Manuscript submitted to
AIMS' Journals
Volume **X**, Number **0X**, XX **200X**

Website: http://AIMsciences.org

pp. **X–XX**

# DIFFUSION LIMIT OF A GENERALIZED MATRIX BOLTZMANN EQUATION FOR SPIN-POLARIZED TRANSPORT

In memory of NAOUFEL BEN ABDALLAH,
our extraordinary PhD-advisor

Stefan Possanner

Institute of Theoretical and Computational Physics
Graz University of Technology
Petersgasse 16, 8010 Graz, Austria

Claudia Negulescu

Laboratoire CMI/LATP
Université de Provence
39, rue Joliot Curie, 13453 Marseille Cedex 13, France

(Communicated by the associate editor name)

Abstract. The aim of the present paper is the mathematical study of a linear Boltzmann equation with different matrix collision operators, modelling the spin-polarized, semi-classical electron transport in non-homogeneous ferromagnetic structures. In the collision kernel, the scattering rate is generalized to a hermitian, positive-definite $2 \times 2$ matrix whose eigenvalues stand for the different scattering rates of, for example, spin-up and spin-down electrons in spintronic applications. We identify four possible structures of linear matrix collision operators that yield existence and uniqueness of a weak solution of the Boltzmann equation for a general Hamilton function. We are able to prove positive-(semi)definiteness of a solution for an operator that features an anti-symmetric structure of the gain respectively the loss term with respect to the occurring matrix products. Furthermore, in order to obtain matrix drift-diffusion equations, we perform the diffusion limit with one of the symmetric operators assuming parabolic spin bands with uniform band gap and in the case that the precession frequency of the spin distribution vector around the exchange field of the Hamiltonian scales with order $\varepsilon^2$. Numerical simulations of the here obtained macroscopic model were carried out in non-magnetic/ferromagnetic multilayer structures and for a magnetic Bloch domain wall. The results show that our model can be used to improve the understanding of spin-polarized transport in spintronics applications.

2000 *Mathematics Subject Classification.* Primary: 76P99, 76R50; Secondary: 81R25.
*Key words and phrases.* Spintronics, kinetic matrix models, spin transport, spin-charge coupling.
.

1. **Introduction.** The coupling between the spin- and the charge degree of freedom of an electron system is a growing research topic in physics and mathematics. What is simply called 'spintronics' (spin-electronics) has become a vast field with many promising applications and plenty of challenging problems to be solved. The field includes, for example, quantum computing [20, 37] (qubits), spin-dependent transport in ferromagnets [14] (giant magneto-resistance effect or GMR effect), semiconductor spintronics [42, 13] (spin field-effect transistors, magnetic resonant tunneling diodes) and spin-transfer torques in ferromagnets [31, 19, 4] (current-induced magnetic switching and domain wall motion). The benefits of spintronics lie in the fact that the magnetic state of a system can be changed by manipulating charges with electric fields, which can be handled rather easily and more precisely as compared to magnetic fields. In most of the spintronic applications, spin-polarized electron transport in solids plays a crucial role. By spin-polarized transport we mean that, in addition to the charge distribution of an electron system, it is necessary to keep track of its spin distribution to obtain a correct description. Magnetic impurities, a ferromagnetic environment, strong spin-orbit coupling [9, 12] or an applied magnetic field often require the spin-polarized treatment of transport in these systems.

The spin of an electron represents a two-state quantum system [1]. This means that once a direction is chosen in real space, the electron spin can be determined to be either parallel (spin-up) or anti-parallel (spin-down) to that direction. Prior to the measurement, a general spin state (or spin-coherent state) is a quantum superposition of the spin-up and spin-down basis states. The density matrix of a spin-coherent state is a hermitian $2 \times 2$ matrix, where the spin-coherence is represented by non-vanishing off-diagonal elements. From a mathematical point of view, spin systems resemble electron-hole systems in Graphene [23]. For such systems, there exist various matrix transport models on the microscopic (von Neumann and Wigner equation), the kinetic (Boltzmann equation [29, 40, 24, 2]) and the macroscopic level (drift-diffusion and fluiddynamic equations [41, 28, 2, 39], quantum drift-diffusion and quantum fluiddynamic equations [21, 3]). For the purpose of engineering spintronic devices, macroscopic models are very appealing. On the one hand, they enable efficient numerical simulations on the desired length scale ($10^1 - 10^3\,\mathrm{nm}$) and, on the other hand, they incorporate the scattering of electrons from phonons (non-zero temperature) and impurities (material imperfections). However, spin-coherent drift-diffusion models occurring in literature are still mostly heuristic. Recently, El Hajj and Ben Abdallah [10] introduced a spin-coherent collision operator in the linear BGK approximation to obtain a matrix Boltzmann equation. They performed rigorous diffusion limits in various scalings to derive a number of matrix drift-diffusion models. The rigorous derivation of a spin-coherent collision operator from the microscopic scale is still an open problem.

In this work we address, at first, the kinetic level of spin-coherent transport. Our goal is to set up a matrix Boltzmann equation that incorporates spin-dependent scattering rates, or more precisely, that features a collision kernel with matrix-valued transition probabilities from momentum $\hbar k$ to $\hbar k'$. Such a kinetic equation can be viewed as a generalization of the model in [10] to spin-dependent mean-free paths. In [10], the scattering rates were scalar quantities (which yield one mean free path for both spin species) whereas in our case they are fully occupied hermitian, positive-definite $2 \times 2$ matrices. The eigenvalues of these matrices stand for the

different scattering rates of spin-up and spin-down electrons (yielding two distinct respective mean free paths). The observation of spin-dependent electron resistances in ferromagnets [8, 15] was crucial for triggering the research on spintronics, therefore the generalization of scalar scattering rates to matrix-valued scattering rates is a logical step. The main problem, as compared to the scalar case, is to deal with the matrix products that will occur in the newly defined collision operator.

The effects of spin-dependent mean free paths on non-coherent spin-polarized transport (two-component models) have been studied comprehensively [18, 34, 17, 33, 38, 35]. However, to our knowledge, there exist no works on the consequences of spin-dependent scattering for spin-coherent electron systems. Our approach is to add, on the right-hand-side of the spin-coherent Vlasov equation, the four most simple types of linear matrix collision operators which preserve the hermiticity of the electron distribution matrix. We then apply the method of characteristics and a fixed point argument to check existence and uniqueness of a weak solution of the respective matrix Boltzmann equation. Additionally, using the maximum principle, we check the positive-(semi)definiteness of the solution. We identify one collision operator that satisfies the maximum principle. This operator features an anti-symmetric structure with respect to the matrix products in the gain and the loss term, respectively. The anti-symmetric collision operator is mass- but not spin-conserving. In the subsequent sections of the paper, we focus on a mass- and spin-conserving collision operator, which has a symmetric structure of the gain respectively the loss term. In contrast to the anti-symmetric operator, the symmetric collision operator describes only spin-conserving momentum scattering, no spin-flip processes. The spin-flip scattering is then described by a second collision operator. This strategy permits to treat spin-conserving respectively spin-flip scattering on different timescales. However, the verification of the maximum principle for this two-operator approach remains an open problem.

In the second part of this paper we perform the diffusion limit in a scaled form of the matrix Boltzmann equation, using standard techniques [25] known from the scalar case. The necessary physical assumptions for this step are Boltzmann statistics and local thermal equilibrium (detailed balance) in each spin band. Additionally, we make the strong assumption of parabolic spin bands with uniform band gap, a model that is known in spintronic literature as the Stoner model [16, 22]. Relaxing this assumption should clearly be the topic of following works. However, even in the simple setting of the Stoner model, we obtain, in the macroscopic limit, a matrix drift-diffusion model that features a coupling between the charge- and the spin degree of freedom. The coupling we get is linear in the polarization $p$ of the scattering rates ($0 \leq p < 1$).

The third part of this work contains some numerical studies of the derived spin-coherent drift-diffusion model in one-dimensional multilayer structures and for strongly varying magnetization on the scale of several nanometers (e.g. a magnetic domain wall). We use a standard Crank-Nicolson finite difference scheme to solve the four coupled drift-diffusion equations on a uniform grid. The results show that our model provides a new means for studying spin-polarized transport in arbitrary magnetic structures (e.g. non-collinear multilayers or strongly varying magnetization).

2. **Some notations and Lemmas.** As a help for the better understanding of this work, we start by introducing some relevant notations.

**Definition 2.1** (**Pauli matrices**). By $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ we denote the triple of the three Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

To be consistent, the $2 \times 2$ unit matrix is denoted by

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2}$$

The Pauli matrices satisfy the following properties, for $k, l, m \in \{1, 2, 3\}$,

$$[\sigma_k, \sigma_l] = 2i \sum_m \varepsilon_{klm} \sigma_m \tag{3}$$

$$[\sigma_k, \sigma_l]_+ = 2\delta_{kl} \sigma_0 \tag{4}$$

$$\sigma_k \sigma_l = \delta_{kl} \sigma_0 + i \sum_m \varepsilon_{klm} \sigma_m. \tag{5}$$

Here, $[\sigma_k, \sigma_l] = \sigma_k \sigma_l - \sigma_l \sigma_k$ stands for the commutator of $\sigma_k$ and $\sigma_l$, $[\sigma_k, \sigma_l]_+ = \sigma_k \sigma_l + \sigma_l \sigma_k$ denotes the anti-commutator, $\delta_{km}$ the Kronecker delta, $\varepsilon_{klm}$ the Levi-Civita symbol, defined by

$$\varepsilon_{klm} = \begin{vmatrix} \delta_{k1} & \delta_{k2} & \delta_{k3} \\ \delta_{l1} & \delta_{l2} & \delta_{l3} \\ \delta_{m1} & \delta_{m2} & \delta_{m3} \end{vmatrix}. \tag{6}$$

From (3) one deduces, for $\vec{a}, \vec{b} \in \mathbb{R}^3$,

$$(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = (\vec{a} \cdot \vec{b}) \sigma_0 + i(\vec{a} \times \vec{b}) \cdot \vec{\sigma} \tag{7}$$

$$[\vec{a} \cdot \vec{\sigma}, \vec{b} \cdot \vec{\sigma}] = 2i(\vec{a} \times \vec{b}) \cdot \vec{\sigma}. \tag{8}$$

**Definition 2.2** (**Matrix spaces**). Let $\mathcal{H}_2(\mathbb{C})$ denote the vector space of hermitian $2 \times 2$ matrices. Associated with the Frobenius scalar product $\langle \cdot, \cdot \rangle_2$ and the corresponding norm $|| \cdot ||_2$,

$$\langle A, B \rangle_2 := \mathrm{tr}\,(AB), \qquad ||A||_2 := \sqrt{\mathrm{tr}\,(A^2)} \qquad \forall A, B \in \mathcal{H}_2(\mathbb{C}), \tag{9}$$

the vector space $\mathcal{H}_2(\mathbb{C})$ becomes a Hilbert space, where $A = (a_{ij})$ and $B = (b_{ij})$ with $i, j \in \{1, 2\}$ and

$$\mathrm{tr}\,(AB) = \sum_{ij} a_{ij} b_{ji} \tag{10}$$

denotes the trace of $AB$. By $\mathcal{H}_2^{0,+}(\mathbb{C})$ we denote the subspace of $\mathcal{H}_2(\mathbb{C})$ containing positive semi-definite matrices and by $\mathcal{H}_2^{+}(\mathbb{C})$ we identify the subspace of positive definite matrices.

The space $\mathcal{H}_2(\mathbb{C})$ is spanned by the four matrices $\sigma_0$, $\sigma_1$, $\sigma_2$ and $\sigma_3$. In this basis, the coefficients of a matrix $A \in \mathcal{H}_2(\mathbb{C})$ are denoted by $a_0 \in \mathbb{R}$, $\vec{a} = (a_1, a_2, a_3) \in \mathbb{R}^3$. We have the following isomorphism between $\mathcal{H}_2(\mathbb{C})$ and $\mathbb{R}^4$,

$$A = a_0 \sigma_0 + \vec{a} \cdot \vec{\sigma} \ \in \mathcal{H}_2(\mathbb{C}) \quad \Longleftrightarrow \quad \tilde{A} = (a_0, \vec{a}) \ \in \mathbb{R}^4. \tag{11}$$

The coefficients of $A$ in this Pauli basis are computed as follows,

$$a_0 = \frac{1}{2}\mathrm{tr}\,(A) \qquad ; \qquad \vec{a} = \frac{1}{2}\mathrm{tr}\,(\vec{\sigma}A)\,. \tag{12}$$

In the following, we call the space $\mathbb{R}^3$ of the coefficient vectors $\vec{a}$ of a matrix $A \in \mathcal{H}_2(\mathbb{C})$ in the Pauli basis the *spin space*. Only vectors in spin space are written with the overlined arrow symbol. The eigenvalues of $A \in \mathcal{H}_2(\mathbb{C})$ are given by $a_+ = a_0 + |\vec{a}|$ and $a_- = a_0 - |\vec{a}|$, respectively.

**Lemma 2.3.** *Let $A \in \mathcal{H}_2^+(\mathbb{C})$ with components $(a_0, \vec{a})$ in the Pauli basis, then*

$$A^{1/2} = \frac{1}{2}\left(\sqrt{a_0+|\vec{a}|} + \sqrt{a_0-|\vec{a}|}\right)\sigma_0 + \frac{1}{2}\left(\sqrt{a_0+|\vec{a}|} - \sqrt{a_0-|\vec{a}|}\right)\frac{\vec{a}}{|\vec{a}|}\cdot\vec{\sigma}. \tag{13}$$

**Lemma 2.4.** *Let $A, B \in \mathcal{H}_2(\mathbb{C})$. Then we have $AB + BA \in \mathcal{H}_2(\mathbb{C})$ and $ABA \in \mathcal{H}_2(\mathbb{C})$. Moreover, in the Pauli basis,*

$$\frac{1}{2}AB + \frac{1}{2}BA = (a_0 b_0 + \vec{a}\cdot\vec{b})\sigma_0 + (a_0\vec{b} + b_0\vec{a})\cdot\vec{\sigma}$$

*and*

$$\begin{aligned} A^{1/2}BA^{1/2} = {} & (a_0 b_0 + \vec{a}\cdot\vec{b})\sigma_0 + \\ & + \left[b_0\vec{a} + \left(a_0 - \sqrt{a_0^2 - |\vec{a}|^2}\right)\left(\vec{b}\cdot\frac{\vec{a}}{|\vec{a}|}\right)\frac{\vec{a}}{|\vec{a}|} + \vec{b}\sqrt{a_0^2-|\vec{a}|^2}\right]\cdot\vec{\sigma}. \end{aligned}$$

**Lemma 2.5.** *For $A, B \in \mathcal{H}_2^{0,+}(\mathbb{C})$ we have $ABA \in \mathcal{H}_2^{0,+}(\mathbb{C})$. However, $AB + BA$ is not necessarily in $\mathcal{H}_2^{0,+}(\mathbb{C})$.*

**Lemma 2.6 (Trace properties).** *We have*

$$\mathrm{tr}\,(AB) \geq 0 \quad \forall A, B \in \mathcal{H}_2^{0,+}(\mathbb{C}) \tag{14}$$

$$\mathrm{tr}\left(A^2 + B^2\right) \geq 2\,|\mathrm{tr}\,(AB)| \quad \forall A, B \in \mathcal{H}_2(\mathbb{C}) \tag{15}$$

$$0 \leq \mathrm{tr}\left((AB)^2\right) \leq \mathrm{tr}\left(A^2B^2\right) \leq 2\mathrm{tr}\left(A^2\right)\mathrm{tr}\left(B^2\right) \quad \forall A \in \mathcal{H}_2(\mathbb{C}), B \in \mathcal{H}_2^{0,+}(\mathbb{C}). \tag{16}$$

*Proof.* Relation (15) follows from

$$\begin{aligned} 0 \leq \mathrm{tr}\left((A+B)^2\right) = \mathrm{tr}\left(A^2 + 2AB + B^2\right) \quad &\Longrightarrow \quad \mathrm{tr}\left(A^2+B^2\right) \geq -2\mathrm{tr}\,(AB) \\ 0 \leq \mathrm{tr}\left((A-B)^2\right) = \mathrm{tr}\left(A^2 - 2AB + B^2\right) \quad &\Longrightarrow \quad \mathrm{tr}\left(A^2+B^2\right) \geq 2\mathrm{tr}\,(AB)\,. \end{aligned}$$

To prove (16), let $A = (a_{ij})$ and $B = (b_{ij})$, then $\bar{a}_{ij}$ stands for the complex conjugate of $a_{ij}$. Further, let $\theta$ be a unitary matrix, $\theta\bar{\theta}^t = \sigma_0$, such that $\bar{\theta}^t B\theta$ is diagonal. One has

$$\mathrm{tr}\left((AB)^2\right) = \mathrm{tr}\left((\theta\bar{\theta}^t A\theta\bar{\theta}^t B)^2\right) = \mathrm{tr}\left(\bar{\theta}^t A\theta\bar{\theta}^t B\theta\bar{\theta}^t A\theta\bar{\theta}^t B\theta\right) = \mathrm{tr}\left((A'B'_D)^2\right).$$

