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ENERGY-TRANSPORT MODELS FOR SPIN TRANSPORT IN FERROMAGNETIC SEMICONDUCTORS*

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Abstract. Explicit energy-transport equations for the spinorial carrier transport in ferromagnetic semiconductors are calculated from a general spin energy-transport system that was derived by Ben Abdallah and El Hajj from a spinorial Boltzmann equation. The novelty of our approach is the simplifying assumptions leading to explicit models which extend both spin drift-diffusion and semiclassical energy-transport equations. The explicit models allow us to examine the interplay between the spin and charge degrees of freedom. In particular, the dissipation of the entropy (or free energy) is quantified, and the existence of weak solutions to a time-discrete version of one of the models is proved, using novel truncation arguments. Numerical experiments in one-dimensional multilayer structures using a finite-volume discretization illustrate the effect of the temperature and the polarization parameter.

Keywords. spin transport, energy-transport equations, entropy inequalities, existence of weak solutions, finite-volume method, semiconductors.

AMS subject classifications. 35J47, 35J60, 65M08, 82D37.

1. Introduction

Spintronics is a new emerging field in solid-state physics with the aim to exploit the spin degree of freedom of electrons, which may lead to smaller and faster semiconductor devices with reduced power consumption. The aim of the mathematical modeling of spin-polarized materials is to develop a hierarchy of models that describe the relevant physical phenomena in an accurate way and, at the same time, allow for fast and efficient numerical predictions. A model class which seems to fulfill the requirements of precision and simplicity are moment equations derived from the (spinorial) Boltzmann equation.

In the literature, up to now, mostly lowest-order moment equations for spin transport have been investigated, namely spin drift-diffusion-type equations [8,17–19]. These models are mathematically analyzed in [10, 11, 14, 20]. When hot electron thermalization has to be taken into account, the carrier transport needs to be described by higher-order moment equations including energy transport. This leads to semiclassical energy-transport equations in semiconductors, see, e.g., [1, 2, 5, 13]. A spinorial energy-transport model was derived in [3], but the equations are not explicit such that its structure is not easy to analyze. The goal of this paper is to derive and analyze simplified explicit versions of this model.

The starting point is the spinorial Boltzmann equation for the distribution function $F(x,k,t)$ with values in the space of Hermitian 2×2 matrices,

$$\partial_t F + k\cdot\nabla_x F - \nabla_x V\cdot\nabla_k F = Q(F) + \frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma},F] + Q_{\rm sf}(F), \tag{1.1}$$

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where $x\in\mathbb{R}^3$ denotes the spatial variable, $k\in\mathbb{R}^3$ the wave vector, $t>0$ the time, $\mathrm{i}=\sqrt{-1}$ the imaginary unit, and $[\cdot,\cdot]$ the commutator. The function $V(x,t)$ is the electric potential, which is usually self-consistently defined as the solution of the Poisson equation

$$-\lambda_D^2\Delta V = n_0[F]-C(x), \quad n_0[F]=\frac{1}{2}\mathrm{tr}\int_{\mathbb{R}^3} F dk,$$

where λ_D is the scaled Debye length, $n_0[F]$ the charge density, "tr" the trace of a matrix, and $C(x)$ the doping concentration [13]. Furthermore, $\vec{\Omega}(x)$ is a local magnetization field and $\vec{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ is the vector of the Pauli matrices. We choose the spin-conserving BGK-type collision operator $Q(F)=M[F]-F$, where the Maxwellian $M[F]$ is such that $Q(F)$ conserves mass and energy (in the sense of (3.2)), and the operator $Q_{\mathrm{sf}}(F)$ models spin-flip interactions. Details are given in Section 3.1.

Assuming dominant collisions and a large time scale, moment equations for the electron density $n[A,C]$ and energy density $W[A,C]$ can be derived from equation (1.1) in the diffusion limit [3], leading to

$$\begin{aligned}\partial_t n[A,C]+\operatorname{div} J_n &= F_n[\vec{\Omega},A,C],\\ \partial_t W[A,C]+\operatorname{div} J_W + J_n\cdot\nabla V &= F_W[\vec{\Omega},A,C], \quad x\in\mathbb{R}^3,\ t>0,\end{aligned} \tag{1.2}$$

where J_n and J_W are the particle and energy flux, respectively, and F_n, F_W are some functions; we refer to Section 3.1 for details. Furthermore, A and C are the Lagrange multipliers which are obtained from entropy maximization under the constraints of given mass and energy, and the electron and energy densities are the zeroth- and second-order moments

$$n[A,C]=\int_{\mathbb{R}^3} M[A,C]dk, \quad W[A,C]=\frac{1}{2}\int_{\mathbb{R}^3} M[A,C]|k|^2 dk,$$

where $M[A,C]=\exp(A+C|k|^2/2)$ is the spinorial Maxwellian. Note that A and C are Hermitian matrices in $\mathbb{C}^{2\times 2}$, so $n[A,C]$ and $W[A,C]$ are Hermitian matrices too.

In contrast to the semiclassical situation, the densities cannot be expressed explicitly in terms of the Lagrange multipliers because of the matrix structure. In order to obtain explicit equations, we need to impose simplifying assumptions on A and C. Our strategy is to first formulate the variables in terms of the Pauli basis,

$$A=a_0\sigma_0+\vec{a}\cdot\vec{\sigma}, \quad C=c_0\sigma_0+\vec{c}\cdot\vec{\sigma},$$

where σ_0 is the unit matrix and a_0, $c_0\in\mathbb{R}$, $\vec{a}$, $\vec{c}\in\mathbb{R}^3$. The densities may be expanded in this basis as well, $n[A,C]=n_0\sigma_0+\vec{n}\cdot\vec{\sigma}$, $W[A,C]=W_0\sigma_0+\vec{W}\cdot\vec{\sigma}$, and the Maxwellian becomes

$$M[A,C]=e^{a_0+c_0|k|^2/2}\left(\cosh|\vec{b}(k)|\sigma_0+\frac{\sinh|\vec{b}(k)|}{|\vec{b}(k)|}\vec{b}(k)\cdot\vec{\sigma}\right), \quad \vec{b}(k):=\vec{a}+\vec{c}\frac{|k|^2}{2}. \tag{1.3}$$

The formulation of the energy-transport model (1.2) in terms of the Pauli components $(a_0,\vec{a})$, $(c_0,\vec{c})$ still leads to nonexplicit equations, so we will impose some conditions. We will derive three model classes by assuming $\vec{c}=0$, $\vec{a}=0$, or $\vec{a}=\lambda\vec{c}$ for some $\lambda=\lambda(x,t)$ and show the following results:

- First model class ($\vec{c}=0$): we discretize the one-dimensional equations using a semi-implicit Euler finite-volume scheme and illustrate the effect of the temperature on two multilayer structures.

- Second model class ($\vec{a}=0$): we show the existence of weak solutions to a time-discrete version.
- Third model class ($\vec{a}=\lambda\vec{c}$): we show that the equation for the spin accumulation density $\vec{s}=\vec{n}/|\vec{n}|$ has some similarities with the Landau–Lifshitz equation.
- All model classes: we quantify the dissipation of the entropy (free energy), thus providing not only the monotonicity of the entropy but also gradient estimates.

These assumptions mean that we impose additional properties to the local equilibrium related to the moments n_0, $\vec{n}$, W_0, and $\vec{W}$. Namely, some components of the moments are determined by the other ones, so that the local equilibrium coincides with that one that could be obtained by imposing the conservation of selected fewer moments.

These findings are a first step to understand higher-order spinorial macroscopic models which may lead to improved simulation outcomes.

The paper is organized as follows. The main results are detailed in Section 2. The derivation of the general energy-transport model from the spinorial Boltzmann equation is recalled in Section 3.1 and the general model is formulated in terms of the Pauli components in Section 3.2. In Section 4, the three simplified energy-transport model classes are derived. The entropy structure is investigated in Section 5, and the existence result for the second model is stated and proved in Section 6. Some numerical experiments for the first model are performed in Section 7.

2. Main results

We detail the main results of this paper.

2.1. Derivation of explicit spin energy-transport models.

We derive explicit versions of model (1.2) under three simplifying assumptions on the Pauli components of A and C.

First model: $\vec{c}=0$. If the Lagrange multiplier C is interpreted as a "temperature" tensor, it might be reasonable to suppose that the "spin" part $\vec{c}$ is much smaller than the non-vanishing trace part c_0, which motivates the simplification $\vec{c}=0$. This allows us to write three of the eight scalar moments $(n_0,\vec{n})$ and $(W_0,\vec{W})$ in terms of the remaining moments, leading to equations for five moments. We choose the moments $(n_0,\vec{n},W_0)$, leading to the system (see Section 4.1)

$$\partial_t n_0+\operatorname{div}J_n=0,\qquad J_n=-\big(\nabla(n_0T)+n_0\nabla V\big),\tag{2.1}$$

$$\frac{3}{2}\partial_t(n_0T)+\operatorname{div}J_W+J_n\cdot\nabla V=0,\qquad J_W=-\frac{5}{2}\big(\nabla(n_0T^2)+n_0T\nabla V\big),\tag{2.2}$$

$$\partial_t\vec{n}-\sum_{j=1}^{3}\partial_{x_j}\big(\partial_{x_j}(\vec{n}T)+\vec{n}\partial_{x_j}V\big)+\vec{\Omega}_{\rm e}\times\vec{n}=-\frac{\vec{n}}{\tau_{\rm sf}},\qquad x\in\mathbb{R}^3,\ t>0,\tag{2.3}$$

where $T=2W_0/(3n_0)$ is interpreted as the electron temperature, $\partial_{x_j}=\partial/\partial x_j$, $\vec{\Omega}_{\rm e}$ is the even part of the effective field (with respect to k), and $\tau_{\rm sf}>0$ is the spin-flip relaxation time. In this model, $(n_0,\frac{3}{2}n_0T)$ solves the semiclassical energy-transport equations, and the spin-vector density $\vec{n}$ solves a drift-diffusion-type equation, which is coupled to the equations for $(n_0,\frac{3}{2}n_0T)$ via T only. Our numerical experiments indicate that this coupling is rather weak.

Motivated from [18], we may include a polarization matrix P in the definition of the collision operator $Q(F)$. We choose $Q(F)=P^{1/2}(M[F]-F)P^{1/2}$, where the direction of $P=\sigma_0+p\vec{\Omega}\cdot\vec{\sigma}$ in spin space is the local magnetization $\vec{\Omega}$ and $p\in[0,1)$ represents the spin polarization of the scattering rates. This operator conserves spin, mass, and (in contrast to the operators in [18]) energy. The corresponding spin energy-transport model (still under the assumption $\vec{c}=0$) becomes (see Remark 4.1)

$$\partial_t n_0 + \operatorname{div} \mathcal{J}_n = 0, \qquad \mathcal{J}_n = \eta^{-2}\big(J_n - p\vec{\Omega}\cdot\vec{J}_n\big), \tag{2.4}$$

$$\frac{3}{2}\partial_t(n_0 T) + \operatorname{div}\mathcal{J}_W + \mathcal{J}_n\cdot\nabla V = 0, \qquad \mathcal{J}_W = \eta^{-2}\big(J_W - p\vec{\Omega}\cdot\vec{J}_W\big), \tag{2.5}$$

$$\partial_t \vec{n} + \operatorname{div}\vec{\mathcal{J}} + \vec{\Omega}_{\rm e}\times\vec{n} = -\frac{\vec{n}}{\tau_{\rm sf}}, \qquad x\in\mathbb{R}^3,\ t>0, \tag{2.6}$$

where $\eta = \sqrt{1-p^2}$, J_n, J_W are as above, and

$$\vec{J}_n = -\big(\nabla(\vec{n}T) + \vec{n}\nabla V\big), \quad \vec{J}_W = -\frac{5}{2}\big(\nabla(\vec{n}T^2) + \vec{n}\nabla V\big),$$
$$\vec{\mathcal{J}} = \eta^{-2}\big((1-\eta)(\vec{J}_n\cdot\vec{\Omega})\vec{\Omega} + \eta\vec{J}_n - p\vec{\Omega}J_n\big).$$

Note that we recover the model (2.1)–(2.3) if $p=0$. We compare both models numerically in Section 7. It turns out that the polarization matrix P leads to a stronger mixing of the spin density components, and the heat flux effects causes a smoothing of these components.

