Drift-Diffusion model for spin-polarized electron transport in semiconductors

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Introduction

- **Motivation**: need for future semiconductor devices
- **Idea**: exploit electron spin
- **Main aim**: analyze spin Drift-Diffusion model
- **Starting point**: paper Possanner-Negulescu, 2011

Model

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

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

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

$\gamma > 0$ - 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 $p = p(x) \in [0,1)$.

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

Poisson equation:

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

Main points

$$\begin{cases} \partial_t N + \mathrm{div} J + i\gamma[N, \vec{m}\cdot\vec{\sigma}] = \frac{1}{\tau}\left(\frac{1}{2}\mathrm{tr}(N)\sigma_0 - N\right), & (1) \\ J = -DP^{-1/2}(\nabla N + N\nabla V)P^{-1/2}, \quad (2) & + \textit{Poisson eq}\,(4). \end{cases}$$

Difficulties:

- **Nonlinearity** due to $N\nabla V$
- **Strong coupling** due to matrix-valued variables
- **NO** analytical results: no maximal principle, no regularity theory, no L^∞ estimates

Main ideas and techniques:

- **Different formulations** help for decoupling
- Fixed point theorem, Stampacchia method, Moser-type iteration method

Reformulation I: 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.

$$
\begin{aligned}
&\partial_t n_0 - \operatorname{div}\left(\frac{D}{\eta^2}(J_0 - 2p\vec{J} \cdot \vec{m})\right) = 0, \\
&\partial_t n_k - \operatorname{div}\left(\frac{D}{\eta^2}\left(\eta J_k + (1-\eta)(\vec{J} \cdot \vec{m}) m_k - \frac{p}{2} J_0 m_k\right)\right) \\
&- 2\gamma(\vec{n} \times \vec{m})_k = -\frac{n_k}{\tau}, k = 1, 2, 3, \\
&J_0 = \nabla n_0 + n_0 \nabla V, \vec{J} = \nabla \vec{n} + \vec{n} \nabla V, x \in \Omega, \ t > 0.
\end{aligned}
$$

Boundary and initial conditions:

$$
n_0 = n_D, \vec{n} = 0 \text{ on } \partial\Omega, \ t > 0, \ n_0(0) = n_0^0, \ \vec{n}(0) = \vec{n}^0 \text{ in } \Omega,
$$

Advantage: **system of scalar equations**

Spin-up and spin-down densities formulation

Reformulation II: spin-up / spin-down densities $n_\pm = \frac{1}{2} n_0 \pm \vec{n} \cdot \vec{m}$

$$\partial_t n_+ - \operatorname{div}\big(D(1+p)(\nabla n_+ + n_+ \nabla V)\big) = \frac{1}{2\tau}(n_- - n_+),$$
$$\partial_t n_- - \operatorname{div}\big(D(1-p)(\nabla n_- + n_- \nabla V)\big) = \frac{1}{2\tau}(n_+ - n_-).$$

Boundary and initial conditions:

$$n_+ = n_- = \frac{1}{2} n_D \text{ on } \partial\Omega, \; t > 0, \; n_\pm(0) = \frac{1}{2} n_0^0 \pm \vec{n}^0 \cdot \vec{m} \text{ in } \Omega.$$

Advantage: **decoupling**, helps for boundedness proof

Parallel and perpendicular densities formulation

Reformulation III: parallel / perpendicular densities

$\vec{n}_{\|} = (\vec{n} \cdot \vec{m})\vec{m}$ and $\vec{n}_{\perp} = \vec{n} - (\vec{n} \cdot \vec{m})\vec{m}$:

$$\partial_t \vec{n}_{\|} - \operatorname{div}\left(\frac{D}{\eta^2}\left((\vec{J} \cdot \vec{m})\vec{m} - \frac{p}{2} J_0 \vec{m}\right)\right) = -\frac{\vec{n}_{\|}}{\tau},$$
$$\partial_t \vec{n}_{\perp} - \operatorname{div}\left(\frac{D}{\eta^2}(\nabla \vec{n}_{\perp} + \vec{n}_{\perp} \nabla V)\right) + 2\gamma(\vec{n}_{\perp} \times \vec{m}) = -\frac{\vec{n}_{\perp}}{\tau}.$$

Advantage: **equation for $\vec{n}_{\perp}$ doesn't depend on $\vec{n}_{\|}$**, helps for boundedness proof

Theorem: Existence of bounded weak solutions

$$\begin{cases} \partial_t N + \operatorname{div} J + i\gamma[N, \vec{m}\cdot\vec{\sigma}] = \dfrac{1}{\tau}\left(\dfrac{1}{2}\operatorname{tr}(N)\sigma_0 - N\right), \quad (1) \\ J = -DP^{-1/2}(\nabla N + N\nabla V)P^{-1/2}, \quad (2) \quad + \textit{Poisson eq}\,(4). \end{cases}$$