Here, $A' = \bar{\theta}^t A\theta = (a'_{ij})$ with $(a'_{ii}) \in \mathbb{R}$, and $B'_D$ is a diagonal matrix with eigenvalues $(b'_{ii}) \in \mathbb{R}^+$. We obtain

$$\mathrm{tr}\left((AB)^2\right) = \mathrm{tr}\left((A'B'_D)^2\right) = \sum_{ik} a'_{ik}b'_{kk}a'_{ki}b'_{ii} = \sum_{ik}|a'_{ik}|^2 b'_{kk}b'_{ii} \geq 0, \tag{17}$$

which gives the first inequality in (16). The second inequality follows from

$$\mathrm{tr}\left((A'B'_D)^2\right) = \sum_{ik}|a'_{ik}|^2 b'_{kk}b'_{ii} \leq \sum_{ik}|a'_{ik}|^2 b'^2_{ii} = \mathrm{tr}\left(A'^2 B'^2_D\right) \tag{18}$$

The third inequality in (16) follows from the fact that $A^2$ and $B^2$ are positive hermitian matrices. □

## 3. Preliminaries.

3.1. **Spin-coherent semiclassical electrons.** The state of a spin-coherent semiclassical electron system is characterized by the *distribution matrix* $F : \mathbb{R}^+ \times \mathbb{R}^d_x \times \mathbb{R}^d_k \to \mathcal{H}_2^{0,+}(\mathbb{C})$. Here, $t$ denotes the time and $x$ and $k$ are the respective variables for position and momentum (more precisely, $k$ stands for an electron's wave vector and $\hbar k$ for its crystal momentum). The phase space of the electron system is $\mathbb{R}^d_x \times \mathbb{R}^d_k = \mathbb{R}^{2d}$ where $d$ is the number of space dimensions. In the Pauli basis the distribution matrix is written as $F = (\frac{1}{2} f_0, \vec{f})$. The coefficient $f_0(t,x,k) = \mathrm{tr}\,(F)$ is the scalar distribution function of the electrons ignoring the spin. The vector $\vec{f}(t,x,k) = \frac{1}{2}\mathrm{tr}\,(\vec{\sigma} F)$ represents the vector spin polarization of the electron system and $\hbar\vec{f}$ is the electron spin density at $(t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}$. The two eigenvalues of $F$, denoted by $f_\pm = \frac{1}{2} f_0 \pm |\vec{f}|$, stand for the distribution functions of electrons with spin in the direction $+\vec{f}/|\vec{f}|$ and in the direction $-\vec{f}/|\vec{f}|$, respectively. These directions, determined by the distribution matrix itself, define the $z$-axis of a coordinate system in spin space in which $F$ is diagonal. This coordinate frame defined by $\vec{f}/|\vec{f}|$ depends on $(t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}$. Since it is our purpose to describe the spin-coherence of electrons with respect to a given field $\vec{\Omega}(t,x,k)$ in spin space, it is preferrable to work in a coordinate frame independent of $(t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}$ and to keep track of the direction $\vec{f}/|\vec{f}|$ therein.

The energy density of the system in the state $F$ is computed from the *Hamilton matrix* $H : \mathbb{R}^+ \times \mathbb{R}^{2d} \to \mathcal{H}_2(\mathbb{C})$. We write this matrix as $H = H_b + H_{so}$, where $H_b$ is called the *band matrix* and $H_{so}$ denotes the *spin-orbit matrix*, given by

$$H_b(t,x,k) = h_0(t,x,k)\sigma_0 + \lambda(t,x,k)\vec{\Omega}(t,x)\cdot\vec{\sigma} \tag{19}$$

$$H_{so}(t,x,k) = \vec{h}_{so}(t,x,k)\cdot\vec{\sigma}. \tag{20}$$

Here, $h_0 : \mathbb{R}^+ \times \mathbb{R}^{2d} \to \mathbb{R}$, $\lambda : \mathbb{R}^+ \times \mathbb{R}^{2d} \to \mathbb{R}$, $\vec{\Omega} : \mathbb{R}^+ \times \mathbb{R}^{2d} \to S^2$ (the unit sphere in $\mathbb{R}^3$) and $\vec{h}_{so} : \mathbb{R}^+ \times \mathbb{R}^{2d} \to \mathbb{R}^3$. The eigenvalues of $H_b$ read $h_{b,\uparrow} = h_0 + |\lambda|$ and $h_{b,\downarrow} = h_0 - |\lambda|$. For fixed $t$ and $x$, they represent the two different transport bands eligible for spin-coherent electrons. We refer to the band $h_{b,\uparrow}$ as the *up-band* and to $h_{b,\downarrow}$ as the *down-band*, respectively. The band gap is given by $2|\lambda|$. The unit vector $\vec{\Omega}$ shall play the role of the local direction of magnetization in a ferromagnet, therefore it depends on $t$ and $x$ but not on the momentum $k$ of the electrons. The distribution functions $f_\uparrow$ and $f_\downarrow$ in the up- and in the down-band are given by the orthogonal projection $\Pi_{\uparrow/\downarrow} : \mathcal{H}_2(\mathbb{C}) \to \mathbb{R}$ of $F$ on the eigenspace associated to the respective eigenvalue of $H_b$,

$$f_\uparrow = \Pi_\uparrow(F) = \left\langle \frac{1}{2}(\sigma_0 + \vec{\Omega}\cdot\vec{\sigma}), F \right\rangle_2 = \frac{1}{2} f_0 + \vec{\Omega}\cdot\vec{f} \tag{21}$$

$$f_\downarrow = \Pi_\downarrow(F) = \left\langle \frac{1}{2}(\sigma_0 - \vec{\Omega}\cdot\vec{\sigma}), F \right\rangle_2 = \frac{1}{2} f_0 - \vec{\Omega}\cdot\vec{f}. \tag{22}$$

A possible absence of spin-coherence is reflected by

$$\pm\,\vec{f} \parallel \vec{\Omega} \quad \Longleftrightarrow \quad [F, H_b] = 0. \tag{23}$$

In this case, the equations (21) and (22) yield $f_\uparrow = \frac{1}{2} f_0 \pm |\vec{f}|$ and $f_\downarrow = \frac{1}{2} f_0 \mp |\vec{f}|$ where $|\vec{f}|$ is the usual scalar spin polarization in two-component models.

The matrix $H_{so}$ stands for contributions to the electron energy arising from the spin-orbit coupling that electrons experience when moving through a crystal lattice.

The field $\vec{h}_{so}$ may, for example, contain terms like the Elliott-Yafet, the D'yakonov-Perel' or the Rashba spin-orbit couplings [42]. The separation of $H$ into $H_b$ and $H_{so}$ was made in order to single out the field $\vec{\Omega}$, which plays a central role in the theory developed in this work. The total Hamilton matrix reads

$$H = H_b + H_{so} = h_0\sigma_0 + \vec{h}\cdot\vec{\sigma}, \tag{24}$$

where $\vec{h} = (\lambda\vec{\Omega} + \vec{h}_{so})$ is called the *pseudo-exchange field*.

Given a distribution matrix $F$, the energy $E : \mathbb{R}^+ \times \mathbb{R}^{2d} \to \mathbb{R}$ of the system at $(t, x, k)$ is obtained by

$$E(t,x,k) = \langle H, F\rangle_2 = h_0(t,x,k)f_0(t,x,k) + 2\vec{h}(t,x,k)\cdot\vec{f}(t,x,k). \tag{25}$$

The ballistic dynamics of the spin-coherent semi-classical electron system is described by the matrix Vlasov equation [11, 26],

$$\begin{cases} \partial_t F + \dfrac{1}{\hbar}\left(\nabla_k h_0\cdot\nabla_x F - \nabla_x h_0\cdot\nabla_k F\right) + \dfrac{i}{\hbar}[F, \vec{h}\cdot\vec{\sigma}] = 0 \\ F(t=0,x,k) = F_{in}(x,k) \\ F_{in}(x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C}) \qquad \forall (x,k). \end{cases} \tag{26}$$

The commutator $[F, \vec{h}\cdot\vec{\sigma}]$ describes the precession of the spin polarization $\vec{f}$ of the electron system around the pseudo-exchange field $\vec{h}$. Equation (26) is obtained by passing to the limit $\varepsilon \to 0$ (where $\varepsilon$ stands for the scaled Planck constant $\hbar$) in the Schrödinger equation with the Hamiltonian (24), for the case where the modulus $|\vec{h}|$ of the pseudo-exchange field scales with order $\varepsilon$.[1] Thus, equation (26) is merely the correct semi-classical equation for electrons in a weak exchange field $\vec{h}$. This is the case, for example, if the band gap $\lambda$ is small compared to the Fermi energy of the electron system. To take into account scattering processes (non-ballistic transport), we shall add collision terms at the right-hand-side of the matrix Vlasov equation (26).

3.2. **Spin-coherent collision operators.** For a spin-polarized electron system, there are two kinds of possible collision processes, namely the spin-conserving and the spin-flip collisions. Spin-conserving collisions drive the velocity distribution of the electrons towards thermal equilibrium, i.e., the Fermi-Dirac or the Maxwellian distribution, depending on the used statistics. On the other hand, spin-flip collisions will relax the electron spin density towards its thermal equilibrium field, which is, at each point $x \in \mathbb{R}^d_x$, parallel to the local pseudo-exchange field $\vec{h}$ defined in (24). In ferromagnets, the two processes happen at very different timescales [41], spin-conserving collisions occurring at a much higher frequency than spin-flip collisions.

In the present paper, we shall write seperate collision operators for each of the two processes. Spin-flip processes will be modeled by a relaxation term [10],

$$\frac{1}{\tau_{sf}}Q_{sf}(F) := \frac{1}{\tau_{sf}}\left(\frac{1}{2}\mathrm{tr}\,(F)\,\sigma_0 - F\right), \tag{27}$$

where $\tau_{sf} \in \mathbb{R}^+$ is the average time between two subsequent spin-flip collisions. The focus of this work is on spin-conserving momentum scattering of electrons with (magnetic) impurities. The essential point is that impurity potentials may look different for spin-up and spin-down electrons and that, additionally, the latter feature

[1] The fact that $\hbar$ still appears in (26) is due to rescaling to physical variables after the limiting procedure.

different density of states in spin-polarized materials [36]. Both effects lead to spin-dependent momentum scattering rates. Our goal is to construct a collision operator that, on the one hand, describes the impurity scattering of spin-coherent electrons and, on the other hand, takes into account spin-dependent collision rates. Moreover, the new *spin-coherent collision operator* must satisfy the necessary mathematical properties to yield a well-defined theory. We state four requirements on such an operator:

1. incorporate spin-dependent scattering rates,
2. yield a two-component Boltzmann model if
$$[F(t,x,k), H_b(t,x,k)] = 0 \qquad \forall (t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d},$$
3. be a map with range in $\mathcal{H}_2(\mathbb{C})$,
4. conserve the positive-(semi)definiteness of $F$,

$$F(t=0,x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C}) \quad \Longrightarrow \quad F(t,x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C}) \quad \forall (t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}.$$

Let $S : \mathbb{R}^+ \times \mathbb{R}^{3d} \to \mathcal{H}_2^+(\mathbb{C})$ denote the *scattering matrix*, in the Pauli basis written as

$$S(t,x,k,k') = s_0(t,x,k,k')\sigma_0 + \vec{s}(t,x,k,k') \cdot \vec{\sigma}. \tag{28}$$

This matrix shall describe the rate at which spin-coherent electrons scatter from $k$ to $k'$ due to collisions with (magnetic) impurities. The eigenvalues of $S$, denoted by $s_\uparrow$ and $s_\downarrow$, shall stand for the respective (scaled) scattering rates of electrons in the up-band and in the down-band. An electron distribution $F$ consists only of non-coherent spin-up and spin-down states if it commutes with the band matrix $H_b$, c.f. (23). In this case, the eigenvalues of $F$ should scatter at the rates $s_\uparrow$ and $s_\downarrow$, respectively. Therefore, it is necessary that

$$[S(t,x,k,k'), H_b(t,x,k)] = 0 \qquad \forall (t,x,k,k') \in \mathbb{R}^+ \times \mathbb{R}^{3d}. \tag{29}$$

We construct a linear spin-coherent collision operator $Q_{ij}(F)$ as a sum of a gain term $Q_i^+(F)$ and a loss term $Q_j^-(F)$,

$$\frac{1}{\tau_c} Q_{ij}(F) := \frac{1}{\tau_c} Q_i^+(F) - \frac{1}{\tau_c} Q_j^-(F) \qquad i,j \in \{1,2\}, \tag{30}$$

where we defined $\tau_c \in \mathbb{R}^+$, the time between two subsequent spin-conserving collision processes. The two basic possible structures of the gain and loss term, respectively, read

$$Q_1^+(F) := \int_{\mathbb{R}^d_{k'}} \left( \frac{1}{2} S' F' + \frac{1}{2} F' S' \right) \mathrm{d}k' \tag{31}$$

$$Q_2^+(F) := \int_{\mathbb{R}^d_{k'}} S'^{1/2} F' S'^{1/2} \mathrm{d}k', \tag{32}$$

$$Q_1^-(F) := \frac{1}{2} \Lambda F + \frac{1}{2} F \Lambda \tag{33}$$

$$Q_2^-(F) := \int_{\mathbb{R}^d_{k'}} S^{1/2} F S^{1/2} \mathrm{d}k', \tag{34}$$

where we denoted $F' = F(t,x,k')$, $S' = S(t,x,k',k)$, and $\Lambda = \int S \mathrm{d}k'$. The gain and loss terms are chosen such that they conserve the hermiticity of the electron distribution function $F$. We stress that, according to (30), there are four possible

spin-coherent collision operators that fall into two categories, namely the symmetric operators $Q_{11}$ respectively $Q_{22}$, and the anti-symmetric operators $Q_{12}$ respectively $Q_{21}$. At first the different structures of gain and loss term in the anti-symmetric operators may seem counter-intuitive or unphysical. However, in the theory of open quantum systems [7], the well-known Lindblad equation features a product structure similar to the operator $Q_{21}$.

It is easily seen that the symmetric operators $Q_{11}$ and $Q_{22}$ are mass- and spin-conserving,

$$\int_{\mathbb{R}^d_k} Q_{11}(F)\mathrm{d}k = \int_{\mathbb{R}^d_k} Q_{22}(F)\mathrm{d}k = 0, \tag{35}$$

whereas the anti-symmetric operators $Q_{21}$ and $Q_{12}$ are just mass-conserving,

$$\int_{\mathbb{R}^d_k} Q_{12}(F)\mathrm{d}k = -\int_{\mathbb{R}^d_k} Q_{21}(F)\mathrm{d}k \neq 0 \tag{36}$$

$$\int_{\mathbb{R}^d_k} \mathrm{tr}\left(Q_{12}(F)\right)\mathrm{d}k = \int_{\mathbb{R}^d_k} \mathrm{tr}\left(Q_{21}(F)\right)\mathrm{d}k = 0. \tag{37}$$

Therefore, the anti-symmetric operators contribute to the spin-flip scattering on the time scale $\tau_c$, which contradicts our assumption that spin flip processes should happen on the timescale $\tau_{sf}$.

4. **The model.** Adding the collision operators (27) and (30) on the right-hand side of (26), one obtains the following generalized matrix Boltzmann equation,

$$\begin{cases} \partial_t F + \dfrac{1}{\hbar}\left(\nabla_k h_0 \cdot \nabla_x F - \nabla_x h_0 \cdot \nabla_k F\right) + \dfrac{i}{\hbar}[F, \vec{h}\cdot\vec{\sigma}] = \dfrac{1}{\tau_c} Q_{ij}(F) + \dfrac{1}{\tau_{sf}} Q_{sf}(F) \\ F(t=0,x,k) = F_{in}(x,k) \\ F_{in}(x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C}) \qquad \forall (x,k). \end{cases} \tag{38}$$

Here, $h_0$ and $\vec{h}$ are the components of the Hamilton matrix (24). Equation (38) has been investigated by el Hajj [10] for the case that $S$, occurring in $Q_{ij}(F)$ and defined in (28), is a scalar, $S = s_0\sigma_0$. The case $S \in \mathcal{H}_2^+(\mathbb{C})$ is a new problem which is the topic of this work.

4.1. **Further assumptions.** Let us summarize in this section the physical hypothesis we need for the further development. Generalizations to these assumptions shall be treated in forthcoming works.

**Assumption 4.1** (**Shifted parabolic bands**)**.** We treat the case of two parabolic transport bands. Moreover, the band gap between the two spin bands does not depend on the momentum $k$. Thus, in equation (19) for $H_b$, we assume

$$\begin{cases} h_0 = \dfrac{\hbar^2|k|^2}{2m} + V(t,x) \\ \lambda = \lambda(t,x), \end{cases} \tag{39}$$

where $m$ is the effective mass of the electrons, $\lambda : \mathbb{R}^+ \times \mathbb{R}^d_x \to \mathbb{R}$ is the $k$-independent band gap and $V : \mathbb{R}^+ \times \mathbb{R}^d_x \to \mathbb{R}$ is an external potential energy.

Assumption 4.1 is known in the physics literature as the *Stoner model* [27]. It is a crude simplification of the problem, since transport bands in ferromagnets often do not have parabolic shape. However, the Stoner model is still a basic tool used to understand electron properties in ferromagnets [16, 22]. In this paper, we investigate the effects of spin-dependent scattering in the framework of the Stoner model and leave the case of more complicated bandstructures open for future work.