Second model: $\vec{a}=0$. The Lagrange multiplier A may be related to the particle density. Supposing that the spin effects are rather encoded in $\vec{c}$, one may assume that $\vec{a}=0$. This condition gives as above three constraints and leads to equations for five moments. One may choose, for instance, the variables $(n_0,\vec{n},T)$ or $(n_0,T,\vec{W})$. In the former case, we arrive at the system of coupled equations

$$\partial_t n_0 + \operatorname{div} J_n = 0, \qquad J_n = -\big(\nabla(n_0T) + n_0\nabla V\big), \tag{2.7}$$

$$\frac{3}{2}\partial_t(n_0T) + \operatorname{div} J_W + J_n\cdot\nabla V = 0, \qquad J_W = -\frac{5}{2}\big(\nabla(D(n_+,n_-)n_0T^2) + n_0T\nabla V\big), \tag{2.8}$$

$$\partial_t\vec{n} - \sum_{j=1}^{3}\partial_{x_j}\left(\partial_{x_j}\left(p(n_+,n_-)n_0T\frac{\vec{n}}{|\vec{n}|}\right) + \vec{n}\partial_{x_j}V\right) + \vec{\Omega}_{\rm e}\times\vec{n} = -\frac{\vec{n}}{\tau_{\rm sf}}, \tag{2.9}$$

and $D(n_+,n_-)$, $p(n_+,n_-)$, defined in equation (4.9), depend on the spin-up/spin-down densities $n_\pm := n_0 \pm |\vec{n}|$ (see Section 4.2). Compared to the first model, these coefficients realize a coupling between the charge and spin-vector densities. A similar model can be derived in the variables $(n_0,T,\vec{W})$. This coupling is still rather weak since the function $D(n_+,n_-)$ only takes values in the interval $[1,1.1]$; see Remark 4.2.

Third model: $\vec{a}=\lambda\vec{c}$. Generalizing the above approaches, we suppose that the vectors $\vec{a}$ and $\vec{c}$ are aligned such that $\vec{a}=\lambda\vec{c}$ for some function $\lambda=\lambda(x,t)\neq 0$. The first model is recovered for $\lambda\to\infty$, the second one for $\lambda=0$. This condition provides only two constraints such that we obtain a system for six moments. A possible choice is $(n_\pm, W_\pm, \vec{s})$, where $n_\pm = n_0 \pm |\vec{n}|$, $W_\pm = W_0 \pm |\vec{W}|$, and $\vec{s} = \vec{n}/|\vec{n}|$, which gives the equations

$$\partial_t n_\pm + \operatorname{div} J_{n,\pm} = \mp\frac{n_+ - n_-}{2\tau_{\rm sf}} \mp \frac{1}{2}(n_+T_+ - n_-T_-)|\nabla\vec{s}|^2, \tag{2.10}$$

$$\frac{3}{2}\partial_t(n_\pm T_\pm) + \operatorname{div} J_{W,\pm} + J_{n,\pm}\cdot\nabla V = \mp\frac{3}{4\tau_{\rm sf}}(n_+T_+ - n_-T_-)$$
$$\mp\frac{5}{4}(n_+T_+^2 - n_-T_-^2)|\nabla\vec{s}|^2, \tag{2.11}$$

$$\partial_t \vec{s} - \frac{n_+T_+ - n_-T_-}{n_+ - n_-}\vec{s}\times(\Delta\vec{s}\times\vec{s}) = \left(2\frac{\nabla(n_+T_+ - n_-T_-)}{n_+ - n_-} + \nabla V\right)\cdot\nabla\vec{s} - \vec{\Omega}_{\rm e}\times\vec{s}, \quad (2.12)$$

where $|\nabla\vec{s}| = \sum_{j=1}^3 |\nabla s_j|^2$, the spin-up/spin-down particle and heat fluxes are given by

$$J_{n,\pm} = -\big(\nabla(n_\pm T_\pm) + n_\pm\nabla V\big), \quad J_{W,\pm} = -\frac{5}{2}\big(\nabla(n_\pm T_\pm^2) + n_\pm T_\pm\nabla V\big), \quad (2.13)$$

and the spin-up/spin-down energy densities are $W_\pm = \frac{3}{2}n_\pm T_\pm$. The evolution equations for the spin-up/spin-down densities are similar in structure as the first and second model. For constant "temperature" $T_+ = T_- = 1$, we recover the two-component spin drift-diffusion equations analyzed in [11]. The coupling is realized through the spin-accumulation density $\vec{s}$. The equation for $\vec{s}$ preserves the relation $|\vec{s}| = 1$, and the second-order term $\vec{s}\times(\Delta\vec{s}\times\vec{s})$ also appears in the Landau–Lifshitz equation [15]; see Remark 4.4.

2.2. Entropy inequalities. We derive explicit entropy (or free energy) functionals which are nonincreasing in time along solutions to the corresponding equations.[1] To simplify the computations, we neglect electric effects, i.e., the potential V is assumed to be constant (also see Remark 5.1 for the general situation).

The kinetic entropy of the general spin model (1.2) is given by

$$H = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} {\rm tr}(M\log M)dkdx, \quad (2.14)$$

where the Maxwellian is defined by equation (1.3) and "tr" denotes the trace of a matrix. It was shown in [3, Theorem 2.2] that the entropy is nonincreasing along solutions to model (1.2). Our aim is to quantify the entropy production $-dH/dt$ which provides gradient estimates. To this end, we insert the Maxwellians (2.14) under the simplifying assumptions on $(\vec{a},\vec{c})$ specified above and compute explicit expressions for the entropies. Denoting by H_j the entropy of the jth model presented above, we obtain

$$H_1 = \int_{\mathbb{R}^3}\big(n_+\log(n_+T_+^{-3/2}) + n_-\log(n_-T_-^{-3/2})\big)dx, \quad (2.15)$$

$$H_2 = \frac{5}{2}\int_{\mathbb{R}^3} n_0\log\frac{n_0}{W_+^{3/5} + W_-^{3/5}}dx, \quad \text{where } W_\pm = \frac{3}{2}n_0T \pm |\vec{W}|^2, \quad (2.16)$$

$$H_3 = H_1, \quad (2.17)$$

and the corresponding entropy inequalities read as (see Propositions 5.1-5.3)

$$\begin{aligned}
&\frac{dH_1}{dt} + 4\int_{\mathbb{R}^3}\big(|\nabla\sqrt{n_+T}|^2 + |\nabla\sqrt{n_-T}|^2 + 5n_0|\nabla\sqrt{T}|^2\big)dx \le 0,\\
&\frac{dH_2}{dt} + c\int_{\mathbb{R}^3}\big(|\nabla\sqrt{W_+}|^2 + |\nabla\sqrt{W_-}|^2 + T|\nabla\sqrt{n_0}|^2\big)dx \le 0,\\
&\frac{dH_3}{dt} + c\int_{\mathbb{R}^3}\sum_{s=\pm}\big(T_s|\nabla\sqrt{n_s}|^2 + n_s|\nabla\sqrt{T_s}|^2\big)dx \le 0,
\end{aligned} \quad (2.18)$$

where $c > 0$ is some number and the results hold for smooth solutions.

[1] In contrast to the physical notation, the mathematical entropy is defined here as the negative physical entropy.

2.3. Existence analysis for the second model. The second analytical result concerns the existence analysis for the second model ($\vec{a}=0$) in the variables $(n_0, W_0, \vec{W})$, where $W_0 = \frac{3}{2} n_0 T$. Because of the strong coupling, we are only able to prove the existence of solutions to a time-discrete version without electric field in a bounded domain $\mathcal{D} \subset \mathbb{R}^d$:

$$\frac{1}{h}(n_0 - n_0^0) - \frac{2}{3}\Delta W_0 = 0, \tag{2.19}$$

$$\frac{1}{h}(W_0 - W_0^0) - \frac{8}{15}\Delta\left(\frac{1}{n_0}(W_+^{3/5} + W_-^{3/5})(W_+^{7/5} + W_-^{7/5})\right) = 0, \tag{2.20}$$

$$\frac{1}{h}(\vec{W} - \vec{W}^0) - \frac{5}{18}\Delta\left(\frac{1}{n_0}(W_+^{3/5} + W_-^{3/5})(W_+^{7/5} - W_-^{7/5})\frac{\vec{W}}{|\vec{W}|}\right) = -\frac{\vec{W}}{\tau_{\mathrm{sf}}} \quad \text{in } \mathcal{D}, \tag{2.21}$$

where $(n_0, W_0, \vec{W})$ is the solution at the actual time, $(n_0^0, W_0^0, \vec{W}^0)$ is the solution at the previous time instant, and $h > 0$ is the time step size; see Theorem 6.1. The boundary conditions are given by

$$n_0 = n_0^D, \quad W_0 = W_0^D, \quad \vec{W} = \vec{W}^D \quad \text{on } \partial\mathcal{D}. \tag{2.22}$$

The main difficulty in the existence proof is the derivation of suitable a priori estimates. The entropy-production inequality (2.18) provides estimates which are uniform in h, but they are not sufficient to pass to the limit $h \to 0$ since the gradient estimate (2.18) for $\nabla\sqrt{n_0}$ becomes useless in regions where T is close to zero.

Our proof employs some ideas from [21]. The first idea is to formulate system (2.19)–(2.21) as

$$\begin{aligned}
n_0(u, v_0, \vec{v}) - n_0^0 &= h\Delta u, \\
W_0(u, v_0, \vec{v}) - W_0^0 &= h\Delta v_0, \\
\vec{W}(u, v_0, \vec{v}) - \vec{W}^0 &= h\Delta\vec{v} - (h/\tau_{\mathrm{sf}})\vec{W} \quad \text{in } \mathcal{D},
\end{aligned}$$

where $(u, v_0, \vec{v})$ are some auxiliary variables. The second idea is to truncate the new variables by replacing u by $[u/v_0]_\varepsilon v_0$, where $[\cdot]_\varepsilon$ is a truncation operator satisfying $[u/v_0]_\varepsilon v_0 = u$ for $0 < u/v_0 \le 1/\varepsilon$. The existence of weak solutions to the truncated problem is shown by means of the Leray–Schauder fixed-point theorem. The compactness follows from standard H^1 elliptic estimates. Then, choosing special Stampacchia-type test functions, we prove lower and upper bounds for the new variables, which allow us to remove the truncation. In this step, we exploit the particular structure of the equations.

Unfortunately, our a priori estimates depend on the time step size which prevents the limit $h \to 0$. Even the analysis of the time-discrete equations is highly delicate since the equations are highly nonlinear and a priori estimates are not easy to obtain. The existence of weak solutions to the semiclassical energy-transport equations near equilibrium was proved in [4, 9, 12]. An existence analysis for general initial data was shown in [6] but for uniformly positive definite diffusion matrices only. A semiclassical energy-transport system without electric effects has been investigated in [21]. This system possesses similar difficulties as equations (2.19)–(2.21) but its structure is easier. For details, we refer to Section 6.

