Analysis of spin-coherent drift-diffusion model for spin-polarized transport in semiconductors

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Main theses

- The model – *continuity equations* (for electron density components) + *Poisson equation* (for electric potential) – describes electron transport in semiconductor with magnetic properties
- Equations in the system are *strongly coupled*, system is *nonlinear* (coupling of the densities and potential)
- We present analytical results (existence, uniqueness of the solution, its boundedness, monotonicity of the entropy) and numerical results for 1D.

Model

We studied a spin-coherent **matrix** drift-diffusion model derived in the work [1]:

$N \in \mathbb{C}^{2\times 2}$ - electron density,
$J \in \mathbb{C}^{2\times 2}$ - current,
$\Omega \subset \mathbb{R}^3$ - domain,
V - potential.

$$\partial_t N + \mathrm{div} J + i\gamma[N, \vec{m}\cdot\vec{\sigma}] = \frac{1}{\tau}\left(\frac{1}{2}\mathrm{tr}(N)\sigma_0 - N\right), \quad (1)$$

$$J = -DP^{-1/2}(\nabla N + N\nabla V)P^{-1/2}, \quad (2)$$

$$N = \frac{1}{2}n_D\sigma_0 \quad \text{on } \partial\Omega,\ t>0, \qquad N(0) = N^0 \quad \text{in } \Omega. \quad (3)$$

$$-\lambda_D^2 \Delta V = \mathrm{tr}(N) - C(x) \quad \text{in } \Omega, \qquad V = V_D \quad \text{on } \partial\Omega. \quad (4)$$

$\gamma > 0$ - pseudo-exchange field,
$\vec{m} \in \mathbb{R}^3$ - direction of magnetization,
$\tau > 0$ - spin-flip relaxation time,
$D = D(x) > 0$ - space-dependent diffusion coefficient,
$\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ - triple of the Pauli matrices, σ_0 - unit matrix in $\mathbb{C}^{2\times 2}$,
$P = \sigma_0 + p\vec{m}\cdot\vec{\sigma}$, where $p = p(x) \in [0, 1)$.

The model describes evolution of electron *charge* and *spin* densities in *semiconductor* matter under impact of *electric* and *magnetic* fields.

It takes into account *drift* and *diffusion* of electron charge and spin densities, *precession* of spin around magnetic field direction, *relaxation* of spin.

Difficulties: **strong coupling** of the model equations and the **quadratic-type nonlinearity** of the drift term. Due to this there are no analytical results available for systems like this one.

Theory

Reformulation of the problem (1)-(4) in Pauli basis: $N = \frac{1}{2}n_0\sigma_0 + \vec{n}\cdot\vec{\sigma}$, $J = \frac{1}{2}j_0\sigma_0 + \vec{j}\cdot\vec{\sigma}$.
n_0 - electron charge density,
$\vec{n} = (n_1, n_2, n_3)$ - spin-vector density.

$$\partial_t n_0 - \mathrm{div}\left(\frac{D}{\eta^2}(J_0 - 2p\vec{J}\cdot\vec{m})\right) = 0,$$

$$\partial_t n_k - \mathrm{div}\left(\frac{D}{\eta^2}\left(\eta J_k + (1-\eta)(\vec{J}\cdot\vec{m})m_k - \frac{p}{2}J_0 m_k\right)\right) - 2\gamma(\vec{n}\times\vec{m})_k = -\frac{n_k}{\tau},$$

$$k = 1,..3,\ J_0 = \nabla n_0 + n_0\nabla V,\ \vec{J} = \nabla\vec{n} + \vec{n}\nabla V,\ x\in\Omega,\ t>0.$$

Advantage: system of scalar equations

Main analytical result:

Theorem 1 (Existence of bounded weak solutions)**.** *Let $T > 0$, $\Omega \subset \mathbb{R}^3$ - bounded domain : $\partial\Omega \in C^{1,1}$. Let $\lambda_D, \gamma, D > 0$, $0 \le p < 1$, $\vec{m}\in\mathbb{R}^3 : |\vec{m}| = 1$, $C \in L^\infty(\Omega)$,*

$$0 \le n_D \in H^1(\Omega)\cap L^\infty(\Omega), \quad V_D \in W^{2,q_0}(\Omega), \quad q_0 > 3,$$
$$n_0^0,\ \vec{n}^0\cdot\vec{m},\ |\vec{n}^0| \in L^\infty(\Omega), \quad \frac{1}{2}n_0^0 \pm \vec{n}^0\cdot\vec{m} \ge 0.$$

Then $\exists$ a unique solution $(N = \frac{1}{2}n_0\sigma_0 + \vec{n}\cdot\vec{\sigma}, V)$ to (1) - (4) *such that*

$$n_0, n_k \in W^{1,2}(0,T; H_0^1, L^2), \quad V \in L^\infty(0,\infty; W^{2,q_0}(\Omega)), \quad q_0 > 3,$$
$$0 \le n_0 \pm \vec{n}\cdot\vec{m} \in L^\infty(0,\infty; L^\infty(\Omega)), \quad |\vec{n}| \in L^\infty(0,T; L^\infty(\Omega)).$$

The **key idea** of the proof – exploiting of reformulations with different variables:
- in Pauli basis (n_0, n_1, n_2, n_3)
- spin up/down densities: $n_\pm = \frac{1}{2}n_0 \pm \vec{n}\cdot\vec{m}$
- parallel/perpendicular densities: $\vec{n}_\parallel = (\vec{n}\cdot\vec{m})\vec{m}$ and $\vec{n}_\perp = \vec{n} - (\vec{n}\cdot\vec{m})\vec{m}$.

For existence proof we used **Leray-Schauder** Fixed Point Theorem, for boundedness estimates – **Stampacchia** and **Moser-type iteration** methods.

Von-Neumann entropy:

$$H_Q(t) = \int_\Omega \left(\mathrm{tr}[N(\log N - 1) - N_D(\log N_D - 1)] + \frac{\lambda_D^2}{2}|\nabla(V - V_D)|^2\right)dx$$

Proposition 2 (Monotonicity of H_Q)**.** *Let $\log(n_D/2) + V_D = \mathrm{const.}$ in Ω, (N, V) - a smooth solution to* (1)-(4) *: $\frac{1}{2}n_0 > |\vec{n}|$ in Ω, $t \ge 0$. Then $t \mapsto H_Q(t)$ is nonincreasing for $t > 0$.*

This follows from spectral theory and matrix trace properties.

Entropy $H_Q(t)$ of numerical solution converging to the thermal equilibrium state:

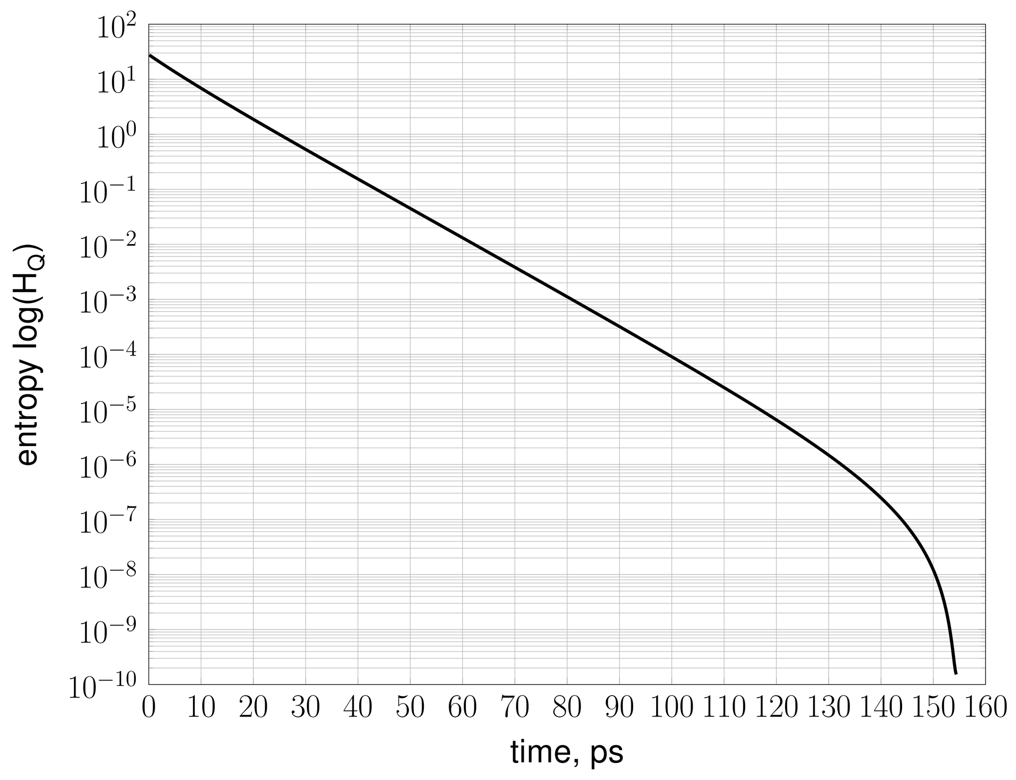

Figure 1: Semilogarithmic plot of the entropy $H_Q(t)$: **exponential decay**

Numerics

We considered 1D problem for 3-layered structure composed of layers of different magnetic and semiconductor properties:

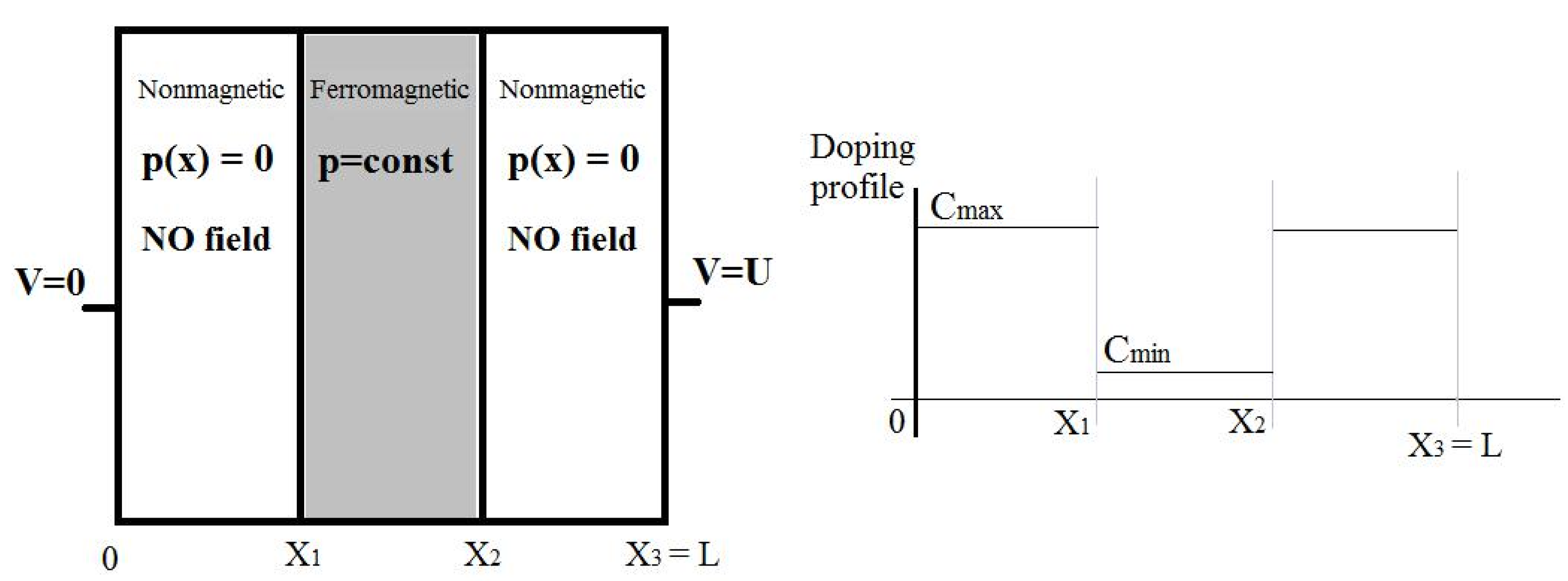

Figure 2: Scheme of the considered problem

This is a "toy problem" which could be considered as a first approximation of *spin transistor*.