**Assumption 4.2 (Boltzmann statistics).** In thermal equilibrium, the distribution matrix has the form $F_{eq} = c\exp(-\beta H_{th})$ where $c \in \mathbb{R}^+$ is a normalization constant, $\beta = 1/k_B T$ is the inverse of the thermal energy and $H_{th}$ denotes the Hamilton matrix (24) of the system without externally applied electric or magnetic fields.

From the assumptions 4.1 and 4.2 we deduce

$$F_{eq}(x,k) = N(x)\mathcal{M}_\beta(k) \qquad \text{with} \qquad [N(x), H_{th}(x,k)] = 0 \quad \forall (x,k) \in \mathbb{R}^{2d}, \tag{40}$$

where $N \in \mathcal{H}_2(\mathbb{C})$ is a hermitian matrix and $\mathcal{M}_\beta$ stands for the scalar Maxwellian at thermal energy $\beta^{-1}$,

$$\mathcal{M}_\beta(k) = \left(\frac{\beta\hbar^2}{2\pi m}\right)^{d/2} \exp\left(-\frac{\beta\hbar^2|k|^2}{2m}\right). \tag{41}$$

**Assumption 4.3 (Detailed balance).** Let $\sigma(A)$ denote the ordered spectrum of $A \in \mathcal{H}_2(\mathbb{C})$. We assume local thermal equilibrium in each band,

$$\sigma(SF_{eq}) = \sigma(S'F'_{eq}). \tag{42}$$

This assumption implies that spin-conserving momentum scattering occurs at a much faster timescale than spin-flip scattering, so that equilibrium is established in each band separately before the whole system reaches equilibrium.

Under the assumption 4.3, from (40) one obtains

$$s_{\uparrow(\downarrow)}\mathcal{M}_\beta = s'_{\uparrow(\downarrow)}\mathcal{M}'_\beta \quad \Longrightarrow \quad \frac{s_\uparrow}{s_\downarrow} = \frac{s'_\uparrow}{s'_\downarrow} \qquad \forall k, k'. \tag{43}$$

In (43) we see that the ratio of the scattering rates for spin-up and spin-down electrons must not depend on $k$. We deduce $s_\uparrow = C(t,x)s_\downarrow$ where $C \in \mathbb{R}^+$. Therefore, the scattering matrix $S$ can be written as

$$S(t,x,k,k') = \alpha(t,x,k,k')P(t,x) \tag{44}$$

$$P(t,x) = \sigma_0 + p(t,x)\vec{\Omega}(t,x)\cdot\vec{\sigma}, \tag{45}$$

where $\alpha \in \mathbb{R}^+$ denotes the scattering rate from $k$ to $k'$ at $(t,x)$ and $P : \mathbb{R}^+ \times \mathbb{R}^d_x \to \mathcal{H}_2(\mathbb{C})$ is called the *polarization matrix*. Note that, because of (29), the direction of $P$ in spin space has to be $\vec{\Omega}$, the direction of the local magnetization. Moreover, the parameter $p$, which satisfies $0 \le p(t,x) < 1$, represents the spin-polarization of the scattering rates, whose ratio $C(t,x)$ is now given by

$$s_\uparrow = \frac{1+|p(t,x)|}{1-|p(t,x)|}s_\downarrow. \tag{46}$$

Further, by inserting the eigenvalues of $S$ written in (44) into (43), one can define the function $\phi$ which is symmetric in $k$ and $k'$ as

$$\phi(t,x,k,k') = \frac{\alpha(t,x,k,k')}{\mathcal{M}_\beta(k')} = \frac{\alpha(t,x,k',k)}{\mathcal{M}_\beta(k)} = \phi(t,x,k',k). \tag{47}$$

4.2. **Symmetric collision operator for the Stoner model.** In the present paper, we shall perform the diffusion limit with the symmetric operator $Q_{22}$ and denote it simply by $Q(F)$,

$$Q(F) := Q_{22}(F). \tag{48}$$

From (44), (45) and (47), one deduces the collision operator (48) in the Stoner model,

$$Q(F) = P^{1/2}K(F)P^{1/2}, \tag{49}$$

where

$$K(F)(k) := K^+(F)(k) - K^-(F)(k) = \mathcal{M}_\beta \int_{\mathbb{R}^d_{k'}} \phi F' \mathrm{d}k' - F\lambda. \tag{50}$$

Here, $\lambda = \int_{\mathbb{R}^d_{k'}} \phi \mathcal{M}'_\beta \mathrm{d}k'$ denotes the collision frequency.

4.3. **Scaled model.** The next step is to scale (38) in a way suitable for performing the diffusion limit. The main assumption is that the time scales $\tau_c$ and $\tau_{sf}$ are very different,

$$\tau_c \ll \tau_{sf} \qquad \Longrightarrow \qquad \varepsilon := \sqrt{\frac{\tau_c}{\tau_{sf}}} \ll 1. \tag{51}$$

Here $\varepsilon$ is a small parameter intended to go to zero. Let $\bar{v} = (\beta m)^{-1/2}$ denote the thermal velocity of the electrons. The length scale $\bar{l}$ we choose is the geometric average of the two occurring mean free paths $l_c = \tau_c \bar{v}$ and $l_{sf} = \tau_{sf}\bar{v}$, respectively,

$$\bar{l} = \sqrt{l_c l_{sf}}. \tag{52}$$

The characteristic time, momentum and energy scales are chosen as

$$\bar{t} = \tau_{sf} \qquad \bar{k} = \frac{m\bar{v}}{\hbar} \qquad \bar{E} = \beta^{-1}. \tag{53}$$

Applying the scaling (52)-(53) to (38) with the collision operator $Q_{ij}(F) = Q_{22}(F) = Q(F)$, $Q(F)$ given by (49), then multiplying by $\tau_{sf}$ and subsequently inserting (51) leads to the diffusion-scaled matrix Boltzmann equation (now in dimensionless variables $t$, $x$ and $k$). The scaling of the pseudo-exchange field $\vec{h} = (\lambda\vec{\Omega} + \vec{h}_{so})$ is crucial for performing the diffusion limit. In this work, we assume the weak coupling $\lambda/\bar{E} = \mathcal{O}(\varepsilon^2)$ and $|\vec{h}_{so}|/\bar{E} = \mathcal{O}(\varepsilon^2)$. Thus, under the hypothesis of the Stoner model (39), the scaled Hamilton matrix (24) reads

$$\begin{cases} H^\varepsilon(t,x,k) = \left(\dfrac{|k|^2}{2} + \hat{V}(t,x)\right)\sigma_0 + \varepsilon^2 \hat{\vec{h}}(t,x,k)\cdot\vec{\sigma} \\ \hat{\vec{h}}(t,x,k) := \vec{\Omega}(t,x) + \hat{\vec{h}}_{so}(t,x,k), \end{cases} \tag{54}$$

where we defined $\hat{V} := V/\bar{E}$ and $\hat{\vec{h}}_{so} = \vec{h}_{so}/\bar{E}$. Using the scaled Hamilton matrix (54) leads to the following scaled version of (38),

$$\begin{cases} \partial_t F^\varepsilon + \dfrac{1}{\varepsilon}\mathcal{T}(F^\varepsilon) + i[F^\varepsilon, \hat{\vec{h}}\cdot\vec{\sigma}] = \dfrac{1}{\varepsilon^2}Q(F^\varepsilon) + Q_{sf}(F) \\ F(t=0,x,k) = F_{in}(x,k) \\ F_{in}(x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C}) \qquad \forall (x,k), \end{cases} \tag{55}$$

where the transport operator $\mathcal{T}(F^\varepsilon)$ is defined by

$$\mathcal{T}(F^\varepsilon) = k\cdot\nabla_x F^\varepsilon - \nabla_x \hat{V}\cdot\nabla_k F^\varepsilon \tag{56}$$

and the scaled collision operator $Q(F^\varepsilon)$ is given by (49) and (50) where $\mathcal{M}_\beta$ is to be replaced by the scaled Maxwellian,

$$\mathcal{M}(k) = \left(\frac{1}{2\pi}\right)^{d/2} \exp\left(-\frac{|k|^2}{2}\right). \tag{57}$$

The aim of the present work is to go to the limit $\varepsilon \to 0$ in equation (55) in order to obtain a macroscopic model, more suitable for numerical simulations. Therefore, we shall make a Hilbert ansatz $F^\varepsilon = F^0 + \varepsilon F^1 + \varepsilon^2 F^2 + \dots$ of the solution and sort the appearing terms in powers of $\varepsilon$. The obtained equations read

$$Q(F^0) = 0 \tag{58}$$

$$Q(F^1) = \mathcal{T}(F^0) \tag{59}$$

$$Q(F^2) = \partial_t F^0 + \mathcal{T}(F^1) + i[F^0, \hat{\vec{h}} \cdot \vec{\sigma}] - Q_{sf}(F^0). \tag{60}$$

Let us summarize now the main steps of this work.

4.4. **Contents of the paper.** Section 5 deals with the analysis of the generalized matrix Boltzmann equation (38). We prove existence and uniqueness of a weak solution. Moreover, it is shown that the solution $F$ satisfies the maximum principle when the anti-symmetric collision operator $Q_{21}(F)$ is used in the Boltzmann equation. Section 6 contains the analysis of the collision operator $Q(F)$ appearing in (55) in a proper mathematical framework. In section 7 we present the main theorem of this work, namely the diffusion limit $\varepsilon \to 0$ in (55). Section 8 contains some numerical results of the macroscopic matrix drift-diffusion equations obtained in the diffusion limit. Some implications for physical applications such as spin-transfer torque devices or domain wall dynamics in ferromagnets are discussed briefly.

5. **Existence, positive-definiteness and uniqueness of a weak solution.** Let us first start by studying the matrix Boltzmann equation (38), in particular proving the existence, positive-(semi)definiteness and uniqueness of a weak solution. Without loss of generality the constants $\hbar$ and $\tau_{sf}$ are set to one. Let us introduce the following Hilbert space:

**Definition 5.1** (**Hilbert space**). By $\mathbb{L}^2_{\mathcal{M}}$ we denote the following space,

$$\mathbb{L}^2_{\mathcal{M}} := \left\{ F : \mathbb{R}^{2d} \to \mathcal{H}_2(\mathbb{C}) \,\middle|\, \int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_k} ||F||_2^2 \mathcal{M}^{-1} \mathrm{d}k\mathrm{d}x < \infty \right\} \tag{61}$$

associated with the scalar product and the corresponding norm

$$(F, G)_{\mathbb{L}^2_{\mathcal{M}}} := \int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_k} \langle F, G \rangle_2 \, \mathcal{M}^{-1} \mathrm{d}k\mathrm{d}x \qquad ||F||_{\mathbb{L}^2_{\mathcal{M}}} = \sqrt{(F,F)_{\mathbb{L}^2_{\mathcal{M}}}}, \tag{62}$$

where $\mathcal{M}$ stands for the scaled Maxwellian (57).

**Assumption 5.2.** Let $h_0 \in L^\infty(0,T; W^{2,\infty}_{loc}(\mathbb{R}^{2d}))$, $\vec{h} \in (L^\infty_{loc}([0,T) \times \mathbb{R}^{2d}))^3$ and let us define the transport operator $\mathcal{T}_{h_0} : D(\mathcal{T}_{h_0}) \to \mathbb{L}^2_{\mathcal{M}}$ by

$$\mathcal{T}_{h_0}(F) := \nabla_k h_0 \cdot \nabla_x F - \nabla_x h_0 \cdot \nabla_k F \tag{63}$$

and where the definition domain and norm are given by

$$D(\mathcal{T}_{h_0}) := \{ F \in \mathbb{L}^2_{\mathcal{M}} \,|\, \mathcal{T}_{h_0}(F) \in \mathbb{L}^2_{\mathcal{M}} \} \tag{64}$$

$$||F||^2_{D(\mathcal{T})} := ||F||^2_{\mathbb{L}^2_{\mathcal{M}}} + ||\mathcal{T}_{h_0}(F)||^2_{\mathbb{L}^2_{\mathcal{M}}}. \tag{65}$$

**Assumption 5.3.** The scattering matrix $S$ defined in (28) is chosen in such a way that (30) is a well-defined linear operator, $Q_{ij} : \mathbb{L}^2_{\mathcal{M}} \to \mathbb{L}^2_{\mathcal{M}}$, satisfying

$$\exists\, c > 0\, s.t. \qquad ||Q_{ij}(F)||^2_{\mathbb{L}^2_{\mathcal{M}}} \leq c\, ||F||^2_{\mathbb{L}^2_{\mathcal{M}}} \qquad \forall F \in \mathbb{L}^2_{\mathcal{M}}. \tag{66}$$

An example is given in section 6.

**Definition 5.4 (Weak solution).** Let $\hbar = \tau_{sf} = 1$ and $F_{in} \in \mathbb{L}^2_{\mathcal{M}}$. For a fixed time $T > 0$, a function $F \in L^2(0, T; \mathbb{L}^2_{\mathcal{M}})$ is called a weak solution of (38) if it satisfies

$$\begin{aligned} -\int_0^T \int\int \langle \partial_t \Psi, F\rangle_2 \,\mathrm{d}x\mathrm{d}k\mathrm{d}t - \int_0^T \int\int \langle \mathcal{T}_{h_0}(\Psi), F\rangle_2 \,\mathrm{d}x\mathrm{d}k\mathrm{d}t + \\ + i\int_0^T \int\int \left\langle \Psi, [F, \vec{h}\cdot\vec{\sigma}]\right\rangle_2 \mathrm{d}x\mathrm{d}k\mathrm{d}t = \int_0^T \int\int \langle \Psi, Q_{ij}(F)\rangle_2 \,\mathrm{d}x\mathrm{d}k\mathrm{d}t + \\ + \int_0^T \int\int \langle \Psi, Q_{sf}(F)\rangle_2 \,\mathrm{d}x\mathrm{d}k\mathrm{d}t + \int\int \langle \Psi, F_{in}\rangle_2 \,\mathrm{d}x\mathrm{d}k \end{aligned} \tag{67}$$

for all test functions $\Psi \in C^1_c([0, T) \times \mathbb{R}^{2d}, \mathcal{H}_2(\mathbb{C}))$.

**Proposition 5.5 (Existence/Uniqueness).** *Let $T > 0$ be fixed. Under the assumptions 5.2, 5.3 and with $F_{in} \in \mathbb{L}^2_{\mathcal{M}}$, the matrix Boltzmann equation (38) admits a unique weak solution $F \in L^\infty(0, T; \mathbb{L}^2_{\mathcal{M}})$.*

*Proof.* Let us define the fixed point map

$$\mathcal{F} : L^2(0, T; \mathbb{L}^2_{\mathcal{M}}) \to L^2(0, T; \mathbb{L}^2_{\mathcal{M}}) \qquad ; \qquad F^{old} \mapsto F^{new}, \tag{68}$$

where $F^{new}$ is a solution of

$$\begin{cases} \partial_t F^{new} + \mathcal{T}_{h_0}(F^{new}) + i[F^{new}, \vec{h}\cdot\vec{\sigma}] - \\ \qquad\qquad - Q_{sf}(F^{new}) + Q_j^-(F^{new}) = Q_i^+(F^{old}) \\ F^{new}(t = 0, x, k) = F_{in}(x, k). \end{cases} \tag{69}$$

The first step is to show that $\mathcal{F}$ is well-defined. For this take $F^{old} \in L^2(0, T; \mathbb{L}^2_{\mathcal{M}})$ and denote by $G_i := Q_i^+(F^{old}) \in L^2(0, T; \mathbb{L}^2_{\mathcal{M}})$. Let us use the decomposition of each matrix $F \in \mathcal{H}_2(\mathbb{C})$ in the Pauli basis $\{\sigma_0, \sigma_1, \sigma_2, \sigma_3\}$, which means $F = \frac{1}{2} f_0 + \vec{f}\cdot\vec{\sigma}$ and where we denote the coefficients by $\tilde{F} = (\frac{1}{2} f_0, \vec{f})$. Using this decomposition, system (69) now writes

$$\begin{cases} \partial_t \tilde{F} + \mathcal{T}_{h_0}(\tilde{F}) + (\mathbf{A} + \mathbf{D}_j)\tilde{F} = \tilde{G}_i \\ \tilde{F}(t = 0, x, k) = \tilde{F}_{in}(x, k). \end{cases} \tag{70}$$

Here, $\mathbf{A} \in M_4(\mathbb{R})$ is the $4 \times 4$ matrix representation of the operator $i[F, \vec{h}\cdot\vec{\sigma}] - Q_{sf}(F)$,