3. A general energy-transport model for spin transport

3.1. Derivation from the spinorial Boltzmann equation. We sketch briefly the derivation of the general energy-transport model (1.2) from the spinorial Boltzmann transport Equation (1.1). Details are given in [3]. We consider the Boltzmann equation in the diffusion scaling,

$$\partial_t F_\varepsilon + \frac{1}{\varepsilon}\big(k\cdot\nabla_x F_\varepsilon - \nabla_x V\cdot\nabla_k F_\varepsilon\big) = \frac{1}{\varepsilon^2}Q(F_\varepsilon) + \frac{\mathrm{i}}{2}[\vec{\Omega}_\varepsilon(x,k)\cdot\vec{\sigma}, F_\varepsilon] + Q_{\mathrm{sf}}(F_\varepsilon), \tag{3.1}$$

The parameter $\varepsilon > 0$ is the scaled mean free path and is supposed to be small. We have assumed the parabolic-band approximation such that the mean velocity equals $v(k) = k$.

The last term in equation (3.1) represents the spin-flip interactions which are specified in (4.1) below. The commutator $[\cdot,\cdot]$ on the right-hand side of equation (3.1) can be rigorously derived from the Schrödinger equation with spin-orbit Hamiltonian in the semiclassical limit [7, Chapter 1]. The term models a precession effect around the effective field [3].

The first term on the right-hand side of equation (3.1) models collisions that conserve mass and energy. For simplicity, we employ the BGK-type operator (named after Bhatnagar, Gross, and Krook) $Q(F) = M[F] - F$, where the Maxwellian $M[F]$ associated to F has the same mass and energy as F,

$$\int_{\mathbb{R}^3} M[F]dk = \int_{\mathbb{R}^3} F dk, \quad \frac{1}{2}\int_{\mathbb{R}^3} M[F]|k|^2 dk = \frac{1}{2}\int_{\mathbb{R}^3} F|k|^2 dk. \tag{3.2}$$

The Maxwellian is constructed from entropy maximization under the constraints of given mass and energy, which yields, in case of Maxwell-Boltzmann statistics, the existence of Lagrange multipliers $A(x,t)$ and $C(x,t)$ such that [3]

$$M[F](x,k,t) = \exp\left(A(x,t) + C(x,t)\frac{|k|^2}{2}\right),$$

where exp is the matrix exponential and A, C are Hermitian 2×2 matrices satisfying (3.2).

The space of Hermitian 2×2 matrices can be spanned by the unit matrix σ_0 and the Pauli matrices $\vec{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$,

$$\sigma_0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \quad \sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_2 = \begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}, \quad \sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

Accordingly, we may write $A = a_0 + \vec{a}\cdot\vec{\sigma}$ and $C = c_0 + \vec{c}\cdot\vec{\sigma}$, where a_0, $c_0\in\mathbb{R}$, $\vec{a} = (a_1,a_2,a_3)$, $\vec{c} = (c_1,c_2,c_3)\in\mathbb{R}^3$, and $\vec{a}\cdot\vec{\sigma} = \sum_{j=1}^3 a_j\sigma_j$. The coefficients in the Pauli basis are computed from $a_0 = \frac{1}{2}\mathrm{tr}(A)$, $\vec{a} = \frac{1}{2}(\vec{\sigma}A)$, and similarly for c_0, $\vec{c}$; see, e.g., [18]. The matrix exponential can be also expanded in the Pauli matrix, giving $M[F] = M_0\sigma_0 + \vec{M}\cdot\vec{\sigma}$, where

$$M_0 = e^{a_0+c_0|k|^2/2}\cosh\left|\vec{a}+\vec{c}\frac{|k|^2}{2}\right|, \quad \vec{M} = e^{a_0+c_0|k|^2/2}\frac{\sinh|\vec{a}+\vec{c}|k|^2/2|}{|\vec{a}+\vec{c}|k|^2/2|}\left(\vec{a}+\vec{c}\frac{|k|^2}{2}\right). \tag{3.3}$$

It is shown in [3, Theorem 3.1] that F_ε converges formally to $M := M[A,C] = \exp(A + C|k|^2/2)$ as $\varepsilon\to 0$, where (A,C) are solutions to the following spin energy-transport system for the electron density $n(x,t)$ and energy density $W(x,t)$, which are related to (A,C) via the moment equations

$$n = \int_{\mathbb{R}^3} M[A,C]dk, \quad W = \frac{1}{2}\int_{\mathbb{R}^3} M[A,C]|k|^2 dk.$$

The general energy-transport equations read as [3, Theorem 3.1]

$$\partial_t n + \operatorname{div}_x J_n = \frac{\mathrm{i}}{2}\int_{\mathbb{R}^3}\left[\vec{\Omega}_{\mathrm{ET}}\cdot\vec{\sigma}, M\right]dk - \frac{1}{4}\int_{\mathbb{R}^3}\left[\vec{\Omega}_{\mathrm{o}}\cdot\vec{\sigma},[\vec{\Omega}_{\mathrm{o}}\cdot\vec{\sigma},M]\right]dk + \int_{\mathbb{R}^3} Q_{\mathrm{sf}}(M)dk, \tag{3.4}$$

$$\begin{aligned}&\partial_t W + \operatorname{div}_x J_W + J_n\cdot\nabla_x V\\ &= \frac{\mathrm{i}}{2}\int_{\mathbb{R}^3}\left[\vec{\Omega}_{\mathrm{o}}\cdot\vec{\sigma},M\right]\frac{|k|^2}{2}dk - \frac{1}{4}\int_{\mathbb{R}^3}\left[\vec{\Omega}_{\mathrm{o}}\cdot\vec{\sigma},[\vec{\Omega}_{\mathrm{o}}\cdot\vec{\sigma},M]\right]\frac{|k|^2}{2}dk + \frac{1}{2}\int_{\mathbb{R}^3} Q_{\mathrm{sf}}(M)|k|^2dk,\end{aligned} \tag{3.5}$$

where the effective field $\vec{\Omega}_{\mathrm{ET}}$ is defined by

$$\vec{\Omega}_{\mathrm{ET}} = (k\cdot\nabla_x - \nabla_x V\cdot\nabla_k)\vec{\Omega}_{\mathrm{o}} + \vec{\Omega}_{\mathrm{e}}, \tag{3.6}$$

and $\vec{\Omega}_{\mathrm{o}}$ and $\vec{\Omega}_{\mathrm{e}}$ are the odd and even parts of $\vec{\Omega}$ (with respect to k), respectively. The tensor-valued fluxes are defined by

$$\begin{aligned} J_n &= -\operatorname{div}_x \Pi - n\nabla_x V + \Pi_{\Omega_{\mathrm{o}}},\\ J_W &= -\operatorname{div}_x Q - (W+\Pi)\nabla_x V + Q_{\Omega_{\mathrm{o}}},\end{aligned} \tag{3.7}$$

and the tensors $\Pi = (\Pi^{j\ell})$, $Q = (Q^{j\ell})$ with $\Pi^{j\ell}$, $Q^{j\ell}\in\mathbb{C}^{2\times 2}$ and $\Pi_{\Omega_{\mathrm{o}}} = (\Pi^j_{\Omega_{\mathrm{o}}})$, $Q_{\Omega_{\mathrm{o}}} = (Q^j_{\Omega_{\mathrm{o}}})$ with $\Pi^j_{\Omega_{\mathrm{o}}}$, $Q^j_{\Omega_{\mathrm{o}}}\in\mathbb{C}^{2\times 2}$ are given by the moments

$$\Pi^{j\ell} = \int_{\mathbb{R}^3} k_j k_\ell M dk, \qquad Q^{j\ell} = \frac{1}{2}\int_{\mathbb{R}^3} k_j k_\ell |k|^2 M dk,$$
$$\Pi^j_{\Omega_{\mathrm{o}}} = \mathrm{i}\int_{\mathbb{R}^3}\left[\vec{\Omega}_{\mathrm{o}}\cdot\vec{\sigma},M\right]k_j dk, \qquad Q^j_{\Omega_{\mathrm{o}}} = \frac{\mathrm{i}}{2}\int_{\mathbb{R}^3}\left[\vec{\Omega}_{\mathrm{o}}\cdot\vec{\sigma},M\right]k_j|k|^2 dk,$$

where $j,\ell = 1,2,3$. The first two terms on the right-hand sides of equations (3.4) and (3.5) are due to spinor effects; they vanish in the classical energy-transport model. The last term on the left-hand side of equation (3.5) is the Joule heating and it is also present in the classical model. The last terms in equations (3.4)–(3.5) express the moments of the spin-flip interactions.

3.2. Formulation in the Pauli basis. In order to derive simplified spin energy-transport models in explicit form, it is convenient to formulate equations (3.4)–(3.5) in the Pauli basis. Recall that $n = n_0\sigma_0 + \vec{n}\cdot\vec{\sigma}$ and $W = W_0\sigma_0 + \vec{W}\cdot\vec{\sigma}$. Furthermore, we expand

$$\int_{\mathbb{R}^3} Q_{\mathrm{sf}}(M)dk = Q_{\mathrm{sf},n,0}\sigma_0 + \vec{Q}_{\mathrm{sf},n}\cdot\vec{\sigma}, \quad \frac{1}{2}\int_{\mathbb{R}^3} Q_{\mathrm{sf}}(M)|k|^2 dk = Q_{\mathrm{sf},W,0}\sigma_0 + \vec{Q}_{\mathrm{sf},W}\cdot\vec{\sigma}. \tag{3.8}$$

LEMMA 3.1 (Energy-transport model in Pauli components). *Equations* (3.4)–(3.5) *can be written in the Pauli components* $(n_0,\vec{n})$ *and* $(W_0,\vec{W})$ *as*

$$\partial_t n_0 - \operatorname{div}_x\left(\frac{2}{3}\nabla_x W_0 + n_0\nabla_x V\right) = Q_{\mathrm{sf},n,0}, \tag{3.9}$$

$$\begin{aligned}&\partial_t \vec{n} - \sum_{j=1}^3 \partial_{x_j}\left(\frac{2}{3}\partial_{x_j}\vec{W} + \vec{n}\partial_{x_j}V + 2\int_{\mathbb{R}^3}(\vec{\Omega}_{\mathrm{o}}\times\vec{M})k_j dk\right)\\ &\quad + \sum_{j=1}^3\int_{\mathbb{R}^3}\partial_{x_j}(\vec{\Omega}_{\mathrm{o}}\times\vec{M})k_j dk + \sum_{j=1}^3 \partial_{x_j}V\int_{\mathbb{R}^3}\partial_{k_j}(\vec{\Omega}_{\mathrm{o}}\times\vec{M})dk + \int_{\mathbb{R}^3}\vec{\Omega}_{\mathrm{e}}\times\vec{M}dk\end{aligned}$$

$$+\int_{\mathbb{R}^3}\big(|\vec\Omega_{\rm o}|^2-\vec\Omega_{\rm o}\otimes\vec\Omega_{\rm o}\big)\cdot\vec M dk=\vec Q_{{\rm sf},n}, \tag{3.10}$$

$$\partial_t W_0-{\rm div}_x\left(\frac16\int_{\mathbb{R}^3}\nabla_x M_0|k|^4dk+\frac53 W_0\nabla_x V\right)$$
$$-\left(\frac23\nabla_x W_0+n_0\nabla_x V\right)\cdot\nabla_x V=Q_{{\rm sf},W,0}, \tag{3.11}$$

$$\partial_t\vec W-\sum_{j=1}^3\bigg\{\partial_{x_j}\left(\frac16\partial_{x_j}\int_{\mathbb{R}^3}\vec M|k|^4dk+\frac53\vec W\partial_{x_j}V+\int_{\mathbb{R}^3}(\vec\Omega_{\rm o}\times\vec M)k_j|k|^2dk\right)$$
$$+\left(\frac23\partial_{x_j}\vec W+\vec n\partial_{x_j}V+2\int_{\mathbb{R}^3}(\vec\Omega_{\rm o}\times\vec M)k_jdk\right)\partial_{x_j}V\bigg\}$$
$$+\frac12\sum_{j=1}^3\partial_{x_j}\int_{\mathbb{R}^3}(\vec\Omega_{\rm o}\times\vec M)k_j|k|^2dk+\frac12\sum_{j=1}^3\partial_{x_j}V\int_{\mathbb{R}^3}\partial_{k_j}(\vec\Omega_{\rm o}\times\vec M)|k|^2dk$$
$$+\frac12\int_{\mathbb{R}^3}(\vec\Omega_{\rm e}\times\vec M)|k|^2dk+\int_{\mathbb{R}^3}\big(|\vec\Omega_{\rm o}|^2-\vec\Omega_{\rm o}\otimes\vec\Omega_{\rm o}\big)\cdot\vec M|k|^2dk=\vec Q_{{\rm sf},W}, \tag{3.12}$$

where $\partial_{x_j}=\partial/\partial x_j$, $\partial_{k_j}=\partial/\partial k_j$.

