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 numerical 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]:

\[
\begin{align*}
\partial_t n + \text{div}(J_n) &= \frac{1}{\tau} (n N - N) - \gamma n, \quad (1) \\
J - D \nabla N &= \frac{1}{\tau} (\nabla V + N) [n^2] J, \quad (2) \\
\nG (n, m, j) &= \frac{1}{\tau} \left( J_m \cdot (n, j) - n \right), \quad (3) \\
\n\gamma > 0 &= \text{pseudo-exchange field}, \quad (4)
\end{align*}
\]

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

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: \( N = \begin{pmatrix} n_0 + \eta & \eta \end{pmatrix}, \quad J = \begin{pmatrix} j_0 + j & j \end{pmatrix} \). 

1D - spin-up/down densities:

\[
\begin{align*}
\partial_t n + \text{div}(J_n) &= \frac{1}{\tau} (n N - N) - \gamma n, \quad (1) \\
J - D \nabla N &= \frac{1}{\tau} (\nabla V + N) [n^2] J, \quad (2) \\
\nG (n, m, j) &= \frac{1}{\tau} \left( J_m \cdot (n, j) - n \right), \quad (3) \\
\n\gamma > 0 &= \text{pseudo-exchange field}, \quad (4)
\end{align*}
\]

Advantage: system of scalar equations

Main analytical result:

Theorem 1 (Existence of bounded weak solutions). Let \( T > 0, \eta \in \mathbb{R}^3 \), bounded domain: \( \Omega \in \mathbb{R}^3 \). Let \( \eta \), \( D, \gamma, \eta \), \( \nu > 0 \), \( \nu \leq p \), \( \nabla \cdot \eta = 0 \), \( \eta \in \mathbb{R}^3 \), \( \sigma > 0 \), \( \tau > 0 \), \( C \in \mathbb{R}^3 \), \( H \in [0, T] \), \( \Omega \). Then \( \exists \) unique solution \( N = \begin{pmatrix} n_0 + \eta & \eta \end{pmatrix}, \quad J = \begin{pmatrix} j_0 + j & j \end{pmatrix} \) to (1)-(4) such that

\[
\begin{align*}
n_0, n_1 &\in \mathbb{W}^{1,2}(\Omega, H; L^2(\Omega)), \quad J, \nabla \in \mathbb{W}^{1,2}(\Omega, H; L^2(\Omega)), \quad \eta > 0, \\
n_0, \nabla \in \mathbb{W}^{1,2}(\Omega, H; L^2(\Omega)), \quad J, \nabla \in \mathbb{W}^{1,2}(\Omega, H; L^2(\Omega)).
\end{align*}
\]

The key idea of the proof -- exploiting of reformulations with different variables:

- in Pauli basis \( (n_0, n_1, j_0, j) \)

Spin up/down densities: \( n_0 = \frac{1}{2} \left( n + j_0 + j \right) \)

Parallel/perpendicular densities: \( \eta = (n, j) \) and \( \eta = (j_0, j) \).

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

von Neumann entropy:

\[
H_N(g) = \int_\Omega \left[ \frac{1}{2} (N_0 g(N - 1) - N_0) + N_0 g(N - 1) + \frac{1}{2} (V_0 - V_0^0) \right] d\Omega
\]

Proposition 2 (Boundedness of \( H_N \)). Let \( \log(N_0 g(N - 1) + \eta) \) be constant in \( \Omega \). \( N = \begin{pmatrix} n_0 & \eta \end{pmatrix} \) is a smooth solution to (1)-(4): \( \frac{d}{dt} H_N (t) \) is nonincreasing for \( t > 0 \).

This follows from spectral theory and matrix trace properties.

Entropic bound \( H_N(t) \) of numerical solution converging to the thermal equilibrium state:

Future work
- Solution in 2D
- Coupling with Landau-Lifshitz-Gilbert equation (gives evolution of \( n \) in time)

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

Differences: discontinuity of coefficients due to abrupt change of magnetic properties, numerical degeneration of Poisson equation (small \( \lambda_0 \)), possible instability due to large \( \lambda_0 \).

Solution strategy was implemented 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 \( \mu \).

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

References