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & -2h_3 & 2h_2 \\ 0 & 2h_3 & -1 & -2h_1 \\ 0 & -2h_2 & 2h_1 & -1 \end{pmatrix},$$

and $\mathbf{D}_j \in M_4(\mathbb{R})$ is the matrix corresponding to the loss term $Q_j^-$, c.f. (33) and (34), with $\Lambda \in \mathcal{H}_2(\mathbb{C}) \Leftrightarrow \tilde{\Lambda} = (\lambda_0, \vec{\lambda})$,

$$\mathbf{D}_1 = \begin{pmatrix} \lambda_0 & \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_1 & \lambda_0 & 0 & 0 \\ \lambda_2 & 0 & \lambda_0 & 0 \\ \lambda_3 & 0 & 0 & \lambda_0 \end{pmatrix},$$

$$\mathbf{D}_2 = \begin{pmatrix} \lambda_0 & \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_1 & r + \frac{\lambda_1^2}{|\vec{\lambda}|^2}(\lambda_0 - r) & \frac{\lambda_1\lambda_2}{|\vec{\lambda}|^2}(\lambda_0 - r) & \frac{\lambda_1\lambda_3}{|\vec{\lambda}|^2}(\lambda_0 - r) \\ \lambda_2 & \frac{\lambda_2\lambda_1}{|\vec{\lambda}|^2}(\lambda_0 - r) & r + \frac{\lambda_2^2}{|\vec{\lambda}|^2}(\lambda_0 - r) & \frac{\lambda_2\lambda_3}{|\vec{\lambda}|^2}(\lambda_0 - r) \\ \lambda_3 & \frac{\lambda_3\lambda_1}{|\vec{\lambda}|^2}(\lambda_0 - r) & \frac{\lambda_3\lambda_2}{|\vec{\lambda}|^2}(\lambda_0 - r) & r + \frac{\lambda_3^2}{|\vec{\lambda}|^2}(\lambda_0 - r) \end{pmatrix},$$

where $r = (\lambda_0^2 - |\vec{\lambda}|^2)^{1/2}$. The matrix $\mathbf{D}_2$ is obtained straightforwardly from Lemmas 2.4 and 2.3. Now let $\mathcal{Z}_{t,x,k}(s) = (\mathcal{X}(s), \mathcal{K}(s))$ denote the characteristics in the phase space of (70) starting at the point $(x,k) \in \mathbb{R}^{2d}$ at time $t$. Its components satisfy the following system of equations,

$$\begin{cases} \dfrac{\partial \mathcal{X}(s)}{\partial s} = \nabla_k h_0(s, \mathcal{X}(s), \mathcal{K}(s)) \\ \dfrac{\partial \mathcal{K}(s)}{\partial s} = -\nabla_x h_0(s, \mathcal{X}(s), \mathcal{K}(s)) \\ \mathcal{X}(t) = x \qquad \mathcal{K}(t) = k. \end{cases} \tag{71}$$

Defining now, for each fixed $(x_0, k_0) \in \mathbb{R}^{2d}$ the function

$$g(t, x_0, k_0) := \tilde{F}(t, \mathcal{Z}_{0,x_0,k_0}(t)), \quad \forall t \in [0,T],$$

one gets the system

$$\begin{cases} \frac{d}{dt} g(t, x_0, k_0) = \\ \qquad = -(\mathbf{A} + \mathbf{D}_j)(t, \mathcal{Z}_{0,x_0,k_0}(t))\, g(t, x_0, k_0) + \tilde{G}_i(t, \mathcal{Z}_{0,x_0,k_0}(t)) \\ g(0, x_0, k_0) = \tilde{F}_{in}(x_0, k_0). \end{cases} \tag{72}$$

Denoting the "evolution matrix" by $R(\cdot; s) : \mathbb{R}^+ \to M_4(\mathbb{C})$, which represents for each $0 \le s \le T$ the unique solution of the following homogeneous system

$$\begin{cases} \frac{d}{dt} R(t; s) = -(\mathbf{A} + \mathbf{D}_j)(t, \mathcal{Z}_{0,x_0,k_0}(t))\, R(t; s), \quad \forall t \in [s, T] \\ R(s; s) = Id, \end{cases}$$

and which satisfies for $0 \le s \le t \le T$

$$||R(t; s)|| \le \exp\left\{ \int_s^t ||(\mathbf{A} + \mathbf{D}_j)(\tau, \mathcal{Z}_{0,x_0,k_0}(\tau)||\, d\tau \right\} \le C, \tag{73}$$

where $C > 0$ is a constant independent on $s, t, x_0, k_0$ and $||\cdot||$ is an operator norm in $\mathcal{L}(\mathbb{C}^4)$, the solution of (72) can be written as

$$g(t, x_0, k_0) = R(t; 0)\, \tilde{F}_{in}(x_0, k_0) + \textstyle\int_0^t R(t; s)\, \tilde{G}_i(s, \mathcal{Z}_{0,x_0,k_0}(s))\, ds. \tag{74}$$

Remarking now that $\tilde{F}(t,x,k) = g(t, \mathcal{Z}_{t,x,k}(0))$, one has the Duhamel formula

$$\tilde{F}(t,x,k) = R(t;0)\,\tilde{F}_{in}(\mathcal{Z}_{t,x,k}(0)) + \\ + \int_0^t R(t;s)\,\tilde{G}_i(s, \mathcal{Z}_{t,x,k}(s))\,ds\,, \quad \forall (t,x,k) \in [0,T]\times\mathbb{R}^{2d}\,, \quad (75)$$

which is a solution of (70) respectively (69) and therefore of (38). The goal is now to prove that the fixed point map $\mathcal{F}$ is a contraction, admitting thus a unique fixed point $F \in L^2([0,T],\mathbb{L}^2_{\mathcal{M}})$. From equation (75) we know that a solution $F \in L^\infty(0,T,\mathbb{L}^2_{\mathcal{M}})$ satisfies the following estimate,

$$||F^{new}(t,\cdot,\cdot)||_{\mathbb{L}^2_{\mathcal{M}}} \leq C\,||F_{in}||_{\mathbb{L}^2_{\mathcal{M}}} + \\ + C\int_0^t \left|\left|Q_i^+(F^{old})(\tau,\cdot,\cdot)\right|\right|_{\mathbb{L}^2_{\mathcal{M}}} \mathrm{d}\tau \quad \forall t\in[0,T]. \quad (76)$$

Squaring gives the following estimate in the $L^\infty$-norm,

$$||F^{new}||^2_{L^\infty(0,T;\mathbb{L}^2_{\mathcal{M}})} \leq 2C\,||F_{in}||^2_{\mathbb{L}^2_{\mathcal{M}}} + 2TC||Q_i^+(F^{old})||^2_{L^2(0,T;\mathbb{L}^2_{\mathcal{M}})},$$

yielding $F^{new} \in L^2(0,T,\mathbb{L}^2_{\mathcal{M}})$. To prove that $\mathcal{F}$ is a contraction we introduce the following norm in $L^2(0,T,\mathbb{L}^2_{\mathcal{M}})$,

$$||G||^2_\delta := \int_0^T e^{-\delta t}\,||G(t,\cdot,\cdot)||^2_{\mathbb{L}^2_{\mathcal{M}}}\,\mathrm{d}t \qquad\qquad \forall G \in L^2(0,T,\mathbb{L}^2_{\mathcal{M}}),$$

where the parameter $\delta > 0$ shall be specified later. We estimate

$$\begin{aligned}
||\mathcal{F}(F_1^{old}) - \mathcal{F}(F_2^{old})||^2_\delta &= ||F_1^{new} - F_2^{new}||^2_\delta \\
&= \int_0^T e^{-\delta t}\,||F_1^{new}(t) - F_2^{new}(t)||^2_{\mathbb{L}^2_{\mathcal{M}}}\,\mathrm{d}t \\
&\leq 2C\int_0^T e^{-\delta t}\int_0^t \left|\left|Q_i^+(F_1^{old})(s) - Q_i^+(F_2^{old})(s)\right|\right|^2_{\mathbb{L}^2_{\mathcal{M}}}\,\mathrm{d}s\mathrm{d}t \\
&= 2C\int_0^T\int_s^T e^{-\delta t}\left|\left|Q_i^+(F_1^{old})(s) - Q_i^+(F_2^{old})(s)\right|\right|^2_{\mathbb{L}^2_{\mathcal{M}}}\,\mathrm{d}t\mathrm{d}s \\
&\leq 2C\int_0^T \left|\left|F_1^{old}(s) - F_2^{old}(s)\right|\right|^2_{\mathbb{L}^2_{\mathcal{M}}} \frac{e^{-\delta s} - e^{-\delta T}}{\delta}\mathrm{d}s \\
&\leq \frac{2C}{\delta}||F_1^{old} - F_2^{old}||^2_\delta,
\end{aligned}$$

yielding that the parameter $\delta$ can be chosen in such a manner that $\mathcal{F}$ is a contraction. Therefore $\mathcal{F}$ admits a unique fixed point in $L^2([0,T],\mathbb{L}^2_{\mathcal{M}})$, solution of the matrix Boltzmann equation (38). □

**Proposition 5.6** (**Positive-(semi)definiteness**). *Let $T > 0$ be fixed. Further let $\phi \in L^\infty([0,T]\times\mathbb{R}^{2d})$ and assume 5.2 and 5.3. The matrix Boltzmann equation (38) with the collision operator $Q_{21}(F)$ conserves the positive-(semi)definiteness of a weak solution $F \in L^\infty(0,T;\mathbb{L}^2_{\mathcal{M}})$,*

$$F_{in}(x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C})\forall (x,k)\in\mathbb{R}^{2d} \Longrightarrow F(t,x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C})\forall(t,x,k)\in[0,T]\times\mathbb{R}^{2d}.$$

*Proof.* To prove this Proposition we shall show that for $F_{in} \in \mathcal{H}_2^{0,+}(\mathbb{C})$, the smallest eigenvalue of $F$, denoted $f_- = \frac{1}{2}f_0 - |\vec{f}|$, satisfies $f_-(t,x,k) \geq 0 \, \forall \, (t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}$. For this, let us find the equation of motion satisfied by $f_-$. Starting from

$$\partial_t F + \mathcal{T}_{h_0}(F) + i[F, \vec{h}\cdot\vec{\sigma}] - Q_{sf}(F) + Q_j^-(F) = G_i \tag{77}$$

where we defined $G_i(t,x,k) := Q_i^+(F^{old})(t,x,k)$, $G_i(t,x,k) \in \mathcal{H}_2(\mathbb{C}) \, \forall (t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}$, and taking the trace, we get

$$\partial_t f_0 + \mathcal{T}_{h_0}(f_0) + \mathrm{tr}\left(Q_j^-(F)\right) = \mathrm{tr}\left(G_i\right). \tag{78}$$

For this we recall:

$$F = \frac{1}{2} f_0 \sigma_0 + \vec{f}\cdot\vec{\sigma} \qquad ; \qquad f_0 = \mathrm{tr}\,(F) \tag{79}$$

$$[F, \vec{h}\cdot\vec{\sigma}] = [\vec{f}\cdot\vec{\sigma}, \vec{h}\cdot\vec{\sigma}] = 2i(\vec{f}\times\vec{h})\cdot\vec{\sigma}. \tag{80}$$

Multiplying now equation (77) with $\frac{1}{2}\vec{\sigma}$, taking the trace and further taking the scalar product with $\vec{f}/|\vec{f}|$ permits to get an equation for $|\vec{f}|$,

$$\partial_t|\vec{f}| + \mathcal{T}_{h_0}(|\vec{f}|) + |\vec{f}| + \frac{1}{2}\mathrm{tr}\left(\vec{\sigma}Q_j^-(F)\right)\cdot\frac{\vec{f}}{|\vec{f}|} = \frac{1}{2}\mathrm{tr}\left(\vec{\sigma}G_i\right)\cdot\frac{\vec{f}}{|\vec{f}|} \tag{81}$$

Subtracting (81) from (78) multiplied by $\frac{1}{2}$ gives, for $f_- = \frac{1}{2}f_0 - |\vec{f}|$,

$$\partial_t f_- + \mathcal{T}_{h_0}(f_-) - |\vec{f}| + \Pi_-(Q_j^-(F)) = \Pi_-(G_i) \tag{82}$$

where the operator $\Pi_- : \mathcal{H}_2(\mathbb{C}) \to \mathbb{R}$ is the projection on the smallest eigenvalue $f_-$ of $F \in \mathcal{H}_2(\mathbb{C})$. We shall now apply the maximum principle to (82). For this, we rewrite the equation in the form

$$\begin{cases} \partial_t f_- + \mathcal{T}_{h_0}(f_-) + \omega_{ij} f_- = \gamma_{ij} \\ f_-(t=0,x,k) = f_{-,in}(x,k), \end{cases} \tag{83}$$

where the coefficients $\omega_{ij} = \omega_{ij}(t,x,k) \in \mathbb{R}$ and $\gamma_{ij} = \gamma_{ij}(t,x,k) \in \mathbb{R} \, \forall (t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}$ are computed in Appendix A for $i,j \in \{1,2\}$. Now let $\mathcal{Z}_{t,x,k}(s) = (\mathcal{X}(s), \mathcal{K}(s))$ denote the characteristics in the phase space of (83) defined by (71). Using the Duhamel formula, we get the following identity for $f_-$

$$\begin{aligned} f_-(t,x,k) = \exp\left(-\int_0^t \omega_{ij}(s, \mathcal{Z}_{t,x,k}(s))\mathrm{d}s\right) f_{-,in}(\mathcal{Z}_{t,x,k}(0)) + \\ + \int_0^t \exp\left(-\int_\tau^t \omega_{ij}(s, \mathcal{Z}_{t,x,k}(s))\mathrm{d}s\right)\gamma_{ij}(\tau, \mathcal{Z}_{t,x,k}(\tau))\mathrm{d}\tau. \end{aligned} \tag{84}$$

We see that $f_-(t,x,k) \geq 0 \forall (t,x,k) \in \mathbb{R}\times\mathbb{R}^{2d}$ is satisfied if $\gamma_{ij}(t,x,k) \geq 0 \forall (t,x,k) \in \mathbb{R}\times\mathbb{R}^{2d}$. The coefficients $\gamma_{ij}$ for the respective choice of the gain and the loss term are written in (147)-(150). Lemma 2.5 yields $F^{old} \in \mathcal{H}_2^{0,+}(\mathbb{C}) \Rightarrow G_2 = Q_2^+(F^{old}) \in \mathcal{H}_2^{0,+}(\mathbb{C})$ and thus $\Pi_-(G_2) \geq 0$. However, $G_1 = Q_1^+(F^{old})$ is not necessarily a positive-(semi)definite matrix if $F^{old} \in \mathcal{H}_2^{0,+}(\mathbb{C})$. Additionally, we observe that one needs an estimate for the term $\Pi_-(G_2)$ in (150) in order to check the maximum principle for $Q_{22}$. This shall be done in a forthcoming work. In conclusion, we have

$$F^{old}(t,x,k) \in \mathcal{H}_2^{0,+}(\mathbb{C}) \quad \Longrightarrow \quad \gamma_{21}(t,x,k) \geq 0 \qquad \forall (t,x,k) \in \mathbb{R}\times\mathbb{R}^{2d}, \tag{85}$$

yielding that the collision operator $Q_{21}$ guarantees that a solution $F$ of (38) satisfies the maximum principle. □

6. **Properties of the collision operator Q(F).** In this section we analyze the spin-coherent collision operator $Q(F)$ occurring in the scaled Boltzmann equation (55). By $Im\,Q$ and $Ker\,Q$ we denote the image and the kernel of $Q$. The variables $t$ and $x$ shall be considered as parameters in this section and will often be omitted.

**Definition 6.1.** By $\mathcal{L}^2_{\mathcal{M}}$ we denote the following Hilbert space,

$$\mathcal{L}^2_{\mathcal{M}} := \left\{ F : \mathbb{R}^d_k \to \mathcal{H}_2(\mathbb{C}) \,\middle|\, \int_{\mathbb{R}^d_k} ||F||_2^2 \mathcal{M}^{-1} \mathrm{d}k < \infty \right\}, \tag{86}$$

equipped with the scalar product and the corresponding norm

$$(F,G)_{\mathcal{L}^2_{\mathcal{M}}} := \int_{\mathbb{R}^d_k} \langle F, G \rangle_2 \, \mathcal{M}^{-1} \mathrm{d}k \qquad\qquad ||F||_{\mathcal{L}^2_{\mathcal{M}}} = \sqrt{(F,F)_{\mathcal{L}^2_{\mathcal{M}}}}, \tag{87}$$

where $\mathcal{M}$ stands for the scaled Maxwellian (57).