Proof. We reformulate equations (3.4)–(3.5) in terms of the Pauli coefficients. For this, set $J_n=(J_n^j)_{j=1,2,3}$, $J_W=(J_W^j)_{j=1,2,3}$ and $J_n^j=J_{n,0}^j\sigma_0+\vec J_n^j\cdot\vec\sigma$, $J_W^j=J_{W,0}^j\sigma_0+\vec J_W^j\cdot\vec\sigma$. We obtain

$$\partial_t n_0+\sum_{j=1}^3\partial_{x_j}J_{n,0}^j=Q_{{\rm sf},n,0}, \tag{3.13}$$

$$\partial_t\vec n+\sum_{j=1}^3\partial_{x_j}\vec J_n^j+\int_{\mathbb{R}^3}\vec\Omega_{\rm ET}\times\vec M dk+\int_{\mathbb{R}^3}\big(|\vec\Omega_{\rm o}|^2-\vec\Omega_{\rm o}\otimes\vec\Omega_{\rm o}\big)\cdot\vec M dk=\vec Q_{{\rm sf},n}, \tag{3.14}$$

$$\partial_t W_0+\sum_{j=1}^3\big(\partial_{x_j}J_{W,0}^j+J_{n,0}^j\partial_{x_j}V\big)=Q_{{\rm sf},W,0}, \tag{3.15}$$

$$\partial_t\vec W+\sum_{j=1}^3\big(\partial_{x_j}\vec J_W^j+\vec J_n^j\partial_{x_j}V\big)+\int_{\mathbb{R}^3}(\vec\Omega_{\rm ET}\times\vec M)|k|^2dk$$
$$+\frac12\int_{\mathbb{R}^3}\big(|\vec\Omega_{\rm o}|^2-\vec\Omega_{\rm o}\otimes\vec\Omega_{\rm o}\big)\cdot\vec M|k|^2dk=\vec Q_{{\rm sf},W}. \tag{3.16}$$

Let us expand the integrals involving $\vec\Omega_{\rm ET}$ and the fluxes. Let $\phi(k)=1$ or $\phi(k)=|k|^2/2$. Then, recalling definition (3.6) for $\vec\Omega_{\rm ET}$,

$$\int_{\mathbb{R}^3}(\vec\Omega_{\rm ET}\times\vec M)\phi(k)dk=\int_{\mathbb{R}^3}\big(k\cdot\nabla_x-\nabla_x V\cdot\nabla_k\big)(\vec\Omega_{\rm o}\times\vec M)\phi(k)dk+\int_{\mathbb{R}^3}(\vec\Omega_{\rm e}\times\vec M)\phi(k)dk$$
$$=\sum_{j=1}^3\partial_{x_j}\int_{\mathbb{R}^3}(\vec\Omega_{\rm o}\times\vec M)k_j\phi(k)dk-\sum_{j=1}^3\partial_{x_j}V\int_{\mathbb{R}^3}(\partial_{k_j}\vec\Omega_{\rm o}\times\vec M)\phi(k)dk$$
$$+\int_{\mathbb{R}^3}(\vec\Omega_{\rm e}\times\vec M)\phi(k)dk.$$

Inserting these expressions into the evolution equations for $\vec n$ and $\vec W$, we recover the three integrals in the second line of equation (3.10) as well as the integrals in the third line, and the first integral in the fourth line of equation (3.12).

It remains to compute the fluxes (3.7). First, we calculate

$$\Pi^{j\ell} = \frac{1}{3}\int_{\mathbb{R}^3} M|k|^2 dk\delta_{j\ell} = \frac{2}{3}W\delta_{j\ell}, \quad Q^{j\ell} = \frac{1}{6}\int_{\mathbb{R}^3} M|k|^4 dk\delta_{j\ell}.$$

Furthermore, using the formula $[\vec{u}\cdot\vec{\sigma},\vec{v}\cdot\vec{\sigma}] = 2\mathrm{i}(\vec{u}\times\vec{v})\cdot\vec{\sigma}$ for $\vec{u}$, $\vec{v}\in\mathbb{R}^3$, we find that $\Pi_{\Omega_o} = \Pi_{\Omega_o,0}\sigma_0 + \vec{\Pi}_{\Omega_o}\cdot\vec{\sigma}$ with $\Pi_{\Omega_o,0} = 0$ and $\vec{\Pi}_{\Omega_o} = -2\int_{\mathbb{R}^3}(\vec{\Omega}_o\times\vec{M})kdk$. Therefore,

$$J^j_{n,0} = -\sum_{\ell=1}^{3}\partial_{x_\ell}\Pi_0^{j\ell} - n_0\partial_{x_j}V + \Pi^j_{\Omega_0,0} = -\frac{2}{3}\partial_{x_j}W_0 - n_0\partial_{x_j}V,$$

$$\vec{J}^j_n = -\sum_{\ell=1}^{3}\partial_{x_\ell}\vec{\Pi}^{j\ell} - \vec{n}\partial_{x_j}V + \vec{\Pi}^j_{\Omega_o} = -\frac{2}{3}\partial_{x_j}\vec{W} - \vec{n}\partial_{x_j}V - 2\int_{\mathbb{R}^3}(\vec{\Omega}_o\times\vec{M})k_j dk.$$

Expanding $Q_{\Omega_o} = Q_{\Omega_o,0}\sigma_0 + \vec{Q}_{\Omega_o}\cdot\vec{\sigma}$ with $Q_{\Omega_o,0} = 0$ and $\vec{Q}_{\Omega_o} = -\int_{\mathbb{R}^3}(\vec{\Omega}_o\times\vec{M})k|k|^2 dk$, it follows that

$$\begin{aligned} J^j_{W,0} &= -\sum_{\ell=1}^{3}\left(\partial_{x_\ell}Q_0^{j\ell} + (W_0\delta_{j\ell} + \Pi_0^{j\ell})\partial_{x_\ell}V\right) + Q^j_{\Omega_o,0} \\ &= -\frac{1}{6}\partial_{x_j}\int_{\mathbb{R}^3} M_0|k|^4 dk - \frac{5}{3}W_0\partial_{x_j}V, \\ \vec{J}^j_W &= -\sum_{\ell=1}^{3}\left(\partial_{x_\ell}\vec{Q}^{j\ell} + (\vec{W}\delta_{j\ell} + \vec{\Pi}^{j\ell})\partial_{x_\ell}V\right) + \vec{Q}^j_{\Omega_o} \\ &= -\frac{1}{6}\partial_{x_j}\int_{\mathbb{R}^3}\vec{M}|k|^4 dk - \frac{5}{3}\vec{W}\partial_{x_j}V - \int_{\mathbb{R}^3}(\vec{\Omega}_o\times\vec{M})k_j|k|^2 dk. \end{aligned}$$

Inserting these expressions into equations (3.13)–(3.16) gives equations (3.9)–(3.12). ∎

4. Simplified spin energy-transport equations

In this section, we derive some explicit models. We assume for simplicity that the odd part of the magnetization vanishes, $\vec{\Omega}_o = 0$, and that the even part $\vec{\Omega}_e$ depends on x only. Moreover, we suppose that the spin-flip interactions are modeled by the relaxation-time operator

$$Q_{\mathrm{sf}}(M) := -\frac{1}{\tau_{\mathrm{sf}}}\left(M - \frac{1}{2}\mathrm{tr}(M)\sigma_0\right) = -\frac{1}{\tau_{\mathrm{sf}}}\vec{M}\cdot\vec{\sigma}, \tag{4.1}$$

where $\tau_{\mathrm{sf}} > 0$ is the average time between two subsequent spin-flip collisions, and we recall that $M = M_0\sigma_0 + \vec{M}\cdot\vec{\sigma}$. In particular, with the notation of equation (3.8),

$$Q_{\mathrm{sf},n,0} = 0, \quad \vec{Q}_{\mathrm{sf},n} = -\frac{\vec{n}}{\tau_{\mathrm{sf}}}, \quad Q_{\mathrm{sf},W,0} = 0, \quad \vec{Q}_{\mathrm{sf},W} = -\frac{\vec{W}}{\tau_{\mathrm{sf}}}.$$

Then system (3.9)–(3.12) reduces to

$$\partial_t n_0 - \mathrm{div}\left(\frac{2}{3}\nabla W_0 + n_0\nabla V\right) = 0, \tag{4.2}$$

$$\partial_t\vec{n} - \sum_{j=1}^{3}\partial_{x_j}\left(\frac{2}{3}\partial_{x_j}\vec{W} + \vec{n}\partial_{x_j}V\right) + \vec{\Omega}_e\times\vec{n} = -\frac{\vec{n}}{\tau_{\mathrm{sf}}}, \tag{4.3}$$

$$\partial_t W_0 - \operatorname{div}\left(\frac{1}{6}\nabla\int_{\mathbb{R}^3} M_0|k|^2dk + \frac{5}{3}W_0\nabla V\right) - \left(\frac{2}{3}\nabla W_0 + n_0\nabla V\right)\cdot\nabla V = 0, \tag{4.4}$$

$$\partial_t\vec{W} - \sum_{j=1}^{3}\left\{\partial_{x_j}\left(\frac{1}{6}\partial_{x_j}\int_{\mathbb{R}^3}\vec{M}|k|^4dk + \frac{5}{3}\vec{W}\partial_{x_j}V\right) + \left(\frac{2}{3}\partial_{x_j}\vec{W} + \vec{n}\partial_{x_j}V\right)\partial_{x_j}V\right\}$$
$$+\vec{\Omega}_{\mathrm{e}}\times\vec{W} = -\frac{\vec{W}}{\tau_{\mathrm{sf}}}. \tag{4.5}$$

Given $(n_0,\vec{n},W_0)$, we define the densities $n_\pm$ and the temperature T by

$$n_\pm = n_0 \pm |\vec{n}|, \quad W_0 = \frac{3}{2}n_0T. \tag{4.6}$$

We also introduce the Gaussian with variance $\theta > 0$,

$$g_\theta(k) = (2\pi\theta)^{-3/2}\exp\left(-\frac{|k|^2}{2\theta}\right), \tag{4.7}$$

whose moments are given by

$$\int_{\mathbb{R}^3} g_\theta(k)\begin{pmatrix}1\\ |k|^2/2\\ |k|^4/6\end{pmatrix}dk = \begin{pmatrix}1\\ 3\theta/2\\ 5\theta^2/2\end{pmatrix}. \tag{4.8}$$

4.1. First model. We show the following result.

THEOREM 4.1 (Spin energy-transport model with $\vec{c}=0$). *For $\vec{c}=0$, system* (4.2)–(4.5) *can be written in the variables $(n_0,T,\vec{n})$ as system* (2.1)–(2.3).

