ \frac{\varepsilon}{2} |\nabla (v_0 - v_0^D)|^2 + \sum_{i=1}^{4} \big\{ u_i (\ln \frac{u_i}{\overline{u}_i} - v_i^D - 1) + \overline{u}_i \mathrm{e}^{v_i^D} \big\} \Big\} \mathrm{d}x.$$

Energy estimates

Theorem. Let (A1) – (A5) be satisfied. Then there exists a $c_1 > 0$ depending only on the data such that

$$F(u(t)) \leq (F(u^0)+1)\mathrm{e}^{c_1 t} \qquad \forall t \in \mathbb{R}_+$$

for any solution (u,v) to (P). If

$$\nabla(v_k^D + \gamma_k v_0^D) = 0,\ k = 1,\dots,4,\ v_i^D = v_j^D,\ ij = 12, 34,\ v_i^D + v_j^D = 0,\ ij = 13, 14, 23, 24,$$

then $F(u(t))$ is bounded and decays monotonously (and exponentially).

Idea of the proof: $v(t) - v^D \in \partial F(u(t))$ a.e. on $\mathbb{R}_+$, Brézis formula $\Longrightarrow$

$$F(u(t)) - F(u(s)) = \int_s^t \langle u'(\tau), v(\tau) - v^D\rangle\,\mathrm{d}\tau = -\int_s^t \langle A(u,v), v(\tau) - v^D\rangle\,\mathrm{d}\tau$$

$$\leq c \int_s^t \sum_{k=1}^4 (\|u_k\|_{L^1} + 1)\Big\{\|\nabla\zeta_k^D\|_{L^\infty}^2 + \sum_{ij=12,34} \|v_i^D - v_j^D\|_{L^\infty} + \sum_{ij=13,14,23,24} \|v_i^D + v_j^D\|_{L^\infty}\Big\}\,\mathrm{d}\tau$$

$s = 0$: since $\|u_k\|_{L^1} \leq F(u) + c$, Gronwalls lemma $\Longrightarrow$ $F(u(t)) \leq (F(u^0) + ct)\,\mathrm{e}^{ct}$

Existence and uniqueness result

Theorem. We assume (A1) – (A5). Then there exists a unique solution to Problem (P).

Guideline for the proof

- regularized problem (P_M) on arbitrarily chosen finite time interval $S = [0, T]$
  regularize state equations, reaction terms (parameter M)
- solvability of (P_M)
  by time discretization, passing to the limit
- a priori estimates
  - ☐ energy estimates (F_M)
  - ☐ Moser techniques to get upper and lower bounds

  independent of M
- solution to (P_M) is a solution to (P) if M is chosen sufficiently large
- uniqueness result

Regularized problem (P_M) on a finite time interval

Problem (P_M):

$$u' + A_M(u,v) = 0, \quad u = E_M v \text{ f.a.a. } t \in S,$$
$$u(0) = u^0, \quad v - v^D \in L^2(S,V), \quad u \in H^1(S,V^*).$$

where

$$\langle E_M v, \overline{v} \rangle = \langle E_0 v_0, \overline{v}_0 \rangle + \int_\Omega \sum_{i=1}^{4} \overline{u}_i \mathrm{e}^{P_M v_i} \overline{v}_i \,\mathrm{d}x, \quad \overline{v} \in V,$$

$$\langle A_M(u,v), \overline{v} \rangle = \int_\Omega \Big\{ \sum_{i=1}^{4} D_i u_i \nabla \zeta_i \cdot \nabla \overline{\zeta}_i + \sum_{ij=12,34} r_{ij} \Big[\big(\mathrm{e}^{P_M v_i} - \frac{u_j}{\overline{u}_j} \big) \overline{v}_i - \big(\frac{u_i}{\overline{u}_i} - \mathrm{e}^{P_M v_j} \big) \overline{v}_j \Big]$$
$$+ \sum_{ij=13,14,23,24} r_{ij}(\cdot, u) \big(\mathrm{e}^{P_{2M}(v_i + v_j)} - 1 \big) (\overline{v}_i + \overline{v}_j) \Big\} \,\mathrm{d}x, \quad \overline{v} \in V,$$

with

$$\zeta_i = v_i + \gamma_i v_0, \quad \overline{\zeta}_i = \overline{v}_i + \gamma_i \overline{v}_0, \quad P_k(y) = \begin{cases} k, & \text{if } y > k \\ y, & \text{if } |y| \le k \\ -k, & \text{if } y < -k \end{cases}$$

Upper and lower bounds

Estimates from above

testing $u' + A_M(u,v) = 0$ (or $u' + A(u,v) = 0$) by

- $$2\,e^{2t}\,(0, z_1, z_2, z_3, z_4), \quad z_i := \big(\frac{u_i}{\overline{u}_i} - K\big)^+$$

where $K \geq \widehat{K} := \max\Big(1, \mathrm{e}^{\max_{i=1,\dots,4}\|v_i^D\|_{L^\infty}}, \max_{i=1,\dots,4}\|\frac{u_i^0}{\overline{u}_i}\|_{L^\infty}\Big)$ suitable chosen

- $$p\,e^{pt}\,(0, z_1^{p-1}, z_2^{p-1}, z_3^{p-1}, z_4^{p-1}), \quad z_i := \big(\frac{u_i}{\overline{u}_i} - \widehat{K}\big)^+, \quad p = 2^n, \quad n \geq 1$$

$+$ Moser iteration

Estimates from below

fix some $i \in \{1,2,3,4\}$, testing by

- $$-p\,e^{pt}\,(0,\dots,0, z^{p-1}\frac{\overline{u}_i}{u_i}, 0,\dots,0), \quad z := \big(\ln\frac{u_i}{\overline{u}_i} + \widetilde{K}\big)^-, \quad p = 2^n, \quad n \geq 1$$

where $\widetilde{K} := \sum_{i=1}^4 \Big(\|\ln\big(\frac{u_i}{\overline{u}_i} + 1\big)\|_{L^\infty(S,L^\infty)} + \|v_i^D\|_{L^\infty}\Big) + \max_{i=1,\dots,4}\|\big(\ln\frac{u_i^0}{\overline{u}_i}\big)^-\|_{L^\infty}$

$+$ Moser iteration

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