**Assumption 6.2.** The polarization matrix $P : \mathbb{R}^+ \times \mathbb{R}^d_x \to \mathcal{H}_2^+(\mathbb{C})$, written in the Pauli basis as $P(t,x) = \sigma_0 + p(t,x)\vec{\Omega}(t,x)\cdot\vec{\sigma}$, is a hermitian, positive-definite matrix with $|\vec{\Omega}| = 1$. Its eigenvalues are $p_\uparrow = 1 + |p|$ and $p_\downarrow = 1 - |p|$ where $0 \le |p| < 1$. The scattering rate $\phi \in L^\infty(\mathbb{R}^{2d})$ is symmetric in $k$ and $k'$ and is bounded from above and below,

$$0 < \phi_1 \le \phi(k,k') \le \phi_2 < \infty \qquad \forall k, k'. \tag{88}$$

**Proposition 6.3 (Spin-coherent collision operator).** *Under assumption 6.2, the spin-coherent collision operator $Q : \mathcal{L}^2_{\mathcal{M}} \to \mathcal{L}^2_{\mathcal{M}}$ written in (49), with the scaled Maxwellian (57), satisfies the following properties:*

*i) $Q : \mathcal{L}^2_{\mathcal{M}} \to \mathcal{L}^2_{\mathcal{M}}$ is a linear, self-adjoint, continuous and non-positive operator.*

*ii) Conservation of mass and spin:*

$$\int_{\mathbb{R}^d_k} Q(F) \mathrm{d}k = 0 \qquad \forall F \in \mathcal{L}^2_{\mathcal{M}}. \tag{89}$$

*iii) The kernel of $Q$ has the form*

$$Ker\,Q = \{ F \in \mathcal{L}^2_{\mathcal{M}} \,|\, \exists\, N \in \mathcal{H}_2(\mathbb{C}) \; s.t. \; F = N\mathcal{M} \} \tag{90}$$

*and we have*

$$(Ker\,Q)^\perp = \left\{ F \in \mathcal{L}^2_{\mathcal{M}} \,\middle|\, \int_{\mathbb{R}^d_k} F \mathrm{d}k = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \right\}. \tag{91}$$

*iv) Let $\mathcal{P} : \mathcal{L}^2_{\mathcal{M}} \to Ker\,Q$ be the orthogonal projection operator on $Ker\,Q$. Then we have the coercitivity relation*

$$\exists\, d > 0 \; s.t. \qquad -(Q(F), F)_{\mathcal{L}^2_{\mathcal{M}}} \ge d\, ||F - \mathcal{P}(F)||_{\mathcal{L}^2_{\mathcal{M}}} \qquad \forall F \in \mathcal{L}^2_{\mathcal{M}}. \tag{92}$$

*v) The image of $Q$ is closed and we have $Im\,Q = (Ker\,Q)^\perp$. Further, the equation $Q(F) = G$ has a solution in $\mathcal{L}^2_{\mathcal{M}}$ if and only if $G \in Im\,Q$. The solution is moreover unique in $(Ker\,Q)^\perp$.*

***Proof of Proposition 6.3.*** First we show that $Q : \mathcal{L}^2_{\mathcal{M}} \to \mathcal{L}^2_{\mathcal{M}}$ is a well defined operator, i.e. $F \in \mathcal{L}^2_{\mathcal{M}} \Rightarrow Q(F) \in \mathcal{L}^2_{\mathcal{M}}$. For this, we shall show

$$\exists\, c > 0 \; s.t. \qquad ||Q(F)||^2_{\mathcal{L}^2_{\mathcal{M}}} \le c\, ||F||^2_{\mathcal{L}^2_{\mathcal{M}}} \qquad \forall F \in \mathcal{L}^2_{\mathcal{M}}. \tag{93}$$

Using Lemma 2.6 and $\mathrm{tr}\,(P)^2 < 1$ one obtains

$$||Q(F)||^2_{\mathcal{L}^2_{\mathcal{M}}} = \int_{\mathbb{R}^d_k} \mathrm{tr}\left(Q^2(F)\right)\mathcal{M}^{-1}\mathrm{d}k \leq \int_{\mathbb{R}^d_k} \mathrm{tr}\left(P^2K^2\right)\mathcal{M}^{-1}\mathrm{d}k \tag{94}$$
$$\leq 2\int_{\mathbb{R}^d_k} \mathrm{tr}\,(P)^2\,\mathrm{tr}\,(K)^2\,\mathcal{M}^{-1}\mathrm{d}k \leq 2\int_{\mathbb{R}^d_k} \mathrm{tr}\,(K)^2\,\mathcal{M}^{-1}\mathrm{d}k.$$

By using $\mathrm{tr}\left(K^2\right) = \mathrm{tr}\left((K^+ - K^-)^2\right) \leq 2\mathrm{tr}\left((K^+)^2 + (K^-)^2\right)$, which follows from (15), in (94), then applying the Cauchy-Schwartz inequality and Assumption 6.2, one obtains

$$\begin{aligned}
||Q(F)||^2_{\mathcal{L}^2_{\mathcal{M}}} &\leq 4\int_{\mathbb{R}^d_k} \mathcal{M}\mathrm{tr}\left(\left(\int_{\mathbb{R}^d_{k'}} \phi F'\mathrm{d}k'\right)^2\right)\mathrm{d}k + 4\int_{\mathbb{R}^d_k} \lambda^2\mathrm{tr}\left(F^2\right)\mathcal{M}^{-1}\mathrm{d}k \\
&\leq 4\int_{\mathbb{R}^d_k} \mathcal{M}\mathrm{tr}\left(\left(\int_{\mathbb{R}^d_{k'}} \phi\frac{F'}{\sqrt{\mathcal{M}'}}\sqrt{\mathcal{M}'}\mathrm{d}k'\right)^2\right)\mathrm{d}k + 4\phi_2^2\int_{\mathbb{R}^d_k} \mathrm{tr}\left(F^2\right)\mathcal{M}^{-1}\mathrm{d}k \\
&\leq 4\int_{\mathbb{R}^d_k} \mathcal{M}\mathrm{tr}\left(\int_{\mathbb{R}^d_{k'}} \phi^2\frac{F'^2}{\mathcal{M}'}\mathrm{d}k'\int_{\mathbb{R}^d_{k'}} \mathcal{M}'\mathrm{d}k'\right)\mathrm{d}k + 4\phi_2^2\int_{\mathbb{R}^d_k} \mathrm{tr}\left(F^2\right)\mathcal{M}^{-1}\mathrm{d}k \\
&\leq 4\phi_2^2\int_{\mathbb{R}^d_{k'}} \mathrm{tr}\left(F'^2\right)\mathcal{M}'^{-1}\mathrm{d}k' + 4\phi_2^2\int_{\mathbb{R}^d_k} \mathrm{tr}\left(F^2\right)\mathcal{M}^{-1}\mathrm{d}k \\
&= 8\phi_2^2\,||F||^2_{\mathcal{L}^2_{\mathcal{M}}},
\end{aligned}$$

which proves (93). Let us continue with the proof of Proposition 6.3.

*i*) The linearity of $Q : \mathcal{L}^2_{\mathcal{M}} \to \mathcal{L}^2_{\mathcal{M}}$ is obvious. Since we already proved the inequality (93) we know that $Q$ is a bounded operator and therefore continuous. The self-adjointness follows from

$$\begin{aligned}
(Q(F),G)_{\mathcal{L}^2_{\mathcal{M}}} &= \mathrm{tr}\int_{\mathbb{R}^d_k} Q(F)\frac{G}{\mathcal{M}}\mathrm{d}k = \mathrm{tr}\int_{\mathbb{R}^d_k}\int_{\mathbb{R}^d_{k'}} \phi P^{1/2}(\mathcal{M}F' - \mathcal{M}'F)P^{1/2}\frac{G}{\mathcal{M}}\mathrm{d}k'\mathrm{d}k \\
&= -\frac{1}{2}\mathrm{tr}\int_{\mathbb{R}^d_k}\int_{\mathbb{R}^d_{k'}} \phi\mathcal{M}\mathcal{M}'P^{1/2}\left(\frac{F'}{\mathcal{M}'} - \frac{F}{\mathcal{M}}\right)P^{1/2}\left(\frac{G'}{\mathcal{M}'} - \frac{G}{\mathcal{M}}\right)\mathrm{d}k'\mathrm{d}k.
\end{aligned}$$

Lemma 2.6 gives the non-positivity of $Q : \mathcal{L}^2_{\mathcal{M}} \to \mathcal{L}^2_{\mathcal{M}}$ by regarding

$$(Q(F),F)_{\mathcal{L}^2_{\mathcal{M}}} = -\frac{1}{2}\int_{\mathbb{R}^d_k}\int_{\mathbb{R}^d_{k'}} \phi\mathcal{M}\mathcal{M}'\mathrm{tr}\left(\left(P^{1/2}\left(\frac{F'}{\mathcal{M}'} - \frac{F}{\mathcal{M}}\right)\right)^2\right)\mathrm{d}k'\mathrm{d}k \leq 0. \tag{95}$$

*ii*) is trivial by integrating (50) over $k$.

*iii*) Assume that $F$ lies in the Kernel of $Q$, $F \in Ker\,Q \Rightarrow Q(F) = 0$
$\Rightarrow (Q(F),F)_{\mathcal{L}^2_{\mathcal{M}}} = 0$. One obtains

$$(Q(F),F)_{\mathcal{L}^2_{\mathcal{M}}} = -\frac{1}{2}\int_{\mathbb{R}^d_k}\int_{\mathbb{R}^d_{k'}} \phi\mathcal{M}\mathcal{M}'\mathrm{tr}\left(\left(P^{1/2}\left(\frac{F'}{\mathcal{M}'} - \frac{F}{\mathcal{M}}\right)\right)^2\right)\mathrm{d}k'\mathrm{d}k = 0$$
$$\forall F \in Ker\,Q.$$

From equation (17) we deduce that, for any $F \in Ker\, Q$, the above expression is zero if and only if $F'/\mathcal{M}' = F/\mathcal{M} = 0\, \forall k, k'$, because $P$ is strictly positive definite. This condition is fulfilled if and only if $F = N\mathcal{M}$ with $N \in \mathcal{H}_2(\mathbb{C})$ independent of $k$ and $k'$. Conversely, it is verified easily from (50) that $F = N\mathcal{M}$ implies $Q(F) = 0 \Rightarrow F \in Ker\, Q$.

By definition $(Ker\, Q)^\perp = \left\{ F \in \mathcal{L}^2_\mathcal{M} \,\middle|\, (F, G)_{\mathcal{L}^2_\mathcal{M}} = 0 \ \forall G \in Ker\, Q \right\}$. This leads to

$$(F, N\mathcal{M})_{\mathcal{L}^2_\mathcal{M}} = \mathrm{tr}\left( N \int_{\mathbb{R}^d_k} F \mathrm{d}k \right) = 0 \ \forall N \in \mathcal{H}_2(\mathbb{C})$$

$$\Longrightarrow \quad \int_{\mathbb{R}^d_k} F \mathrm{d}k = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \ \forall F \in (Ker\, Q)^\perp.$$

*iv*) Since $Q : \mathcal{L}^2_\mathcal{M} \to \mathcal{L}^2_\mathcal{M}$ is linear and continuous, $Ker\, Q \subset \mathcal{L}^2_\mathcal{M}$ is closed. It follows the existence of an orthogonal projection $\mathcal{P} : \mathcal{L}^2_\mathcal{M} \to Ker\, Q$ and further $\mathcal{L}^2_\mathcal{M} = Ker\, Q \oplus^\perp (Ker\, Q)^\perp$ where $\oplus^\perp$ denotes the direct orthogonal sum with respect to $(\cdot, \cdot)_{\mathcal{L}^2_\mathcal{M}}$. We want to show that

$$\exists\, d > 0 \; s.t. \qquad -(Q(F), F)_{\mathcal{L}^2_\mathcal{M}} \geq d\, ||F - \mathcal{P}(F)||_{\mathcal{L}^2_\mathcal{M}} \qquad \forall F \in \mathcal{L}^2_\mathcal{M}. \tag{96}$$

The case $F \in Ker\, Q$ is trivial because then $Q(F) = 0$ and $\mathcal{P}(F) = F$. Let $F \in (Ker\, Q)^\perp$. Then we have to show that $-(Q(F), F)_{\mathcal{L}^2_\mathcal{M}} \geq c\, ||F||_{\mathcal{L}^2_\mathcal{M}}$. Equation (95) yields

$$-(Q(F), F)_{\mathcal{L}^2_\mathcal{M}} = \frac{1}{2} \int_{\mathbb{R}^d_k} \int_{\mathbb{R}^d_{k'}} \phi \mathcal{M}\mathcal{M}' \mathrm{tr}\left( \left( P^{1/2} \left( \frac{F'}{\mathcal{M}'} - \frac{F}{\mathcal{M}} \right) \right)^2 \right) \mathrm{d}k' \mathrm{d}k. \tag{97}$$

From equation (17) and the fact that the smallest eigenvalue of $P$ reads $p_\downarrow = 1 - |p|$ (Assumption 6.2), we deduce

$$\phi \mathrm{tr}\left( \left( P^{1/2} \left( \frac{F'}{\mathcal{M}'} - \frac{F}{\mathcal{M}} \right) \right)^2 \right) \geq \phi_1 \left(1 - |p|\right) \mathrm{tr}\left( \left( \frac{F'}{\mathcal{M}'} - \frac{F}{\mathcal{M}} \right)^2 \right).$$

Inserting this relation into (97) yields

$$\begin{aligned} -(Q(F), F)_{\mathcal{L}^2_\mathcal{M}} &\geq \frac{1}{2} \phi_1 \left(1 - |p|\right) \mathrm{tr} \int_{\mathbb{R}^d_k} \int_{\mathbb{R}^d_{k'}} \mathcal{M}\mathcal{M}' \left( \frac{F'}{\mathcal{M}'} - \frac{F}{\mathcal{M}} \right)^2 \mathrm{d}k' \mathrm{d}k = \\ &= \frac{1}{2} \phi_1 \left(1 - |p|\right) \mathrm{tr} \int_{\mathbb{R}^d_k} \int_{\mathbb{R}^d_{k'}} \mathcal{M}\mathcal{M}' \left( \frac{F'^2}{\mathcal{M}'^2} - \frac{F'F}{\mathcal{M}'\mathcal{M}} - \frac{FF'}{\mathcal{M}\mathcal{M}'} + \frac{F^2}{\mathcal{M}^2} \right) \mathrm{d}k' \mathrm{d}k = \\ &= \phi_1 \left(1 - |p|\right) \mathrm{tr} \int_{\mathbb{R}^d_k} \frac{F^2}{\mathcal{M}} \mathrm{d}k, \end{aligned}$$

where the last line follows from (91).

*v*) First we show that $Im\, Q$ is closed. Let $G_n := Q(F_n)$ be a sequence with $F_n \in \mathcal{L}^2_\mathcal{M}$ and $G_n \in Im\, Q$ so that $G_n \to G \in \mathcal{L}^2_\mathcal{M}$ as $n \to \infty$. One has to show that $G \in Im\, Q$, i.e. there exists $F \in \mathcal{L}^2_\mathcal{M}$ s.t. $Q(F) = G$. To any sequence $F_n \in \mathcal{L}^2_\mathcal{M}$ one can construct $H_n := F_n - \mathcal{P}F_n$ with $Q(H_n) = Q(F_n) = G_n$. One has $H_n \in (Ker\, Q)^\perp$ and

therefore the coercitivity relation (92) yields

$$-\left(Q(H_n-H_m),H_n-H_m\right)_{\mathcal{L}^2_{\mathcal{M}}}\geq c\,||H_n-H_m||^2_{\mathcal{L}^2_{\mathcal{M}}}\,.$$

We also have

$$||Q(H_n)-Q(H_m)||_{\mathcal{L}^2_{\mathcal{M}}}\,||H_n-H_m||_{\mathcal{L}^2_{\mathcal{M}}}\geq-\left(Q(H_n-H_m),H_n-H_m\right)_{\mathcal{L}^2_{\mathcal{M}}}$$

and therefore

$$\frac{1}{c}\,||G_n-G_m||_{\mathcal{L}^2_{\mathcal{M}}}\geq||H_n-H_m||_{\mathcal{L}^2_{\mathcal{M}}}\,.$$

Since $\{G_n\}_{n\in\mathbb{N}}$ is convergent (and thus a Cauchy sequence in $\mathcal{L}^2_{\mathcal{M}}$) one obtains that $\{H_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathcal{L}^2_{\mathcal{M}}$. But $\mathcal{L}^2_{\mathcal{M}}$ is complete and therefore $H_n\to H\in\mathcal{L}^2_{\mathcal{M}}$ as $n\to\infty$. Because $Q$ is continuous, $Q(H_n)\to Q(H)$ as $n\to\infty$ and we assumed that $Q(H_n)=G_n\to G\in\mathcal{L}^2_{\mathcal{M}}$. One obtains $Q(H)=G$ with $H\in\mathcal{L}^2_{\mathcal{M}}$.

We now prove that $Q(F)=G$ has a unique solution $F\in(Ker\,Q)^\perp$. It is clear that for $G\in Im\,Q$ there exists a solution $F\in\mathcal{L}^2_{\mathcal{M}}$. Let $F\in\mathcal{L}^2_{\mathcal{M}}$ be such a solution, then $(F-\mathcal{P}F)\in(Ker\,Q)^\perp$ is also a solution. Suppose that there are two solutions $F_a,F_b\in(Ker\,Q)^\perp$, $F_a\neq F_b$ such that $Q(F_a)=Q(F_b)=G$. One obtains

$$Q(F_a-F_b)=0\quad\Rightarrow\quad F_a-F_b\in Ker\,Q\cap(Ker\,Q)^\perp=\{0\}\quad\Rightarrow\quad F_a=F_b.$$

□

7. **Diffusion limit.** In this section we shall finally investigate the diffusion limit $\varepsilon\to0$ of the matrix Boltzmann equation (55) in order to obtain a macroscopic model, which is used in the next section for some numerical experiments.