Proof. Under the assumption $\vec{c}=0$, the higher-order moments in equations (4.4)–(4.5) can be computed explicitly. Indeed, the Pauli expansion of the Maxwellian (3.3) simplifies to

$$M_0 = e^{a_0+c_0|k|^2/2}\cosh|\vec{a}|, \quad \vec{M} = e^{a_0+c_0|k|^2/2}\sinh|\vec{a}|\frac{\vec{a}}{|\vec{a}|}.$$

Observe that $c_0<0$ is necessary to ensure the integrability of M_0 and $\vec{M}$. The above expressions can be reformulated by introducing the new Lagrange multipliers

$$\kappa_\pm := \left(\frac{2\pi}{-c_0}\right)^{3/2}e^{a_0\pm|\vec{a}|}, \quad \theta := -\frac{1}{c_0}, \quad \vec{\gamma} := \frac{\vec{a}}{|\vec{a}|}.$$

Then $M_0 = \frac{1}{2}(\kappa_+ + \kappa_-)g_\theta(k)$, $\vec{M} = \frac{1}{2}(\kappa_+ - \kappa_-)g_\theta(k)\vec{\gamma}$, where g_θ is defined in equation (4.7). As a consequence, we have

$$n_0 = \int_{\mathbb{R}^3} M_0dk = \frac{1}{2}(\kappa_+ + \kappa_-), \quad \vec{n} = \int_{\mathbb{R}^3}\vec{M}dk = \frac{1}{2}(\kappa_+ - \kappa_-)\vec{\gamma},$$
$$W_0 = \frac{1}{2}\int_{\mathbb{R}^3} M_0|k|^2dk = \frac{3}{4}\theta(\kappa_+ + \kappa_-),$$

and we infer from equation (4.6) that $\kappa_\pm = n_\pm$, $\vec{\gamma} = \vec{n}/|\vec{n}|$, and $\theta = T$. Then the Pauli coefficients become $M_0 = n_0g_T(k)$, $\vec{M} = \vec{n}g_T(k)$ and

$$\vec{W} = \frac{1}{2}\int_{\mathbb{R}^3}\vec{M}|k|^2dk = \frac{3}{2}\vec{n}T, \quad \frac{1}{6}\int_{\mathbb{R}^3} M_0|k|^4dk = \frac{5}{2}n_0T^2.$$

Inserting these expressions into system (4.2)–(4.5) shows the result. □

REMARK 4.1. The derivation of model (2.4)–(2.6) is similar to that one in [3], therefore we sketch it only. The Maxwellian is here given by

$$M[F](k) = (2\pi\theta[F])^{-3/2} e^{-|k|^2/(2\theta[F])} \int_{\mathbb{R}^3} F(k')dk',$$
$$\text{where } \theta[F] = \frac{1}{3}\frac{\int_{\mathbb{R}^3} \mathrm{tr}(PF(k))|k|^2 dk}{\int_{\mathbb{R}^3} \mathrm{tr}(PF(k))dk}.$$

The formal limit $\varepsilon \to 0$ in equation (3.1) gives $Q(F^0)=0$, where $F^0 = \lim_{\varepsilon\to 0} F_\varepsilon$, showing that $F^0 = M[F^0]$. Next, we perform a Hilbert expansion $F_\varepsilon = M[F] + \varepsilon F^1 + O(\varepsilon^2)$ and assume that F^1 is odd with respect to k. Since 1, $|k|^2/2$ are even functions, F^1 does not contribute to the moments $n = \int_{\mathbb{R}^3} F dk$, $W = \frac{1}{2}\int_{\mathbb{R}^3} F|k|^2 dk$. It holds that $W = \frac{3}{2}nT$, where $T := \theta[F^0]$. After a computation which is similar to the derivation of the semi-classical energy-transport equations, we obtain the moment equations

$$\partial_t n + \mathrm{div}\, G_n + \mathrm{i}[n, \vec{\Omega}\cdot\vec{\sigma}] = \frac{1}{2}\mathrm{tr}(n) - n, \quad G_n = -P^{-1/2}\big(\nabla(nT) + n\nabla V\big)P^{-1/2},$$
$$\frac{3}{2}\partial_t(nT) + \mathrm{div}\, G_W + G_n\cdot\nabla V = 0, \quad G_W = -\frac{5}{3}P^{-1/2}\big(\nabla(nT^2) + nT\nabla V\big)P^{-1/2}.$$

In order to formulate these equations in the Pauli components, we observe that for any 2×2 Hermitian matrix $A = a_0\sigma_0 + \vec{a}\cdot\vec{\sigma}$, it holds that $P^{1/2}AP^{1/2} = b_0\sigma_0 + \vec{b}\cdot\vec{\sigma}$, where

$$\begin{pmatrix} b_0 \\ \vec{b} \end{pmatrix} = \eta^{-2}\begin{pmatrix} 1 & -p\vec{\Omega}^\top \\ -p\vec{\Omega} & (1-\eta)\vec{\Omega}\otimes\vec{\Omega} + \eta\sigma_0 \end{pmatrix}\begin{pmatrix} a_0 \\ \vec{a} \end{pmatrix}, \quad \eta = \sqrt{1-p^2}.$$

We omit the calulcation and only note that this leads to model (2.4)–(2.6).

4.2. Second model.

THEOREM 4.2 (Spin energy-transport model with $\vec{a}=0$, version I). *For $\vec{a}=0$, system (4.2)–(4.5) can be written in the variables $(n_0, T, \vec{n})$ as system (2.7)–(2.9), where the diffusion coefficient $D(n_+, n_-)$ and the polarization factor $p(n_+, n_-)$ are defined by*

$$D(n_+, n_-) = \frac{2n_0(n_+^{7/3} + n_-^{7/3})}{(n_+^{5/3} + n_-^{5/3})^2}, \quad p(n_+, n_-) = \frac{n_+^{5/3} - n_-^{5/3}}{n_+^{5/3} + n_-^{5/3}}, \tag{4.9}$$

and the spin-up/spin-down densities are given by $n_\pm = n_0 \pm |\vec{n}|$.

Proof. For $\vec{a}=0$, the Pauli components of the Maxwellian take the form

$$M_0 = e^{a_0 + c_0|k|^2/2}\cosh\left(|\vec{c}|\frac{|k|^2}{2}\right), \quad \vec{M} = e^{a_0 + c_0|k|^2/2}\sinh\left(|\vec{c}|\frac{|k|^2}{2}\right)\frac{\vec{c}}{|\vec{c}|}. \tag{4.10}$$

The integrability of M_0 and $\vec{M}$ implies that $c_0 \pm |\vec{c}| < 0$. In the new Lagrange multiplier variables

$$K := (2\pi)^{3/2} e^{a_0}, \quad \theta_\pm := -\frac{1}{c_0 \pm |\vec{c}|}, \quad \vec{\gamma} := \frac{\vec{c}}{|\vec{c}|} \tag{4.11}$$

these components can be rewritten as

$$M_0 = \frac{K}{2}\big(\theta_+^{3/2} g_{\theta_+}(k) + \theta_-^{3/2} g_{\theta_-}(k)\big), \quad \vec{M} = \frac{K}{2}\big(\theta_+^{3/2} g_{\theta_+}(k) - \theta_-^{3/2} g_{\theta_-}(k)\big)\vec{\gamma}.$$

Taking into account equation (4.8), this shows that

$$n_0 = \int_{\mathbb{R}^3} M_0 dk = \frac{K}{2}\left(\theta_+^{3/2} + \theta_-^{3/2}\right), \quad \vec{n} = \int_{\mathbb{R}^3} \vec{M} dk = \frac{K}{2}\left(\theta_+^{3/2} - \theta_-^{3/2}\right)\vec{\gamma},$$
$$W_0 = \frac{1}{2}\int_{\mathbb{R}^3} M_0 |k|^2 dk = \frac{3K}{4}\left(\theta_+^{5/2} + \theta_-^{5/2}\right),$$

and consequently, $n_\pm := n_0 \pm |\vec{n}| = K\theta_\pm^{3/2}$, $\vec{\gamma} = \vec{n}/|\vec{n}|$. This implies that $W_0 = \frac{3}{4}(n_+\theta_+ + n_-\theta_-)$ and $n_-/n_+ = (\theta_-/\theta_+)^{3/2}$. Hence,

$$\begin{aligned}\frac{3}{2} n_0 T = W_0 &= \frac{3}{4}\frac{\theta_+}{n_+^{2/3}}\left(n_+^{5/3} + \left(\frac{n_+}{n_-}\right)\frac{\theta_+}{\theta_-} n_-\right) \\ &= \frac{3\theta_+}{4 n_+^{2/3}}\left(n_+^{5/3} + n_-^{5/3}\right) = \frac{3\theta_-}{4 n_-^{2/3}}\left(n_+^{5/3} + n_-^{5/3}\right).\end{aligned}$$

We obtain the following form for the Pauli components of M:

$$M_0 = \frac{1}{2}\left(n_+ g_{\theta_+}(k) + n_- g_{\theta_-}(k)\right), \quad \vec{M} = \frac{1}{2}\left(n_+ g_{\theta_+}(k) + n_- g_{\theta_-}(k)\right)\frac{\vec{n}}{|\vec{n}|}.$$

It remains to compute the higher-order moments:

$$\vec{W} = \frac{1}{2}\int_{\mathbb{R}^3} \vec{M}|k|^2 dk = \frac{3}{4}(n_+\theta_+ - n_-\theta_-)\frac{\vec{n}}{|\vec{n}|} = \frac{3}{2} n_0 T \frac{n_+^{5/3} - n_-^{5/3}}{n_+^{5/3} + n_-^{5/3}}\frac{\vec{n}}{|\vec{n}|},$$
$$\frac{1}{6}\int_{\mathbb{R}^3} M_0 |k|^4 dk = \frac{5}{4}(n_+\theta_+^2 + n_-\theta_-^2) = 5 n_0^2 T^2 \frac{n_+^{7/3} + n_-^{7/3}}{(n_+^{5/3} + n_-^{5/3})^2}.$$

Inserting these expressions into equations (4.2)–(4.4) concludes the proof. ◻

Remark 4.2. Equations (2.7)–(2.9) are fully coupled since the diffusion coefficient $D(n_+,n_-)$ depends on the spin vector density through $|\vec{n}| = (n_+ - n_-)/2$. However, it turns out that $1 \le D(n_+,n_-) \le 1.1$ for $|\vec{n}| \le n_0$, which means that the dependence of the energy $\frac{3}{2} n_0 T$ on the spin vector density $\vec{n}$ is in fact very weak. When the spin vector density vanishes, $\vec{n} = 0$, it follows that $n_+ = n_- = n_0$ and $D(n_+,n_-) = 1$, and we recover the classical energy-transport model.