Difficulties: **discontinuity** of coefficients due to abrupt change of magnetic properties, **numerical degeneration** of Poisson equation (small λ_D^2), possible instability due to **large** ∇V.

Solution was implemented with finite volumes method, implicit in time; *Gummel iteration scheme* was used for mutual solution of continuity and Poisson equations.

Solution of continuity equations with given (linear) potential was exploited as a *reference solution* as it was already presented in the work [1].

Influence of potential nonlinearity is significant, especially for smaller spin polarization p:

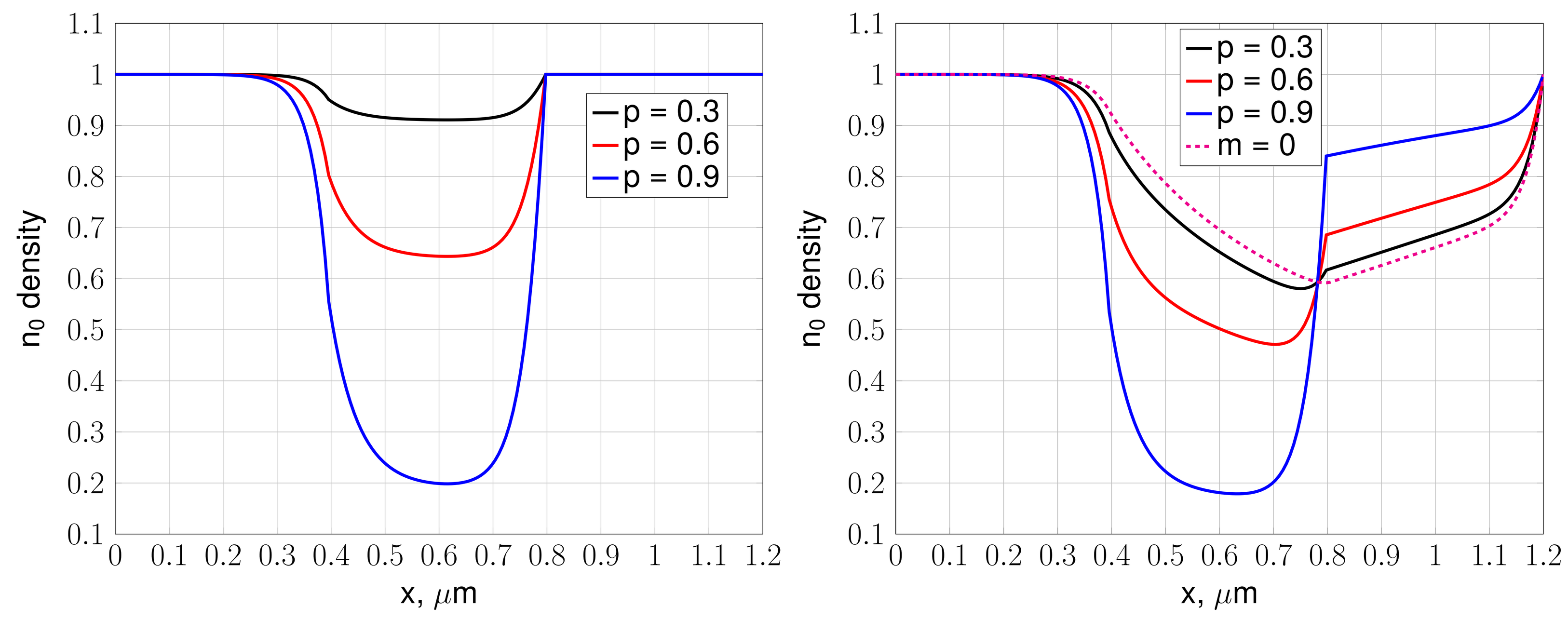

Figure 3: Charge density n_0: solution of continuity equations with given (linear) potential (left), solution of full drift-diffusion-Poisson model (right).