**Theorem 7.1** (**Diffusion limit**). *Let $\mathcal{T}_d:\mathcal{H}_2(\mathbb{C})\to(\mathcal{H}_2(\mathbb{C}))^d$ denote the following transport operator:*

$$\mathcal{T}_d(N):=(-\nabla_x\hat{V}(x)-\nabla_x)N(x).$$

*Under the assumption 6.2, in the limit $\varepsilon\to0$, the solution $F^\varepsilon$ of the matrix Boltzmann equation (55) converges weakly to $F^0=N(t,x)\mathcal{M}(k)$ where $N(t,x)\in\mathcal{H}_2^{0,+}(\mathbb{C})\forall(t,x)\in\mathbb{R}^+\times\mathbb{R}^d_x$ and $\mathcal{M}$ stands for the scalar Maxwellian (57). Moreover, $N$ satisfies the following drift-diffusion equation,*

$$\partial_tN+\nabla_x\cdot\mathcal{J}+i\left[N,(\vec{\Omega}+\hat{\vec{g}}_{so})\cdot\vec{\sigma}\right]-\frac{1}{2}\mathrm{tr}\,(N)\,\sigma_0+N=0. \tag{98}$$

*The current density $\mathcal{J}\in(\mathcal{H}_2(\mathbb{C}))^d$ reads*

$$\mathcal{J}=\mathbb{D}A(N), \tag{99}$$

*where the diffusion matrix $\mathbb{D}\in\mathbb{R}^{d\times d}$ is given by*

$$\mathbb{D}=\int_{\mathbb{R}^d_k}k\otimes\theta(k)\mathrm{d}k, \tag{100}$$

*with $\theta(k)\in\mathbb{R}^d\,\forall k\in\mathbb{R}^d_k$ being the unique solution of*

$$\int_{\mathbb{R}^d_{k'}}\phi(\mathcal{M}\theta'-\mathcal{M}'\theta)\mathrm{d}k'=-k\mathcal{M} \tag{101}$$

*that satisfies $\int_{\mathbb{R}^d_k}\theta\mathrm{d}k=0$. The matrix $A(N)(t,x)\in(\mathcal{H}_2(\mathbb{C}))^d\,\forall(t,x)\in\mathbb{R}^+\times\mathbb{R}^d_x$ is given by*

$$A(N)=P^{-1/2}\mathcal{T}_d(N)P^{-1/2}. \tag{102}$$

*The term $\hat{\vec{g}}_{so}$ in the commutator of (98) stems from the spin-orbit contribution to the pseudo-exchange field,*

$$\hat{\vec{g}}_{so}(t,x) = \int_{\mathbb{R}^d_k} \mathcal{M}(k)\hat{\vec{h}}_{so}(t,x,k)\mathrm{d}k. \tag{103}$$

**Remark 1.** By expressing $\mathcal{J}$ given in (99) in the Pauli basis, $\mathcal{J} = \left(\frac{1}{2}j_0, \vec{j}\right)$ with $j_0 \in \mathbb{R}^d_x$ and $\vec{j} \in \mathbb{R}^d_x \times \mathbb{R}^3$, one obtains a coupling between $n_0 \in \mathbb{R}^+$ and $\vec{n} \in \mathbb{R}^3$, the charge- and the spin degree of freedom, respectively. Writing $N = \left(\frac{1}{2}n_0, \vec{n}\right)$ and for simplicity assuming that $\hat{\vec{g}}_{so} = 0$, the charge and spin currents read

$$j_0 = \frac{\mathbb{D}}{1-|p|^2}\left[\mathcal{T}_d(n_0) - 2p\mathcal{T}_d(\vec{n})\cdot\vec{\Omega}\right] \tag{104}$$

$$\vec{j} = \frac{\mathbb{D}}{1-|p|^2}\left[\sqrt{1-|p|^2}\mathcal{T}_d(\vec{n}) + (1-\sqrt{1-|p|^2})(\mathcal{T}_d(\vec{n})\cdot\vec{\Omega})\vec{\Omega} - \frac{p}{2}\mathcal{T}_d(n_0)\vec{\Omega}\right]. \tag{105}$$

The respective parallel and transverse components of the spin-current with respect to the local magnetization $\vec{\Omega}$ read

$$\vec{j}\cdot\vec{\Omega} = \frac{\mathbb{D}}{1-|p|^2}\left[\mathcal{T}_d(\vec{n})\cdot\vec{\Omega} - \frac{p}{2}\mathcal{T}_d(n_0)\right] \tag{106}$$

$$\vec{j} - (\vec{j}\cdot\vec{\Omega})\vec{\Omega} = \frac{\mathbb{D}\sqrt{1-|p|^2}}{1-|p|^2}\left[\mathcal{T}_d(\vec{n}) - (\mathcal{T}_d(\vec{n})\cdot\vec{\Omega})\vec{\Omega}\right]. \tag{107}$$

7.1. **Formal approach.** Here, we present a formal proof of Theorem 7.1. We consider the equations obtained from the Hilbert ansatz for $F^\varepsilon$ written in (58)-(60). Proposition 6.3 yields

$$Q(F^0) = 0 \quad \Longrightarrow \quad F^0(t,x,k) = N(t,x)\mathcal{M}(k) \qquad N : \mathbb{R}^+ \times \mathbb{R}^d_x \to \mathcal{H}_2(\mathbb{C}). \tag{108}$$

Moreover,

$$\int_{\mathbb{R}^d_k} \mathcal{T}(F^0)\mathrm{d}k = \nabla_x N \cdot \int_{\mathbb{R}^d_k} k\mathcal{M}\mathrm{d}k - N\nabla_x V \cdot \int_{\mathbb{R}^d_k} \nabla_k \mathcal{M}\mathrm{d}k = 0. \tag{109}$$

Therefore $\mathcal{T}(F^0) \in (Ker\, Q)^\perp = Im\, Q$ which gives the existence and uniqueness of $F^1 \in (Ker\, Q)^\perp$ s.t. $Q(F^1) = \mathcal{T}(F^0)$. From (59) one obtains

$$Q(F^1) = \mathcal{T}(F^0) = \nabla_x N \cdot k\mathcal{M} - N\nabla_x V \cdot \nabla_k \mathcal{M} = -\mathcal{T}_d(N)\cdot k\mathcal{M}. \tag{110}$$

To solve (110) we make the Ansatz $F^1 = A(t,x)\cdot\theta(k)$ with $A(t,x) \in (\mathcal{H}_2(\mathbb{C}))^d$ and $\theta(k) \in \mathbb{R}^d$ for $(t,x,k) \in \mathbb{R}^+ \times \mathbb{R}^{2d}$. We obtain

$$Q(A\cdot\theta) = P^{1/2}AP^{1/2} \cdot \int_{\mathbb{R}^d_{k'}} \phi(\mathcal{M}\theta' - \mathcal{M}'\theta)\mathrm{d}k'. \tag{111}$$

From Proposition 6.3 we get that

$$\int_{\mathbb{R}^d_{k'}} \phi(\mathcal{M}\theta' - \mathcal{M}'\theta)\mathrm{d}k' = -k\mathcal{M} \tag{112}$$

has a unique solution $\theta \in (Ker\, Q)^\perp$ that satisfies $\int_{\mathbb{R}^d_k} \theta(k)\mathrm{d}k = 0$. It follows that $F^1 = A\cdot\theta$ is the unique solution of $Q(F^1) = -\mathcal{T}_d(N)\cdot k\mathcal{M}$ if the matrix $A$ satisfies

$$P^{1/2}AP^{1/2} = \mathcal{T}_d(N). \tag{113}$$

Integration of equation (60) with respect to $k$ now yields

$$\partial_t N + \int_{\mathbb{R}^d_k} \mathcal{T}(A\cdot\theta)\mathrm{d}k + i[N,(\vec{\Omega}+\hat{\vec{g}}_{so})\cdot\vec{\sigma}] - \frac{1}{2}\mathrm{tr}\,(N)\,\sigma_0 + N = 0, \tag{114}$$

where

$$\hat{\vec{g}}_{so}(t,x) = \int_{\mathbb{R}^d_k} \mathcal{M}(k)\hat{\vec{h}}_{so}(t,x,k)\mathrm{d}k. \tag{115}$$

Now we shall define, for $k\in\mathbb{R}^d$ and $\theta\in\mathbb{R}^d$, the tensor product $k\otimes\theta\in\mathbb{R}^{d\times d}$ as

$$(k\otimes\theta)_{ij} := k_i\theta_j \qquad ; \qquad i,j\in\{1,\dots,d\}. \tag{116}$$

Moreover, for $A\in(\mathcal{H}_2(\mathbb{C}))^d$, we define $A:=(A_1,\dots,A_d)$ where the components $A_i\in\mathcal{H}_2(\mathbb{C})$ for $i\in\{1,\dots,d\}$. Then we shall use the following notation for the gradient with respect to $u\in\mathbb{R}^d$ of $A\in(\mathcal{H}_2(\mathbb{C}))^d$, $\nabla_u:(\mathcal{H}_2(\mathbb{C}))^d\to(\mathcal{H}_2(\mathbb{C}))^{d\times d}$,

$$(\nabla_u A)_{ij} := \partial_{u_j}A_i \qquad ; \qquad i,j\in\{1,\dots,d\}. \tag{117}$$

Finally, for $b\in\mathbb{R}^{d\times d}$ and $C\in(\mathcal{H}_2(\mathbb{C}))^{d\times d}$, $b:C\in\mathcal{H}_2(\mathbb{C})$ denotes the Frobenius product

$$b:C = \sum_{ij} b_{ij}C_{ji} \qquad ; \qquad i,j\in\{1,\dots,d\}. \tag{118}$$

With the preceeding definitions, the integral appearing in equation (114) can now be written as

$$\begin{aligned}\int_{\mathbb{R}^d_k}\mathcal{T}(A\cdot\theta)\mathrm{d}k &= \int_{\mathbb{R}^d_k}[(k\otimes\theta):\nabla_x A - A\cdot\nabla_k\theta\nabla_x\hat{V}]\mathrm{d}k = \\ &= \nabla_x\cdot\left[\left(\int_{\mathbb{R}^d_k} k\otimes\theta\mathrm{d}k\right)A\right],\end{aligned} \tag{119}$$

where $\nabla_k\theta\in\mathbb{R}^{d\times d}$ is defined by (117). Equation (119) leads to the definition of the diffusion matrix $\mathbb{D}\in\mathbb{R}^{d\times d}$ and the current density $\mathcal{J}\in(\mathcal{H}_2(\mathbb{C}))^d$, respectively,

$$\mathbb{D} := \int_{\mathbb{R}^d_k} k\otimes\theta\mathrm{d}k \tag{120}$$

$$\mathcal{J} := \mathbb{D}A, \tag{121}$$

where we mean

$$\mathcal{J}_i = (\mathbb{D}A)_i = \sum_j \mathbb{D}_{ij}A_j \qquad ; \qquad i,j\in\{1,\dots,d\} \tag{122}$$

for the components $\mathcal{J}_i\in\mathcal{H}_2(\mathbb{C})$ of $\mathcal{J}$.

8. **Numerical Results.** In this section we present some numerical solutions of the spin-coherent drift-diffusion equations (98)-(103). We will consider the one-dimensional case, $d=1$, for different multilayer structures. The multilayers consist of alternating non-magnetic ($N$) and ferromagnetic ($F$) layers, respectively. An $N$-layer is characterized by $\vec{\Omega}=0$ (no magnetization) in its domain, thus having no spin polarization of scattering rates, leading to $P=\sigma_0$ in (102). By contrast, the $F$-layers feature non-vanishing magnetization, $\vec{\Omega}\neq 0$, and non-vanishing spin polarization of scattering rates, $0<p<1$ in (45). In order to focus on the effects of $p\neq 0$ in ferromangets, we do not take into account spin-orbit couplings and assume $\hat{\vec{g}}_{so}=0$. Moreover, to solve for $\theta$ in (101), we assume that $\phi = 1/\tau_c = const.$ is the

same in every layer. This leads to $\theta = \tau_c k \mathcal{M}$ and from (100), after rescaling, one obtains the diffusion coefficient

$$\mathbb{D} = \frac{\tau_c k_B T}{m}, \tag{123}$$

where $T$ is the temperature of the electron system and $k_B$ stands for the Boltzmann constant. Therefore, the rescaled, one-dimensional version of (98)-(103) we consider now reads

$$\begin{cases} \partial_t N + \mathbb{D}\partial_x A(N) + i\dfrac{\gamma}{\hbar}\left[N, \vec{\Omega}\cdot\vec{\sigma}\right] - \dfrac{1}{\tau_{sf}}\left(\dfrac{1}{2}\mathrm{tr}\,(N)\,\sigma_0 - N\right) = 0 \\ A(N) = P^{-1/2}\left(-\dfrac{\partial_x V}{k_B T}N - \partial_x N\right)P^{-1/2}. \end{cases} \tag{124}$$

In the following let us denote $\eta = \sqrt{1-|p|^2}$. Applying Remark 1 to (124), the system of equations to be solved becomes

$$\begin{cases} \partial_t n_0 + \partial_x j_0 = 0 \\ \partial_t \vec{n} + \partial_x \vec{j} - \dfrac{2\gamma}{\hbar}\vec{n}\times\vec{\Omega} + \dfrac{1}{\tau_{sf}}\vec{n} = 0 \\ j_0 = \dfrac{\mathbb{D}}{\eta^2}\left[-\dfrac{\partial_x V}{k_B T}n_0 - \partial_x n_0 - 2p\left(-\dfrac{\partial_x V}{k_B T}\vec{n} - \partial_x\vec{n}\right)\cdot\vec{\Omega}\right] \\ \vec{j} = \dfrac{\mathbb{D}}{\eta^2}\Bigg\{\eta\left(-\dfrac{\partial_x V}{k_B T}\vec{n} - \partial_x\vec{n}\right) + (1-\eta)\left[\left(-\dfrac{\partial_x V}{k_B T}\vec{n} - \partial_x\vec{n}\right)\cdot\vec{\Omega}\right]\vec{\Omega} - \\ \qquad\qquad - \dfrac{p}{2}\left(-\dfrac{\partial_x V}{k_B T}n_0 - \partial_x n_0\right)\vec{\Omega}\Bigg\}, \end{cases} \tag{125}$$

where $n_0$ is the electron charge density and $\vec{n}$ is the non-equilibrium spin density. Initial and boundary conditions are specified for each of the investigated problems separately in the respective subsections. At interfaces between domains with different sets of parameters we require continuity of the densities $n_0$ respectively $\vec{n}$ and of the currents $j_0$ respectively $\vec{j}$. We use a standard Crank-Nicolson finite difference scheme to solve the system (125) in a three-layer and in a five-layer structure. In addition, charge and spin transport through a magnetic domain wall, which is essentially a rapid change of the direction of magnetization $\vec{\Omega}$ over some nanometers, is investigated.

For all simulations, in the equations (125), we set $\mathbb{D} = 10^{-3}\,\mathrm{m^2 s^{-1}}$, $k_B T = 0.025\,\mathrm{eV}$ and $\tau_{sf} = 10^{-12}\,\mathrm{s}$. Moreover, we set $2\gamma\tau_{sf}/\hbar = 4.0$ for the simulations of the five-layer structure, c.f. section 8.2, and $2\gamma\tau_{sf}/\hbar = 20.0$ for the domain wall simulations, c.f. section 8.3. These parameter values are in the range of the parameters cited in [41]. The injected charge density is always $n_0 = 1.0$.

8.1. **Three-layer system: $N/F/N$.** The first system we investigate is composed of three layers, each of which has a thickness of 400 nm, thus the total thickness is $L = 1200\,\mathrm{nm}$. The structure is non-metal/ferromagnet/non-metal where the interfaces are located at $x_1 = 400\,\mathrm{nm}$ and $x_2 = 800\,\mathrm{nm}$. In the three different

domains, we choose the following parameters:

$$x \in (0, x_1]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad p(x) = 0, \tag{126}$$

$$x \in (x_1, x_2]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad p(x) = const., \tag{127}$$

$$x \in (x_2, L]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad p(x) = 0. \tag{128}$$

We apply a constant electric field that is given by $-\Delta V/L$. The system (125) is subjected to the following initial and boundary conditions:

$$\begin{cases} n_0(t=0,x) = 1.0 \quad \forall x \in (0, L] \\ \vec{n}(t=0,x) = 0 \quad \forall x \in (0, L] \\ n_0(t, x=0) = 1.0 \quad \forall t \\ n_0(t, x=L) = 1.0 \quad \forall t \\ \partial_x \vec{n}(t,x)\Big|_{x=0} = 0 \quad \forall t \\ \partial_x \vec{n}(t,x)\Big|_{x=L} = 0 \quad \forall t. \end{cases} \tag{129}$$

The system (125), (129) is solved on an equally spaced grid with 50 points in each layer. The time step was set to $0.005\,\tau_{sf}$. Grid spacing and time step were chosen such that further refinement did not change the results. We conducted two series of simulations. The results, representing steady state solutions obtained after running the system (125) for long enough time, are depicted in Figures 1 and 2, respectively. In the first series, we set $\Delta V = -1.0\,\mathrm{V}$ and vary the parameter $p$ of the scattering polarization in the ferromagnet. The discontinuity of $p$ (and $\vec{\Omega}$, respectively) at the interfaces between the magnetic/non-magnetic layers acts as a source of non-equilibrium spin-polarization in $z$-direction as soon as a voltage is applied. This so-called 'spin injection' is a well known property of magnetic/non-magnetic multilayers [34]. In our new spin-coherent model, it arises from the particular form of the charge current density $j_0$ in (125). Consider the $N/F$ interface at $x = x_1$ in Figure 1. Under an applied bias $\partial_x V < 0$, when there is no initial spin polarization of the current ($\vec{n} = 0$) and $n_0(x) = const. \,\forall\, x$, the 'inflow' $j_0^-(x_1)$ into the interface from $x < x_1$ is smaller than the 'outflow' $j_0^+(x_1)$ into $x > x_1$ because $\eta^2 = 1 - p^2 < 1$ when $p > 0$. In steady state we have $j_0^-(x_1) = j_0^+(x_1)$, thus the discontinuity of $\eta$ has been compensated by a decrease of the charge density $n_0$ in the ferromagnet, which, by the equation for the spin current $\vec{j}$ in (125), leads to a non-equilibrium spin polarization $\vec{n}$ at $x = x_1$. This is a rather simplified yet intuitive explanation of what happens at the interfaces, however, the actual coupling between $n_0$ and $\vec{n}$ is more complicated and is only obtained from the self-consistent solution of (125). The broadening of the peaks of $\vec{n} = (0, 0, n_3)$ at the interfaces is due to spin diffusion, that is, the created spin density decreases exponentially away from the interfaces on the scale of the spin diffusion length, which is of the order of 100 nm. The peaks at the interfaces are asymmetric because the electric field drives the electrons carrying the non-equilibrium spin polarization from left to

right. Curves with higher peaks of $n_3$ correspond to larger values of $p$ and steeper slopes of $n_0$ at $x = x_1$. Note that in the domain $x > x_2$, one finds a significant reduction of the charge density $n_0$ for large scattering polarizations, $0.6 < p < 1$. In the second series of simulations, depicted in Figure 2, we set $p = 0.33$ in the