The model in Theorem 4.1 can be formulated in the variables $(n_0, W_0, \vec{W})$, and this formulation is used below in the existence analysis.

Theorem 4.3 (Spin energy-transport model with $\vec{a} = 0$, version II). *For $\vec{a} = 0$, system (4.2)–(4.5) can be written in the variables $(n_0, T, \vec{W})$ as*

$$\partial_t n_0 - \operatorname{div}\left(\nabla(n_0 T) + n_0 \nabla V\right) = 0, \tag{4.12}$$

$$\frac{3}{2}\partial_t(n_0 T) - \operatorname{div}\left(\nabla Z_0 + \frac{5}{2} n_0 T \nabla V\right) - \left(\nabla(n_0 T) + n_0 \nabla V\right)\cdot \nabla V = 0, \tag{4.13}$$

$$\begin{aligned}\partial_t \vec{W} - \sum_{j=1}^3 \partial_{x_j}\left(\partial_{x_j}\vec{Z} + \frac{5}{3}\vec{W}\partial_{x_j} V\right) - \sum_{j=1}^3 \left(\frac{2}{3}\partial_{x_j}\vec{W} + \vec{n}\nabla_{x_j} V\right)\partial_{x_j} V& \\ + \vec{\Omega}_{\rm e} \times \vec{W} = -\frac{\vec{W}}{\tau_{\rm sf}},&\end{aligned} \tag{4.14}$$

where the spin-vector density $\vec{n}$ and the auxiliary quantities Z_0 and $\vec{Z}$ are given by

$$\vec{n} = n_0 \frac{W_+^{3/5} - W_-^{3/5}}{W_+^{3/5} + W_-^{3/5}} \frac{\vec{W}}{|\vec{W}|},$$

$$Z_0 = \frac{5}{18 n_0} \big(W_+^{3/5} + W_-^{3/5}\big)\big(W_+^{7/5} + W_-^{7/5}\big), \tag{4.15}$$

$$\vec{Z} = \frac{5}{18 n_0} \big(W_+^{3/5} + W_-^{3/5}\big)\big(W_+^{7/5} - W_-^{7/5}\big) \frac{\vec{W}}{|\vec{W}|}, \tag{4.16}$$

and $W_\pm = W_0 \pm |\vec{W}|$, $W_0 = \frac{3}{2} n_0 T$.

Proof. With the new Lagrange multipliers introduced in the proof of Theorem 4.1, we find that

$$n_0 = \int_{\mathbb{R}^3} M_0 dk = \frac{K}{2}\big(\theta_+^{3/2} + \theta_-^{3/2}\big), \quad W_0 = \frac{1}{2}\int_{\mathbb{R}^3} M_0 |k|^2 dk = \frac{3K}{4}\big(\theta_+^{5/2} + \theta_+^{5/2}\big), \tag{4.17}$$

$$\vec{W} = \frac{1}{2}\int_{\mathbb{R}^3} \vec{M} |k|^2 dk = \frac{3K}{4}\big(\theta_+^{5/2} - \theta_-^{5/2}\big)\vec{\gamma}. \tag{4.18}$$

As $c_0 < 0$ is required to ensure integrability of the Maxwellian, it holds that $\theta_+ \geq \theta_-$, such that we deduce from (4.18) that

$$\vec{\gamma} = \frac{\vec{W}}{|\vec{W}|}, \quad |\vec{W}| = \frac{3K}{4}(\theta_+^{5/2} - \theta_-^{5/2}). \tag{4.19}$$

Let $W_\pm = W_0 \pm |\vec{W}|$. Then

$$W_\pm = \frac{3K}{4}\big(\theta_+^{5/2} + \theta_+^{5/2}\big) \pm \frac{3K}{4}\big(\theta_+^{5/2} - \theta_-^{5/2}\big) = \frac{3K}{2}\theta_\pm^{5/2},$$

which is equivalent to $\theta_\pm = (2W_\pm/(3K))^{2/5}$. Inserting this expression into the first equation of (4.17), we obtain

$$n_0 = \frac{K}{2}\left(\left(\frac{2W_+}{3K}\right)^{3/5} + \left(\frac{2W_-}{3K}\right)^{3/5}\right) = \frac{K^{2/5}}{2^{2/5} 3^{3/5}}\big(W_+^{3/5} + W_-^{3/5}\big).$$

Thus, the constant K can be written as

$$K = 2 \cdot 3^{3/2} n_0^{5/2} (W_+^{3/5} + W_-^{3/5})^{-5/2}, \tag{4.20}$$

and we can eliminate K in the formulation of $\theta_\pm$:

$$\theta_\pm = \left(\frac{2W_\pm}{3K}\right)^{2/5} = \frac{W_\pm^{2/5}}{3n_0}\big(W_+^{3/5} + W_-^{3/5}\big). \tag{4.21}$$

The spin-vector density is then computed as follows:

$$\begin{aligned}\vec{n} &= \int_{\mathbb{R}^3} \vec{M} dk = \frac{K}{2}\big(\theta_+^{3/2} - \theta_-^{3/2}\big)\frac{\vec{W}}{|\vec{W}|} \\ &= \frac{3^{3/2} n_0^{5/2}}{(W_+^{3/5} + W_-^{3/5})^{5/2}} \left(\frac{W_+^{3/5} + W_-^{3/5}}{3n_0}\right)^{3/2} \big(W_+^{3/5} - W_-^{3/5}\big)\frac{\vec{W}}{|\vec{W}|}\end{aligned}$$

$$= n_0 \frac{W_+^{3/5} - W_-^{3/5}}{W_+^{3/5} + W_-^{3/5}} \frac{\vec{W}}{|\vec{W}|}.$$

It remains to compute the fourth-order moments. Using $W_\pm = \frac{3}{2}K\theta_\pm^{5/2}$ and equation (4.21), we have

$$\frac{1}{6}\int_{\mathbb{R}^3} M_0|k|^4dk = \frac{5K}{4}\left(\theta_+^{7/2}+\theta_-^{7/2}\right) = \frac{5}{6}(\theta_+W_+ + \theta_-W_-)$$
$$= \frac{5}{18n_0}\left(W_+^{3/5}+W_-^{3/5}\right)\left(W_+^{7/5}+W_-^{7/5}\right).$$

In an analogous way, we calculate

$$\frac{1}{6}\int_{\mathbb{R}^3} \vec{M}|k|^4dk = \frac{5}{18n_0}\left(W_+^{3/5}+W_-^{3/5}\right)\left(W_+^{7/5}-W_-^{7/5}\right)\frac{\vec{W}}{|\vec{W}|}.$$

Inserting these expressions into (4.2)–(4.5), the result follows. ☐

Remark 4.3. If $\vec{W}=0$, it follows that $W_\pm = W_0 = \frac{3}{2}n_0T$, $\vec{n}=0$, $Z_0 = \frac{5}{2}n_0T^2$, and we recover the semiclassical energy-transport model. It is possible to see that $1 \le Z_0/(\frac{5}{2}n_0T^2) \le 1.08$, which shows that the coupling is rather weak. This is expected since the coupling in system (2.7)–(2.9) is weak too.

4.3. Third model.

Theorem 4.4 (Spin energy-transport model for $\vec{a}=\lambda\vec{c}$). *Under the assumption $\vec{a}=\lambda\vec{c}$ for some $\lambda=\lambda(x,t)\ge 0$, system* (4.2)–(4.5) *can be written in the variables $(n_\pm, W_\pm, \vec{s})$ as system* (2.10)–(2.13), *where $(n_\pm, T_\pm, \vec{s})$ are linked to $(n_0, \vec{n}, W_0, \vec{W})$ via*

$$n_\pm = n_0 \pm |\vec{n}|, \quad \frac{3}{2}n_\pm T_\pm = W_0 \pm |\vec{W}|, \quad \vec{s} = \frac{\vec{n}}{|\vec{n}|}. \tag{4.22}$$

Proof. First, we compute the moments in order to make system (4.2)–(4.5) explicit. Under the assumption that $\vec{a}=\lambda\vec{c}$ for some $\lambda\ge 0$, the Pauli components of the Maxwellian become

$$M_0 = \frac{1}{2}\exp\left(a_0+\lambda|\vec{c}|+\frac{1}{2}(c_0+|\vec{c}|)|k|^2\right)+\frac{1}{2}\exp\left(a_0-\lambda|\vec{c}|+\frac{1}{2}(c_0-|\vec{c}|)|k|^2\right),$$
$$\vec{M} = \frac{1}{2}\left\{\exp\left(a_0+\lambda|\vec{c}|+\frac{1}{2}(c_0+|\vec{c}|)|k|^2\right)-\exp\left(a_0-\lambda|\vec{c}|+\frac{1}{2}(c_0-|\vec{c}|)|k|^2\right)\right\}\frac{\vec{c}}{|\vec{c}|}.$$

Introducing the new Lagrange multipliers

$$\kappa_\pm := (2\pi\theta_\pm)^{3/2}e^{a_0\pm\lambda|\vec{c}|}, \quad \theta_\pm := -\frac{1}{c_0\pm|\vec{c}|}, \quad \vec{\gamma} := \frac{\vec{c}}{|\vec{c}|},$$

the Pauli components of M can be rewritten as

$$M_0 = \frac{1}{2}(k_+g_{\theta_+}+k_-g_{\theta_-}), \quad \vec{M} = \frac{1}{2}(k_+g_{\theta_+}-k_-g_{\theta_-})\vec{\gamma},$$

where $g_{\theta_\pm}$ is defined in equation (4.7). Since the Maxwellian has to be integrable, we have $c_0+|\vec{c}|<0$ and consequently, $\theta_+\ge\theta_->0$ and $\kappa_+\ge\kappa_->0$. It follows that

$$n_0 = \frac{1}{2}(\kappa_++\kappa_-), \qquad \vec{n} = \frac{1}{2}(\kappa_+-\kappa_-)\vec{\gamma},$$

$$W_0 = \frac{3}{4}(\kappa_+\theta_+ + \kappa_-\theta_-), \qquad \vec{W} = \frac{3}{4}(\kappa_+\theta_+ - \kappa_-\theta_-)\vec{\gamma}.$$

These expressions allow us to identify the new Lagrange multipliers with $n_\pm = n_0 \pm |\vec{n}|$, $W_\pm = W_0 \pm |\vec{W}|$, and $\vec{s} = \vec{n}/|\vec{n}|$:

$$n_\pm = k_\pm, \quad W_\pm = \frac{3}{2}k_\pm\theta_\pm, \quad \vec{s} = \frac{\vec{n}}{|\vec{n}|} = \frac{\vec{W}}{|\vec{W}|} = \vec{\gamma}.$$

The last expression represents a constraint of the spin part of the particle density and energy. Moreover, the definition $T_\pm = 2W_\pm/(3n_\pm)$ implies that $T_\pm = \theta_\pm$. Thus, the Pauli components of the Maxwellian take the form

$$M_0 = \frac{1}{2}(n_+ g_{T_+} + n_- g_{T_-}), \quad \vec{M} = \frac{1}{2}(n_+ g_{T_+} - n_- g_{T_-})\vec{s}. \tag{4.23}$$