Theorem

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*

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

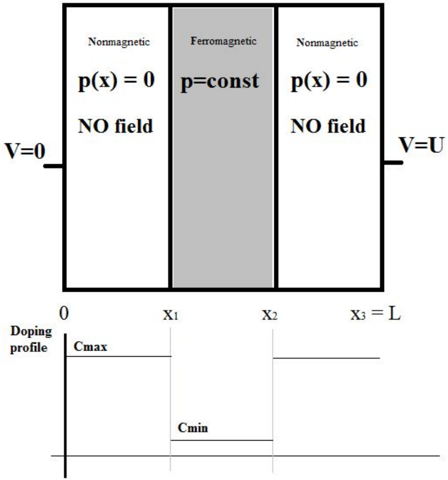
Scheme of the proof

$$\begin{cases} \partial_t n_+ - \operatorname{div}\big(D(1+p)(\nabla n_+ + n_+\nabla V)\big) = \dfrac{1}{2\tau}(n_- - n_+), \\ \partial_t n_- - \operatorname{div}\big(D(1-p)(\nabla n_- + n_-\nabla V)\big) = \dfrac{1}{2\tau}(n_+ - n_-). \end{cases}$$

$$\partial_t \vec{n}_\perp - \operatorname{div}\left(\frac{D}{\eta^2}(\nabla \vec{n}_\perp + \vec{n}_\perp \nabla V)\right) + 2\gamma(\vec{n}_\perp \times \vec{m}) = -\frac{\vec{n}_\perp}{\tau}.$$

- Leray-Schauder for H^1 existence for $(n_0, \vec{n})$
- Boundedness
  1. Stampacchia technique for L^∞ bounds of $n_\pm = \frac{1}{2}n_0 \pm \vec{n}\cdot\vec{m}$ $\Rightarrow n_0,\ \vec{n}\cdot\vec{m} \in L^\infty(0,\infty; L^\infty(\Omega))$
  2. Moser-type iterations (L^q estimates, $q \to \infty$) $\Rightarrow L^\infty$ bound for $\vec{n}_\perp \Rightarrow L^\infty$ bound for $\vec{n} = \vec{n}_\perp + (\vec{n}\cdot\vec{m})\vec{m}$

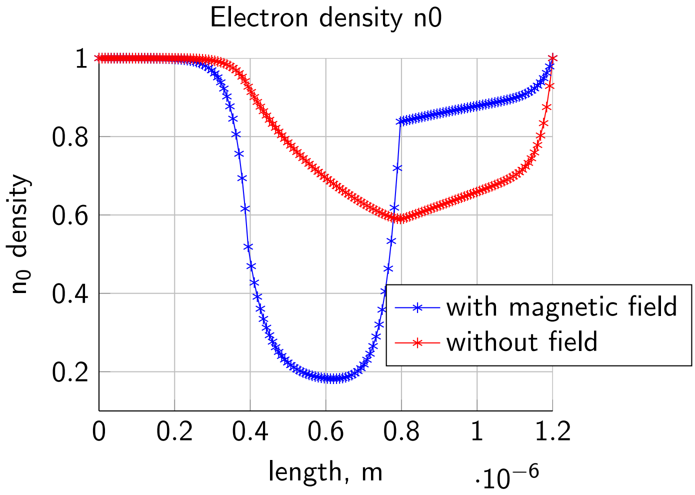
Numerical solution



- Stationary 1D simulation
- Finite Volume Discretization
- Scharfetter-Gummel scheme

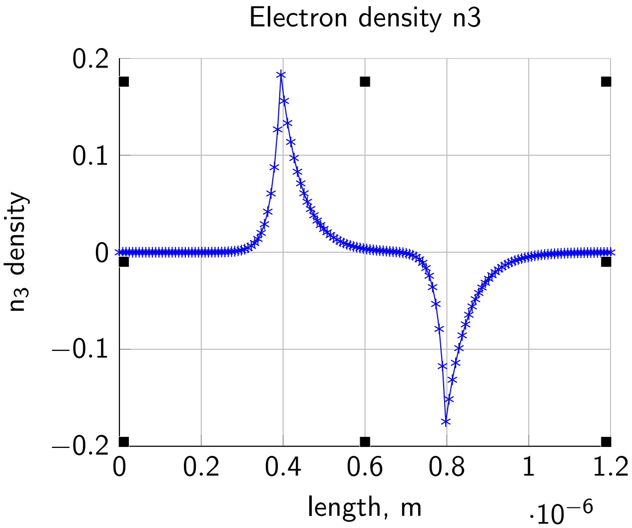
$$\begin{cases} x \in (0, x_1] : \ \vec{m} = 0, p(x) = 0, \\ x \in (x_1, x_2] : \ \vec{m} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, p(x) = p, \\ x \in (x_2, x_3] : \ \vec{m} = 0, p(x) = 0 \end{cases}$$

Results: n_0 density



- Discontinuity of derivative at interfaces
- Influence of magnetic field is stronger with increasing of p (spin polarization)

Results: n_3 density



- Gives distribution of spin vector density
- $n_1 = n_2 = 0$ since $m_1 = m_2 = 0$

Summary

- Matrix drift-diffusion system for spin-coherent transport in semiconductors was investigated: existence, uniqueness and boundedness of the solution is proved
- Numerical solution for multilayered 1D semiconductor device was presented

Outlook

- Analysis for $\vec{m} \neq const$
- 2D simulation

Thank you!