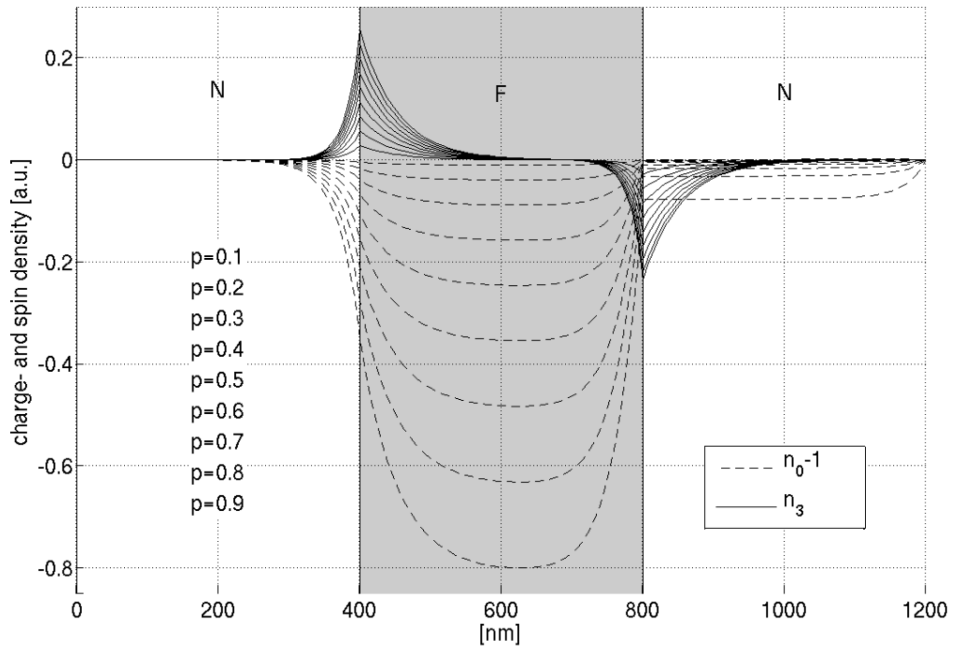


FIGURE 1. Simulated charge density $n_0 - 1$ and non-equilibrium spin density $\vec{n} = (0, 0, n_3)$ in a three-layer structure (non-magnet/ferromagnet/non-magnet) with applied voltage $\Delta V = -1.0\,\mathrm{V}$ for different values of the scattering polarization parameter $p$ in the ferromagnet. The magnetization in the $F$-layer is in the $z$-direction, $\vec{\Omega} = (0, 0, 1)$.

ferromagnetic domain and vary the applied voltage $\Delta V$. Again, curves with higher peaks of $n_3$ correspond to larger values of $\Delta V$ and steeper slopes of $n_0$ at $x = x_1$. With increasing applied bias, the peaks become more and more asymmetric and the decay length (spin-diffusion length) of $n_3$ becomes larger.

8.2. **Five-layer system:** $N/F_1/N/F_2/N$**.** The second system under consideration is a five-layer system with total thickness $L = 900\,\mathrm{nm}$. Sandwiched between two non-magnetic contact layers (200 nm each), we put two magnetic layers with a thickness of 200 nm and different directions of magnetization $\vec{\Omega}_1$ and $\vec{\Omega}_2$, respectively, which are separated by a thin non-magnetic spacer layer of 50 nm. We have interfaces at $x_1 = 200\,\mathrm{nm}$, $x_2 = 400\,\mathrm{nm}$, $x_3 = 450\,\mathrm{nm}$ and $x_4 = 650\,\mathrm{nm}$. The five

domains have the following properties:

$$x \in (0, x_1]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad p(x) = 0, \tag{130}$$

$$x \in (x_1, x_2]: \quad \vec{\Omega}_1(x) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad p_1(x) = const., \tag{131}$$

$$x \in (x_2, x_3]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad p(x) = 0, \tag{132}$$

$$x \in (x_3, x_4]: \quad \vec{\Omega}_2(x) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad p_2(x) = const., \tag{133}$$

$$x \in (x_4, L]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad p(x) = 0. \tag{134}$$

The system (125), (129) is solved on a grid with 30 points in the 200 nm layers

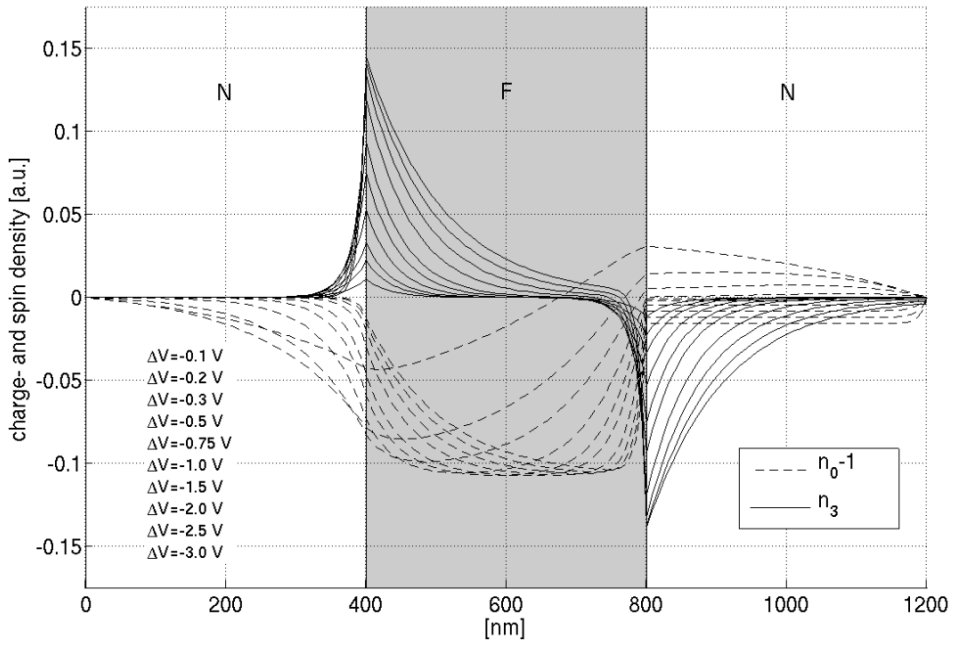


FIGURE 2. Simulated charge density $n_0 - 1$ and non-equilibrium spin density $\vec{n} = (0, 0, n_3)$ in a three-layer structure (non-magnet/ferromagnet/non-magnet) for different applied voltages $\Delta V$. The scattering polarization in the ferromagnet is $p = 0.33$, the magnetization in the $F$-layer points in the $z$-direction, $\vec{\Omega} = (0, 0, 1)$.

and 10 points in the 50 nm spacer layer. The time step was set to $0.01\,\tau_{sf}$. Grid

spacing and time step were chosen such that further refinement did not change the results. The applied voltage is $\Delta V = -1.0\,\mathrm{V}$ and the scattering polarization in both magnetic layers is $p = p_1 = p_2 = 0.33$. The steady state of this system is depicted in Figure 3. As in the three-layer case, c.f. section 8.1, the interfaces $x_1$-$x_4$ act as sources of non-equilibrium spin polarization. In the 5-layer setup, the $F_1$-layer leads to a spin polarization in $z$-direction whereas the $F_2$-layer causes a spin polarization in $y$-direction. Moreover, the non-magnetic spacer layer is thin enough such that a non-vanishing component of $\vec{n}$ perpendicular to $\vec{\Omega}_2$ arrives at the interface $x_3 = 450\,\mathrm{nm}$. The perpendicular component then rotates around $\vec{\Omega}_2$ and decays on a length scale that is determined by the strength of the exchange coupling $2\gamma\tau_{sf}/\hbar$ which was set to 4.0 in this simulation. A perpendicular component of the

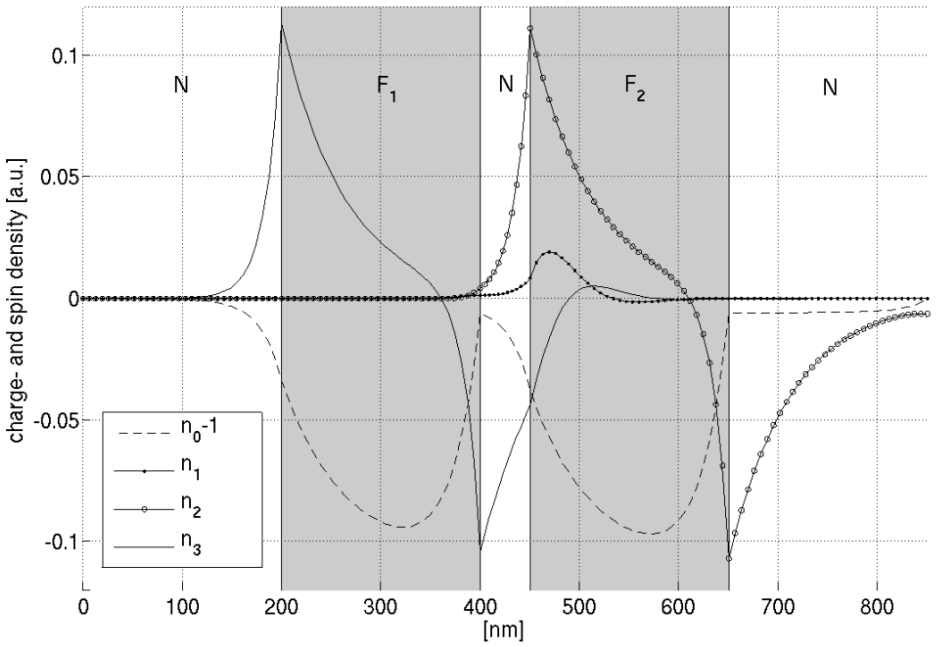


FIGURE 3. Simulated charge density $n_0 - 1$ and non-equilibrium spin density $\vec{n} = (n_1, n_2, n_3)$ in a five-layer structure (non-magnet/ferromagnet/non-magnet/ferromagnet/non-magnet) with applied voltage $\Delta V = -1.0\,\mathrm{V}$. The scattering polarization in the two ferromagnetic layers is $p = 0.33$. In the $F_1$-layer the magnetization points in the $z$-direction, $\vec{\Omega}_1 = (0, 0, 1)$, whereas in the $F_2$-layer the magnetization points in the $y$-direction, $\vec{\Omega}_2 = (0, 1, 0)$.

spin density with respect to the local magnetization can lead to magnetization dynamics if the current density $j_0$ is large enough [30, 5, 32]. This so-called 'spin-transfer torque' is the subject of ongoing research in the field of microelectronics [31, 19]. The spin-coherent drift-diffusion model developed in this work, when coupled to an equation of motion for $\vec{\Omega}$ (e.g. the Landau-Lifshitz equation [6]), is a possible approach towards a better understanding of these processes. As is demonstrated in Figure 3, our model has the advantage that it accounts for creation of non-equilibrium spin polarization at *each* interface in a multilayer structure.

8.3. **Magnetic domain wall.** The third system we consider is a ferromagnet with a thickness $L = 120\,\text{nm}$. At $x = 0$, the magnetization $\vec{\Omega}$ points in the $+z$-direction whereas at $x = L$ it points in the $-z$-direction. In the center of the ferromagnet, between $x_1 = 50\,\text{nm}$ and $x_2 = 70\,\text{nm}$, we place a small region $F_{DW}$ in which the magnetization $\vec{\Omega}$ rotates from $+z$ to $-z$ without acquiring an $x-$component, $\vec{\Omega}_1(x) = 0\,\forall\, x \in (x_1, x_2]$. The region $F_{DW}$ thus models a magnetic Bloch (domain) wall [4]. More precisely, we have:

$$x \in (0, x_1]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad p(x) = const., \tag{135}$$

$$x \in (x_1, x_2]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ \sin\left[\frac{\pi(x-x_1)}{x_2-x_1}\right] \\ \cos\left[\frac{\pi(x-x_1)}{x_2-x_1}\right] \end{pmatrix}, \quad p(x) = const., \tag{136}$$

$$x \in (x_2, L]: \quad \vec{\Omega}(x) = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \quad p(x) = const. \tag{137}$$

The scattering polarization is assumed to be the same in all domains. In this section, we solve the system (125), (129) but associated with von Neumann conditions for the charge density $n_0$ at $x = L$,

$$\partial_x n_0(t, x)\Big|_{x=L} = 0 \quad \forall t. \tag{138}$$

The von Neumann condition was chosen so that the electron charge density can evolve freely at the right boundary of the domain. The grid has 40 points in each layer and the time step was set to $\tau_{sf} \cdot 10^{-5}$. Grid spacing and time step were chosen such that further refinement did not change the results. We conducted two series of simulations, the results being depicted in Figures 4 and 5, respectively. We plot the respective parallel and perpendicular components of $\vec{n}$ with respect to the local magnetization $\vec{\Omega}$, given by $n_\parallel = \vec{n} \cdot \vec{\Omega}$ and $n_\perp = |\vec{n} - (\vec{n} \cdot \vec{\Omega})\vec{\Omega}|$. Figure 4 displays the case where $\Delta V = -0.2\,\text{V}$ and the scattering polarization $p$ is modulated between 0.1 and 0.7. For increasing $p$, one observes increasing $n_\perp$ and stronger variations of $n_\parallel$ in the $F_{DW}$ domain. Moreover, large $p$ leads to a significant difference between the charge densities on the two sides of the domain wall. In a second series, we set $p = 0.2$ and modulate the applied voltage $\Delta V$ between $-0.1\,\text{V}$ and $-1.0\,\text{V}$. The obtained results are displayed in Figure 5. Similar to the previous case, larger applied voltages lead to larger values of $n_\perp$ and stronger variations of $n_\parallel$ in the $F_{DW}$ domain. However, at $\Delta V \approx -0.7\,\text{V}$, we observe a saturation of the maximum value of the perpendicular component $n_\perp$, hence it stops increasing when the applied bias is increased further. In contrast, $n_\parallel$ and the offset of $n_0$ between the left and the right side of the domain wall still increase, but at a lower rate. This can be seen from the two curves for $\Delta V = -0.75\,\text{V}$ and $\Delta V = -1.0\,\text{V}$. To this point, we have not yet extracted the explanation for this behavior from (125).

9. **Conclusions.** In the present work, the authors introduced four spin-coherent collision operators that yield a mathematically well-posed matrix Boltzmann equation, describing the spin-coherent electron transport in ferromagnetic structures and which incorporates spin-dependent scattering rates. Existence and uniqueness of a weak solution to this equation were shown in Proposition 5.5. Moreover,

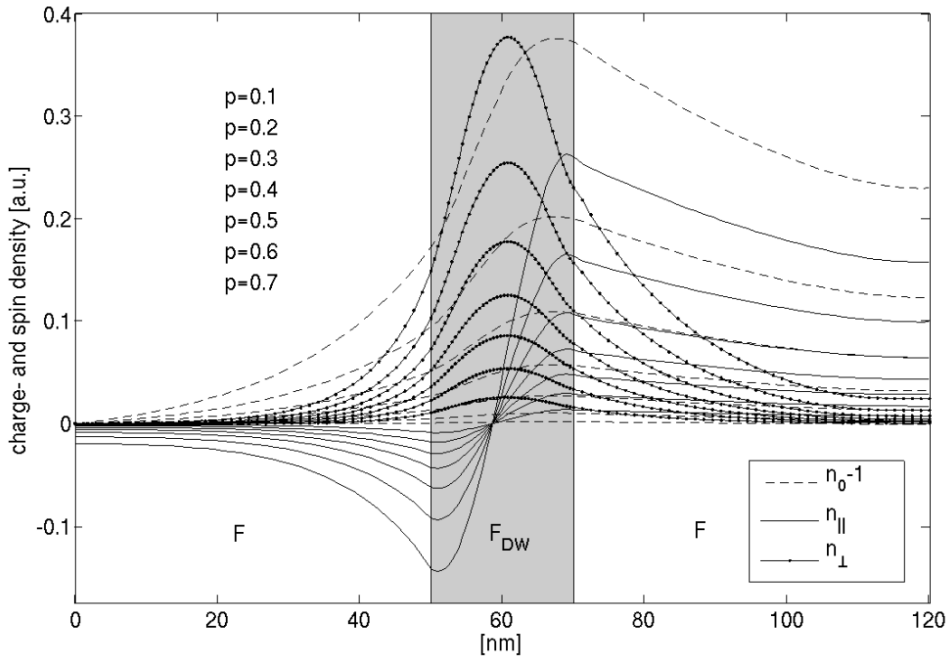


FIGURE 4. Simulated charge density $n_0 - 1$ and the parallel and perpendicular components, $n_\parallel$ and $n_\perp$, respectively, of the non-equilibrium spin density $\vec{n}$ with respect to the local magnetization $\vec{\Omega}(x)$ for different values of the scattering polarization parameter $p$. The respective magnetizations in the two $F$-domains are constant and anti-parallel and a domain wall was realized in the $F_{DW}$-domain, where $\vec{\Omega}(x)$ is given by (136). The applied voltage is $\Delta V = -0.2\,\mathrm{V}$.

the maximum principle was verified for the anti-symmetric collision operator $Q_{21}$ in Proposition 5.6. Assuming parabolic spin bands with momentum-independent band gap (Stoner model), further assuming Boltzmann statistics and applying the condition of detailed balance, the symmetric collision operator $Q_{22}$ was investigated from a rigorous mathematical point of view (Proposition 6.3). We then performed the diffusion limit in the scaled matrix Boltzmann equation, the small parameter $\varepsilon^2$ being the ratio of the respective time scales of spin conserving and spin altering collision processes. The obtained spin-coherent drift-diffusion equation (Theorem 7.1) contains a coupling between the charge- and the spin degree of freedom of the electron system that is linear in the polarization $p$ of the scattering rates. The new macroscopic model was applied to simulate spin-polarized transport in three different one-dimensional structures, namely a three- and a five-layer magnetic/non-magnetic multilayer and a magnetic domain wall. The simulations show that our model can improve the understanding of spin-polarized electron transport, which is important in spintronic research fields such as spin-transfer torque devices and current-induced domain wall motion.