Computing the higher-order moments

$$\frac{1}{6}\int_{\mathbb{R}^3} M_0 |k|^4 dk = \frac{1}{12}\int_{\mathbb{R}^3}(n_+ g_{\theta_+} + n_- g_{\theta_-})|k|^4 dk = \frac{5}{4}(n_+ T_+^2 + n_- T_-^2),$$
$$\frac{1}{6}\int_{\mathbb{R}^3} \vec{M}|k|^4 dk = \frac{5}{4}(n_+ T_+^2 - n_- T_-^2)\vec{s},$$

system (4.2)–(4.5) becomes

$$\partial_t n_0 - \operatorname{div}\left(\frac{2}{3}\nabla W_0 + n_0 \nabla V\right) = 0, \tag{4.24}$$

$$\partial_t \vec{n} - \operatorname{div}\left(\frac{2}{3}\nabla \vec{W} + \vec{n}\nabla V\right) + \vec{\Omega}_{\rm e} \times \vec{n} = -\frac{\vec{n}}{\tau_{\rm sf}}, \tag{4.25}$$

$$\partial_t W_0 - \operatorname{div}\left(\frac{5}{9}\nabla\left(\frac{W_+^2}{n_+} + \frac{W_-^2}{n_-}\right) + \frac{5}{3}W_0\nabla V\right) - \left(\frac{2}{3}\nabla W_0 + n_0\nabla V\right)\cdot\nabla V = 0, \tag{4.26}$$

$$\partial_t \vec{W} - \operatorname{div}\left(\frac{5}{9}\nabla\left(\left(\frac{W_+^2}{n_+} + \frac{W_-^2}{n_-}\right)\vec{s}\right) + \frac{5}{3}\vec{W}\nabla V\right) - \left(\frac{2}{3}\nabla\vec{W} + \vec{n}\nabla V\right)\cdot\nabla V$$
$$+ \vec{\Omega}_{\rm e} \times \vec{W} = -\frac{\vec{W}}{\tau_{\rm sf}}. \tag{4.27}$$

The next step is to reformulate this system in terms of $(n_\pm, W_\pm, \vec{s})$. First, we derive equation (2.10). For this, we take the scalar product of equation (4.25) and $\vec{s} = \vec{n}/|\vec{n}| = \vec{W}/|\vec{W}|$, leading to

$$\partial_t|\vec{n}| - \operatorname{div}\left(\frac{2}{3}\nabla|\vec{W}| + |\vec{n}|\nabla V\right) + \nabla\vec{s}\cdot\left(\frac{2}{3}\nabla\vec{W} + \vec{n}\nabla V\right) = -\frac{|\vec{n}|}{\tau_{\rm sf}}. \tag{4.28}$$

Observing that $|\vec{s}| = 1$ implies that $\nabla\vec{s}\cdot\vec{s} = 0$, we find that $\nabla\vec{s}\cdot\nabla\vec{W} = \nabla\vec{s}\cdot\nabla(|\vec{W}|\vec{s}) = |\vec{W}||\nabla\vec{s}|^2$ and $\nabla\vec{s}\cdot\vec{n} = 0$. Hence, equation (4.28) becomes

$$\partial_t|\vec{n}| - \operatorname{div}\left(\frac{2}{3}\nabla|\vec{W}| + |\vec{n}|\nabla V\right) + \frac{2}{3}|\vec{W}||\nabla\vec{s}|^2 = -\frac{|\vec{n}|}{\tau_{\rm sf}}.$$

Taking the sum and difference of equation (4.2) for n_0 and the previous equation, we obtain equation (2.10) using $n_\pm = n_0 \pm |\vec{n}|$ and $|\vec{W}| = \frac{3}{4}(n_+T_+ - n_-T_-)$.

Second, we derive equation (2.11). Multiplying equation (4.27) by $\vec{s}=\vec{W}/|\vec{W}|$ yields

$$\begin{aligned}\partial_t|\vec{W}|-\operatorname{div}\left(\frac{5}{9}\nabla\left(\frac{W_+^2}{n_+}-\frac{W_-^2}{n_-}\right)+\frac{5}{3}|\vec{W}|\nabla V\right)\\ +\nabla\vec{s}\cdot\left(\frac{5}{9}\nabla\left(\left(\frac{W_+^2}{n_+}-\frac{W_-^2}{n_-}\right)\vec{s}\right)+\frac{5}{3}|\vec{W}|\nabla V\right)\\ -\vec{s}\cdot\left(\frac{2}{3}(\nabla V\cdot\nabla)\vec{W}+\vec{n}|\nabla V|^2\right)=-\frac{|\vec{W}|}{\tau_{\mathrm{sf}}},\end{aligned}$$

and adding and subtracting this equation from expression (4.26) and employing $\vec{s}\cdot\vec{n}=|\vec{n}|$ shows that $\frac{3}{2}n_\pm T_\pm=W_\pm=W_0\pm|\vec{W}|$ solves equation (2.11).

Third, we derive equation (2.12). We take the product of $\widetilde{P}:=(\mathbb{I}-\vec{s}\otimes\vec{s})/|\vec{n}|$ and expression (4.25) (here, $\mathbb{I}$ is the unit matrix in $\mathbb{R}^{3\times3}$.) This matrix has the following properties: $\widetilde{P}\vec{n}=0$, $\widetilde{P}\partial_t\vec{n}=\partial_t\vec{s}$, and $\widetilde{P}\nabla\vec{n}=\nabla\vec{s}$. A computation shows that

$$\partial_t\vec{s}-\operatorname{div}\left(\widetilde{P}\left(\frac{2}{3}\nabla\vec{W}+\vec{n}\nabla V\right)\right)+\nabla\widetilde{P}\cdot\left(\frac{2}{3}\nabla\vec{W}+\vec{n}\nabla V\right)+\vec{\Omega}_{\mathrm{e}}\times\vec{s}=0. \tag{4.29}$$

We reformulate the second and third term:

$$\begin{aligned}\widetilde{P}\left(\frac{2}{3}\nabla\vec{W}+\vec{n}\nabla V\right)&=\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}\frac{1}{|\vec{W}|}(\mathbb{I}-\vec{s}\otimes\vec{s})\nabla\vec{W}=\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}\nabla\vec{s},\\ (\nabla\widetilde{P}\cdot\nabla\vec{W})_i&=\sum_{j=1}^3\nabla\widetilde{P}_{ij}\cdot\nabla W_j\\ &=\sum_{j=1}^3\left(\frac{1}{|\vec{n}|^2}(\delta_{ij}-s_is_j)\nabla|\vec{n}|-\frac{1}{|\vec{n}|}(s_i\nabla s_j+s_j\nabla s_i)\right)\cdot\nabla W_j\\ &=-\frac{1}{|\vec{n}|^2}|\vec{W}|\nabla|\vec{n}|\cdot\nabla s_i-\frac{1}{|\vec{n}|}|\vec{W}||\nabla\vec{s}|^2s_i-\frac{1}{|\vec{n}|}\nabla|\vec{W}|\nabla s_i\\ &=-\frac{|\vec{W}|}{|\vec{n}|}\nabla\log(|\vec{n}||\vec{W}|)\cdot\nabla s_i-\frac{|\vec{W}|}{|\vec{n}|}|\nabla\vec{s}|^2s_i,\\ \nabla\widetilde{P}\cdot\vec{n}\nabla V&=(\nabla V\cdot\nabla)(\widetilde{P}\vec{n})-\widetilde{P}(\nabla V\cdot\nabla)\vec{n}=-\nabla V\cdot\nabla\vec{s}.\end{aligned}$$

Therefore, equation (4.29) becomes

$$\begin{aligned}\partial_t\vec{s}&=\operatorname{div}\left(\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}\nabla\vec{s}\right)+\left(\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}\nabla\log(|\vec{n}||\vec{W}|)+\nabla V\right)\cdot\nabla\vec{s}+\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}|\nabla\vec{s}|^2\vec{s}-\vec{\Omega}_{\mathrm{e}}\times\vec{s}\\ &=\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}(\Delta\vec{s}+|\nabla\vec{s}|^2\vec{s})+\left\{\nabla\left(\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}\right)+\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}\nabla\log(|\vec{n}||\vec{W}|)+\nabla V\right\}\cdot\nabla\vec{s}-\vec{\Omega}_{\mathrm{e}}\times\vec{s}\\ &=\frac{2}{3}\frac{|\vec{W}|}{|\vec{n}|}\vec{s}\times(\Delta\vec{s}\times\vec{s})+\left(\frac{4}{3}\frac{\nabla|\vec{W}|}{|\vec{n}|}+\nabla V\right)\cdot\nabla\vec{s}-\vec{\Omega}_{\mathrm{e}}\times\vec{s}\\ &=\frac{2}{3}\frac{W_+-W_-}{n_+-n_-}\vec{s}\times(\Delta\vec{s}\times\vec{s})+\left(\frac{4}{3}\frac{\nabla(W_+-W_-)}{n_+-n_-}+\nabla V\right)\cdot\nabla\vec{s}-\vec{\Omega}_{\mathrm{e}}\times\vec{s}.\end{aligned}$$

Then, using $W_\pm=\frac{3}{2}n_\pm T_\pm$, equation (2.12) follows. □

REMARK 4.4. If the temperature is constant, $T_+ = T_- = 1$, equation (2.12) for the spin accumulation vector becomes

$$\partial_t \vec{s} - \vec{s} \times (\Delta \vec{s} \times \vec{s}) = \nabla(\log|\vec{n}|^2 + V) \cdot \nabla \vec{s} - \vec{\Omega}_{\rm e} \times \vec{s}.$$

If $\vec{\Omega}_{\rm e} = \Delta \vec{s}$, this resembles the Landau–Lifshitz equation with the exception of the first term on the right-hand side, which provides an additional field contribution. Note that this term does not vanish in termal equilibrium where $V = -\log n_0$.

5. Entropy structure

In this section, we investigate the entropy structure of the spin energy-transport equations derived in the previous section. Recall that the entropy of the general model is given by

$$H = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \mathrm{tr}(M \log M) dk dx,$$

where $M = M_0\sigma_0 + \vec{M} \cdot \vec{\sigma}$ is the Maxwellian. We introduce $M_\pm = M_0 \pm |\vec{M}|$ and $P_\pm = \frac{1}{2}(\sigma_0 \pm (\vec{M}/|\vec{M}|) \cdot \vec{\sigma})$. Then (P_+, P_-) is a set of complete orthogonal projections since $P_\pm^2 = P_\pm$, $P_+P_- = 0$, and $P_+ + P_- = \sigma_0$. Therefore, for any function $f : \mathbb{R} \to \mathbb{R}$,

$$\begin{aligned} f(M) &= f(M_+)P_+ + f(M_-)P_- \\ &= \frac{1}{2}\big(f(M_+) + f(M_-)\big)\sigma_0 + \frac{1}{2}\big(f(M_+) - f(M_-)\big)\frac{\vec{M}}{|\vec{M}|} \cdot \vec{\sigma}. \end{aligned}$$

In particular, since the Pauli matrices are traceless,

$$H = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (M_+ \log M_+ + M_- \log M_-) dk dx. \tag{5.1}$$

5.1. Entropy inequality for the first model.

We wish to explore the entropy structure of the first model (2.1)–(2.3) ($\vec{c} = 0$), neglecting the electric field:

$$\partial_t n_0 = \Delta(n_0 T), \quad \frac{3}{2}\partial_t(n_0 T) = \frac{5}{2}\Delta(n_0 T^2), \quad \partial_t \vec{n} = \Delta(\vec{n} T) - \vec{\Omega}_{\rm e} \times \vec{n} - \frac{\vec{n}}{\tau_{\rm sf}}, \tag{5.2}$$

where $x \in \mathbb{R}^3$, $t > 0$. We claim that the entropy is given by equation (2.15). Indeed, since $\vec{c} = 0$ by assumption, $M = g_T(k)(n_0\sigma_0 + \vec{n} \cdot \vec{\sigma})$, where $g_T(k)$ is defined in equation (4.7) (see the proof of Theorem 4.1). Then $M_\pm = g_T(k) n_\pm$ and equation (5.1) shows that

$$\begin{aligned} H_1 &= \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} g_T(k)\big(n_+ \log(n_+ g_T(k)) + n_- \log(n_- g_T(k))\big) dx dk \\ &= \frac{1}{2} \int_{\mathbb{R}^3} (n_+ \log n_+ + n_- \log n_-) dx + \int_{\mathbb{R}^3} (n_+ + n_-) \int_{\mathbb{R}^3} g_T(k) \log g_T(k) dk dx \\ &= \frac{1}{2} \int_{\mathbb{R}^3} (n_+ \log n_+ + n_- \log n_-) dx - \int_{\mathbb{R}^3} (n_+ + n_-) \left(\frac{3}{2} + \frac{3}{2}\log(2\pi T)\right) dx. \end{aligned}$$

Thus, since $\int_{\mathbb{R}^3} (n_+ + n_-) dx$ is constant in time, we find that, up to a constant,

$$H_1 = \int_{\mathbb{R}^3} \big(n_+ \log(n_+ T^{-3/2}) + n_- \log(n_- T^{-3/2})\big) dx,$$

which is exactly equation (2.15). Recall that $n_\pm = n_0 \pm |\vec{n}|$.