On the contrary solution with Poisson equation for n_3 differs from solution with linear potential only slightly:

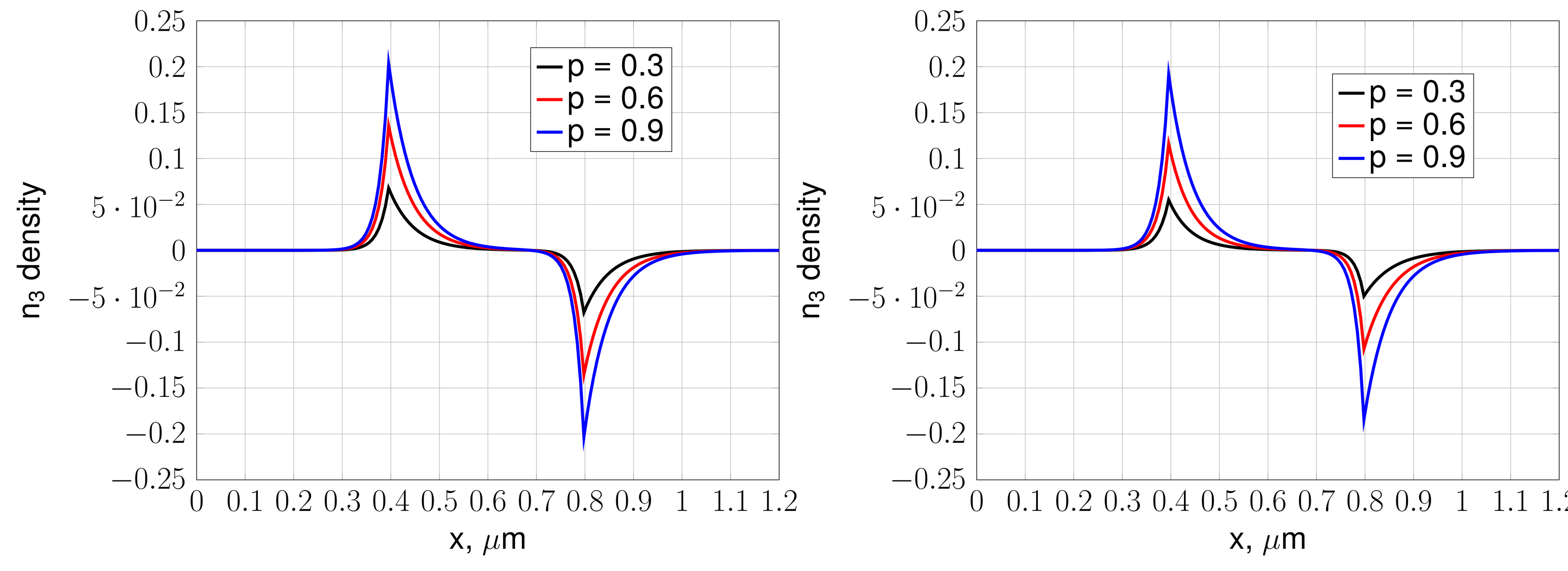

Figure 4: Charge density n_3: solution of continuity equations with given (linear) potential (left), solution of full drift-diffusion-Poisson model (right).

Conclusion: Implemented numerics gives distribution of charge and spin densities, respectively charge and spin currents, but for now only in 1D.

Future work

-Solution in 2D
-Coupling with Landau-Lifschits-Gilbert equation (gives evolution of $\vec{m}$ in time)

References

[1] S. Possanner and C. Negulescu. Diffusion limit of a generalized matrix Boltzmann equation for spin-polarized transport. *Kinetic Related Models* 4 (2011), 1159-1191.