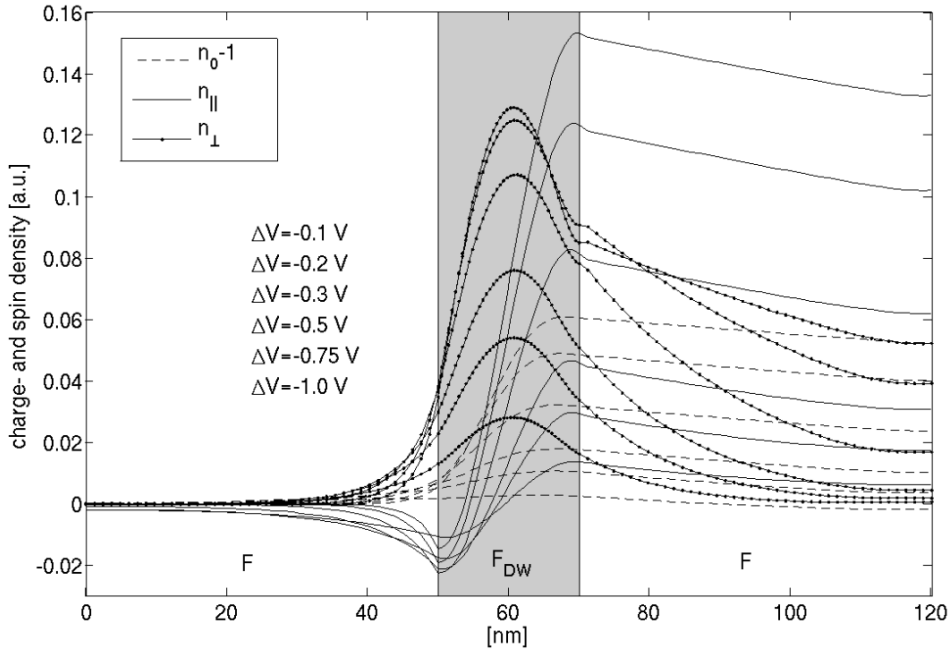


FIGURE 5. Simulated charge density $n_0 - 1$ and the parallel and perpendicular components, $n_\parallel$ and $n_\perp$, respectively, of the non-equilibrium spin density $\vec{n}$ with respect to the local magnetization $\vec{\Omega}(x)$ for different applied voltages $\Delta V$. The respective magnetizations in the two $F$-domains are constant and anti-parallel and a domain wall was realized in the $F_{DW}$-domain, where $\vec{\Omega}(x)$ is given by (136). The scattering polarization is $p = 0.2$.

**Appendix** A. **Computation of the coefficients $\omega_{ij}$ and $\gamma_{ij}$.** Here, we shall compute the coefficients $\omega_{ij}$ respectively $\gamma_{ij}$, $i, j \in \{1, 2\}$, appearing in equation (83) for the eigenvalue $f_-$ of the distribution matrix $F$. Starting from (82) and looking at (78) and (81) we deduce

$$\Pi_-(Q_j^-(F)) = \frac{1}{2}\mathrm{tr}\left(Q_j^-(F)\right) - \frac{1}{2}\mathrm{tr}\left(\vec{\sigma}Q_j^-(F)\right)\cdot\frac{\vec{f}}{|\vec{f}|}. \tag{139}$$

The loss terms $Q_j^-(F)$ are defined in (33)-(34). We recall that $\Lambda = \int S\mathrm{d}k'$, $\Lambda = \lambda_0\sigma_0 + \vec{\lambda}\cdot\vec{\sigma}$ and $F = \frac{1}{2}f_0\sigma_0 + \vec{f}\cdot\vec{\sigma}$ in the Pauli basis. From Lemma 2.4 we deduce

$$\frac{1}{2}\mathrm{tr}\left(Q_1^-(F)\right) = \frac{1}{2}\mathrm{tr}\left(Q_2^-(F)\right) = \frac{1}{2}\lambda_0 f_0 + \vec{\lambda}\cdot\vec{f}. \tag{140}$$

Moreover, we have

$$\frac{1}{2}\mathrm{tr}\left(\vec{\sigma}Q_1^-(F)\right)\cdot\frac{\vec{f}}{|\vec{f}|}=\lambda_0|\vec{f}|+\frac{1}{2}f_0\vec{\lambda}\cdot\frac{\vec{f}}{|\vec{f}|} \tag{141}$$

$$\frac{1}{2}\mathrm{tr}\left(\vec{\sigma}Q_2^-(F)\right)\cdot\frac{\vec{f}}{|\vec{f}|}=\frac{1}{2}f_0\vec{\lambda}\cdot\frac{\vec{f}}{|\vec{f}|}+|\vec{f}|\int_{\mathbb{R}^d_{k'}}\sqrt{s_0^2-|\vec{s}|^2}\mathrm{d}k'+ \tag{142}$$

$$+|\vec{f}|\int_{\mathbb{R}^d_{k'}}\left(s_0-\sqrt{s_0^2-|\vec{s}|^2}\right)\left(\frac{\vec{f}}{|\vec{f}|}\cdot\frac{\vec{s}}{|\vec{s}|}\right)^2\mathrm{d}k'.$$

Let us introduce the angle $\eta$ between $\vec{\lambda}$ and $\vec{f}$ via

$$\cos(\eta)=\frac{\vec{\lambda}}{|\vec{\lambda}|}\cdot\frac{\vec{f}}{|\vec{f}|}=\frac{\vec{s}}{|\vec{s}|}\cdot\frac{\vec{f}}{|\vec{f}|}, \tag{143}$$

where the second equality is a consequence of (29), stating that the direction $\vec{s}/|\vec{s}|$ of $S$ must not depend on $k'$. Then, inserting (140) and (141) respectively (142) into (139), a straightforward calculation yields

$$\Pi_-(Q_1^-(F))=f_-\left(\lambda_0-|\vec{\lambda}|\cos(\eta)\right) \tag{144}$$

$$\Pi_-(Q_2^-(F))=f_-\left(\lambda_0-|\vec{\lambda}|\cos(\eta)\right)+|\vec{f}|\sin^2(\eta)\int_{\mathbb{R}^d_{k'}}\left(s_0-\sqrt{s_0^2-|\vec{s}|^2}\right)\mathrm{d}k' \tag{145}$$

Inserting (144) respectively (145) into (82) we obtain the coefficients $\omega_{ij}$ and $\gamma_{ij}$, $i,j\in\{1,2\}$, defined in (83),

$$\omega_{11}=\omega_{12}=\omega_{21}=\omega_{22}=\frac{1}{\tau_c}\left(\lambda_0-|\vec{\lambda}|\cos(\eta)\right) \tag{146}$$

$$\gamma_{11}=\frac{1}{\tau_c}\Pi_-(G_1)+\frac{1}{\tau_{sf}}|\vec{f}| \tag{147}$$

$$\gamma_{21}=\frac{1}{\tau_c}\Pi_-(G_2)+\frac{1}{\tau_{sf}}|\vec{f}| \tag{148}$$

$$\gamma_{12}=\frac{1}{\tau_c}\Pi_-(G_1)+|\vec{f}|\left(\frac{1}{\tau_{sf}}-\frac{1}{\tau_c}\sin^2(\eta)\int_{\mathbb{R}^d_{k'}}\left(s_0-\sqrt{s_0^2-|\vec{s}|^2}\right)\mathrm{d}k'\right) \tag{149}$$

$$\gamma_{22}=\frac{1}{\tau_c}\Pi_-(G_2)+|\vec{f}|\left(\frac{1}{\tau_{sf}}-\frac{1}{\tau_c}\sin^2(\eta)\int_{\mathbb{R}^d_{k'}}\left(s_0-\sqrt{s_0^2-|\vec{s}|^2}\right)\mathrm{d}k'\right). \tag{150}$$

**Acknowledgments.** The authors would like to send a special and warm thank to their PhD advisor, Naoufel Ben Abdallah, from whom they learned a lot and who was also at the origin of the present work. This work has been supported by the Austrian Science Fund, Vienna, under the contract number P21326-N16 and by the ANR QUATRAIN ("Quantum transport in nanoscale structures").

## REFERENCES

[1] L.E. Ballentine, "Quantum Mechanics. A Modern Development", Revised edition, World Scientific Publishing, River Edge, NJ, 1998.

[2] L. Barletti and G. Frosali, *Diffusive limit of the two-band k.p model for semiconductors*, J. Stat. Phys. **139** (2010), 280–306.

[3] L. Barletti and F. Méhats, *Quantum drift-diffusion modeling of spin transport in nanostructures*, J. Math. Phys. **51** (2010), 053304, 20pp.

[4] G.S.D. Beach, M. Tsoi, and J.L. Erskine, *Current-induced domain wall motion*, J. Magn. Magn. Mater. **320** (2008), 1272–1281.
[5] L. Berger, *Emission of spin waves by a magnetic multilayer traversed by a current*, Phys. Rev. B **54** (1996), 9353–9358.
[6] D.V. Berkov and J. Miltat, *Spin-torque driven magnetization dynamics: micromagnetic modeling*, J. Magn. Magn. Mater. **320** (2008), 1238–1259.
[7] H.-P. Breuer and F. Petruccione, "The Theory of Open Quantum Systems", Oxford University Press, New York, 2002.
[8] I.A. Campbell, A. Fert, and A.R. Pomeroy, *Evidence for two current conduction in iron*, Phil. Mag. **15** (1967), 977–981, arXiv:0711.4478.
[9] M.I. Dyakonov (ed.), "Spin Physics in Semiconductors", Springer-Verlag, Berlin Heidelberg, 2008.
[10] R. El Hajj, *Diffusion models for spin transport derived from the spinor Boltzmann equation*, Comm. Math. Sci. (to appear).
[11] R. El Hajj, *Etude mathématique et numérique de modèles de transport: application à la spintronique*, Ph.D. thesis, Institut de Mathématiques de Toulouse (IMT), Université Paul Sabatier, 2008.
[12] H.A. Engel, E.I. Rashba, and B.I. Halperin, *Theory of spin Hall effects in semiconductors*, Handbook of Magnetism and Advanced Magnetic Materials, John Wiley & Sons, Ltd, 2007, arXiv:cond-mat/0603306v3.
[13] C. Ertler, A. Matos-Abiague, M. Gmitra, M. Turek, and J. Fabian, *Perspectives in spintronics: magnetic resonant tunneling, spin-orbit coupling, and GaMnAs*, J. Phys. Conf. Ser. **129** (2008), 012021, arXiv:0811.0500.
[14] A. Fert, *Nobel lecture: Origin, development, and future of spintronics*, Rev. Mod. Phys. **80** (2008), 1517–1530.
[15] A. Fert and I.A. Campbell, *Electrical resistivity of ferromagnetic nickel and iron based alloys*, J. Phys. F: Metal Phys. **6** (1976), 849–871.
[16] O. Gunnarsson, *Band model for magnetism of transition metals in the spin-density-functional formalism*, J. Phys. F: Metal Phys. **6** (1976), 587.
[17] R.Q. Hood and R.M. Falicov, *Boltzmann-equation approach to the negative magnetoresistance of ferromagnetic-normal-metal multilayers*, Phys. Rev. B **46** (2007), 8287.
[18] M. Johnson and R.H. Silsbee, *Interfacial charge-spin coupling: injection and detection of spin magnetization in metals*, Phys. Rev. Lett. **55** (1985), 1790.
[19] J.A. Katine and E.E. Fullerton, *Device implications of spin-transfer torques*, J. Magn. Magn. Mater. **320** (2008), 1217–1226.
[20] D. Loss and D.P. DiVincenzo, *Quantum computation with quantum dots*, Phys. Rev. A **57** (1998), 120–126.
[21] O. Morandi and F. Schürrer, *Wigner model for quantum transport in graphene*, J. Phys. A (accepted) (2011), arXiv:1102.2416.
[22] W. Nolting and A. Ramakanth, "Quantum Theory of Magnetism", Springer-Verlag Berlin Heidelberg, 2009.
[23] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, *Two-dimensional gas of massless Dirac fermions in graphene*, Nature **438** (2005), 197–200.
[24] F. Piéchon and A. Thiaville, *Spin transfer torque in continuous textures: semiclassical Boltzmann approach*, Phys. Rev. B **75** (2007), 174414.
[25] F. Poupaud, *Diffusion approximation of the linear semiconductor equation: analysis of boundary layers*, Asympt. Anal. **4** (1991), 293–317.
[26] Y. Qi, S. Zhang, *Spin diffusion at finite electric and magnetic fields*, Phys. Rev. B **67** (2003), 052407.
[27] D.C. Ralph and M.D. Stiles, *Spin transfer torques*, J. Magn. Magn. Mater. **320** (2008), 1190–1216.
[28] S. Saikin, *A drift-diffusion model for spin-polarized transport in a two-dimensional non-degenerate electron gas controlled by spin-orbit interaction*, J. Phys.: Condens. Matter **16** (2010), 5071–5081, arXiv:cond-mat/0311221v3.
[29] E. Simanek, *Spin accumulation and resistance due to a domain wall*, Phys. Rev. B **63** (2001), 224412.
[30] J.C. Slonczewski, *Current-driven excitation of magnetic multilayers*, J. Magn. Magn. Mater. **159** (1996), L1–L7.

[31] M.D. Stiles and J. Miltat, *Spin-transfer torque and dynamics*, Top. Appl. Phys. **101** (2006), 225.
[32] M. Tsoi, A.G.M. Jansen, J. Bass, W.-C. Chiang, M. Seck, V. Tsoi, and P. Wyder, *Excitation of a magnetic multilayer by an electric current*, Phys. Rev. Lett. **80** (1998), 4281.
[33] T. Valet and A. Fert, *Theory of the perpendicular magnetoresistance in magnetic multilayers*, Phys. Rev. B **48** (1993), 7099.
[34] P.C. van Son, H. van Kempen, and P. Wyder, *Boundary resistance of the ferromagnetic-nonferromagnetic metal interface*, Phys. Rev. Lett. **58** (1987), 2271.
[35] L. Villegas-Lelovsky, *Hydrodynamic model for spin-polarized electron transport in semiconductors*, J. Appl. Phys. **101** (2007), 053707.
[36] C. Vouille, A. Barthélémy, F. Elokan Mpondo, A. Fert, P. A. Schroeder, S. Y. Hsu, A. Reilly, and R. Loloee, *Microscopic mechanisms of giant magnetoresistance*, Phys. Rev. B **60** (1999), 6710.
[37] M. Wenin and W. Pötz, *Optimal control of a single qubit by direct inversion*, Phys. Rev. A **74** (2006), 022319.
[38] J. Xiao, A. Zangwill, and M.D. Stiles, *A numerical method to solve the Boltzmann equation for a spin valve*, Eur. Phys. J. B **59** (2007), 415–427.
[39] N. Zamponi, L. Barletti, *Quantum electronic transport in graphene: a kinetic and fluid-dynamic approach*, Mathematical Methods in Applied Sciences **34** (2010), 807–818.
[40] J. Zhang, P.M. Levy, S. Zhang, and V. Antropov, *Identification of transverse spin currents in noncollinear magnetic structures*, Phys. Rev. Lett. **93** (2004), 256602, arXiv:cond-mat/0405610v1.
[41] S. Zhang, P.M. Levy, and A. Fert, *Mechanisms of spin-polarized current-driven magnetization switching*, Phys. Rev. Lett. **88** (2002), 236601.
[42] I. Zutic, J. Fabian, and Das Sarma S., *Spintronics: fundamentals and applications*, Rev. Mod. Phys. **76** (2004), 323–410.

Received xxxx 20xx; revised xxxx 20xx.

*E-mail address*: possanner@tugraz.at
*E-mail address*: claudia.negulescu@cmi.univ-mrs.fr