Proposition 5.1 (Entropy inequality for system (5.2)). *The entropy* (2.15), *considered as a function of time, is nonincreasing along (smooth) solutions* $(n_0,T,\vec n)$ *to equation* (5.2), *and*

$$\frac{dH_1}{dt}+4\int_{\mathbb{R}^3}\big(|\nabla\sqrt{n_+T}|^2+|\nabla\sqrt{n_-T}|^2\big)dx+20\int_{\mathbb{R}^3}n_0|\nabla\sqrt{T}|^2\big)dx$$
$$+\frac12\int_{\mathbb{R}^3}(n_+-n_-)(\log n_+-\log n_-)\left(\frac{1}{\tau_{\rm sf}}+T\left|\nabla\frac{\vec n}{|\vec n|}\right|^2\right)dx=0. \tag{5.3}$$

Proof. We compute

$$\begin{aligned}\frac{dH_1}{dt}&=\int_{\mathbb{R}^3}\sum_{s=\pm}\left(\log(n_sT^{-3/2})\partial_tn_s-\frac32\frac1T\partial_t(n_sT)\right)dx\\
&=\int_{\mathbb{R}^3}\bigg(\log\big((n_0+|\vec n|)T^{-3/2}\big)\partial_t(n_0+|\vec n|)-\frac32\frac1T\partial_t(n_0T+|\vec n|T)\\
&\quad+\log\big((n_0-|\vec n|)T^{-3/2}\big)\partial_t(n_0-|\vec n|)-\frac32\frac1T\partial_t(n_0T-|\vec n|T)\bigg)dx\\
&=\int_{\mathbb{R}^3}\left\{\log\left(\frac{n_0^2-|\vec n|^2}{T^3}\right)\partial_tn_0+\log\left(\frac{n_0+|\vec n|}{n_0-|\vec n|}\right)\frac{\vec n}{|\vec n|}\cdot\partial_t\vec n-\frac2T\partial_t\left(\frac32n_0T\right)\right\}dx. \end{aligned}\tag{5.4}$$

Inserting expression (2.1) in the first term and integrating by parts, we find that

$$\int_{\mathbb{R}^3}\log\left(\frac{n_0^2-|\vec n|^2}{T^3}\right)\partial_tn_0dx=-\int_{\mathbb{R}^3}\nabla\log\left(\frac{n_0^2-|\vec n|^2}{T^3}\right)\cdot\nabla(n_0T)dx.$$

Furthermore, using experssion (2.3) in the second term on the right-hand side of equation (5.4) and integrating by parts gives

$$\begin{aligned}&\int_{\mathbb{R}^3}\log\left(\frac{n_0+|\vec n|}{n_0-|\vec n|}\right)\frac{\vec n}{|\vec n|}\cdot\partial_t\vec ndx\\
&=-\int_{\mathbb{R}^3}\nabla\left(\log\left(\frac{n_0+|\vec n|}{n_0-|\vec n|}\right)\right)\frac{\vec n}{|\vec n|}\cdot\nabla(\vec nT)dx\\
&\quad-\int_{\mathbb{R}^3}\log\left(\frac{n_0+|\vec n|}{n_0-|\vec n|}\right)\nabla\frac{\vec n}{|\vec n|}\cdot\nabla(\vec nT)dx-\frac{1}{\tau_{\rm sf}}\int_{\mathbb{R}^3}|\vec n|\log\left(\frac{n_0+|\vec n|}{n_0-|\vec n|}\right)dx.\end{aligned}$$

Since $\nabla(\vec n/|\vec n|)\cdot(\vec n/|\vec n|)=0$ (note that $\vec n/|\vec n|$ is a unit vector) and

$$\begin{aligned}\nabla\frac{\vec n}{|\vec n|}\cdot\nabla(\vec nT)&=\nabla\frac{\vec n}{|\vec n|}\cdot\nabla\left(|\vec n|T\frac{\vec n}{|\vec n|}\right)=|\vec n|T\left|\nabla\frac{\vec n}{|\vec n|}\right|^2,\\
\frac{\vec n}{|\vec n|}\cdot\nabla(\vec nT)&=\frac{\vec n}{|\vec n|}\cdot(T\nabla\vec n+\vec n\nabla T)=T\nabla|\vec n|+|\vec n|\nabla T=\nabla(|\vec n|T),\end{aligned}$$

it follows that

$$\begin{aligned}&\int_{\mathbb{R}^3}\log\left(\frac{n_0+|\vec n|}{n_0-|\vec n|}\right)\frac{\vec n}{|\vec n|}\cdot\partial_t\vec ndx\\
&=-\int_{\mathbb{R}^3}\nabla\log\left(\frac{n_0+|\vec n|}{n_0-|\vec n|}\right)\cdot\nabla(|\vec n|T)dx\end{aligned}$$

$$-\int_{\mathbb{R}^3}\log\left(\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}\right)|\vec{n}|T\left|\nabla\frac{\vec{n}}{|\vec{n}|}\right|^2dx-\frac{1}{\tau_{\rm sf}}\int_{\mathbb{R}^3}|\vec{n}|\log\left(\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}\right)dx.$$

Finally, we employ equation (2.2) to reformulate the last term on the right-hand side of equation (5.4):

$$\begin{aligned}-\int_{\mathbb{R}^3}\frac{2}{T}\partial_t\left(\frac{3}{2}n_0T\right)dx&=5\int_{\mathbb{R}^3}\nabla\frac{1}{T}\cdot\nabla(n_0T^2)dx\\&=-5\int_{\mathbb{R}^3}\nabla\log T\cdot\nabla(n_0T)dx-5\int_{\mathbb{R}^3}\frac{n_0}{T}|\nabla T|^2dx.\end{aligned}$$

Summarizing these expressions, we have

$$\begin{aligned}\frac{dH_1}{dt}=&-\int_{\mathbb{R}^3}\left\{\nabla\log\left(\frac{n_0^2-|\vec{n}|^2}{T^3}\right)\cdot\nabla(n_0T)dx+\nabla\log\left(\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}\right)\cdot\nabla(|\vec{n}|T)\right.\\&\left.+5\nabla\log T\cdot\nabla(n_0T)+5\frac{n_0}{T}|\nabla T|^2\right\}dx\\&-\int_{\mathbb{R}^3}\left\{\log\left(\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}\right)|\vec{n}|T\left|\nabla\frac{\vec{n}}{|\vec{n}|}\right|^2+\frac{1}{\tau_{\rm sf}}|\vec{n}|\log\left(\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}\right)\right\}dx\\=&\,I_1+I_2.\end{aligned}$$

The integrals in I_2 correspond, up to the minus sign, to the second and third integrals in equation (5.3). It remains to show that I_1 corresponds to the first integral in equation (5.3), up to the sign. Indeed, since $\log(n_0^2-|\vec{n}|^2)=\log n_++\log n_-$ and $\log((n_0+|\vec{n}|)/(n_0-|\vec{n}|))=\log n_+-\log n_-$, we have

$$\begin{aligned}I_1=&-\int_{\mathbb{R}^3}\nabla\log(n_0^2-|\vec{n}|^2)\cdot\nabla(n_0T)dx\\&-\int_{\mathbb{R}^3}\nabla\log\left(\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}\right)\cdot\nabla(|\vec{n}|T)dx-2\int_{\mathbb{R}^3}\nabla\log T\cdot\nabla(n_0T)dx\\=&-\int_{\mathbb{R}^3}\big(\nabla\log n_+\cdot\nabla(n_+T)+\nabla\log n_-\cdot\nabla(n_-T)+\nabla\log T\cdot\nabla(n_+T+n_-T)\big)dx\\=&-\int_{\mathbb{R}^3}\big(\nabla\log(n_+T)\cdot\nabla(n_+T)+\nabla\log(n_-T)\cdot\nabla(n_-T)\big)dx.\end{aligned}$$

This ends the proof. ∎

Remark 5.1. When system (2.1)–(2.3) includes the electric field, a computation similar to the proof of Proposition 5.1 shows that the entropy-production identity reads as

$$\begin{aligned}\frac{dH_1}{dt}&+\int_{\mathbb{R}^3}\left(\frac{|\nabla(n_+T)+n_+T\nabla V|^2}{n_+T}+\frac{|\nabla(n_-T)+n_-T\nabla V|^2}{n_-T}\right)dx\\&+10\int_{\mathbb{R}^3}(n_++n_-)|\nabla\sqrt{T}|^2)dx\\&+\frac{1}{2}\int_{\mathbb{R}^3}(n_+-n_-)(\log n_+-\log n_-)\left(\frac{1}{\tau_{\rm sf}}+T\left|\nabla\frac{\vec{n}}{|\vec{n}|}\right|^2\right)dx=0.\end{aligned}$$

Thus, the presence of the electric field complicates the existence of a priori bounds.

5.2. Entropy inequality for the second model. We show that there exists an entropy for the second model (4.12)–(4.14) ($\vec{a}=0$) for vanishing electric field,

$$\partial_t n_0 = \Delta(n_0 T), \quad \frac{3}{2}\partial_t(n_0 T) = \Delta Z_0, \quad \partial_t \vec{W} = \Delta \vec{Z} - \vec{\Omega}_{\rm e} \times \vec{W} - \frac{\vec{W}}{\tau_{\rm sf}}, \tag{5.5}$$

where $x \in \mathbb{R}^3$, $t>0$, and $(Z_0, \vec{Z})$ are defined in equations (4.15)–(4.16), i.e.

$$Z_0 = \frac{5}{18 n_0}\big(W_+^{3/5} + W_-^{3/5}\big)\big(W_+^{7/5} + W_-^{7/5}\big),$$
$$\vec{Z} = \frac{5}{18 n_0}\big(W_+^{3/5} + W_-^{3/5}\big)\big(W_+^{7/5} - W_-^{7/5}\big)\frac{\vec{W}}{|\vec{W}|}.$$

We claim that the general entropy (2.14) becomes an entropy for the second model when the Maxwellian $M = M_0\sigma_0 + \vec{M}\cdot\vec{\sigma}$ is given by expression (4.10), and this entropy equals, up to a constant, expression (2.16). Note that if $\vec{W}=0$, we obtain $W_\pm = W_0 = \frac{3}{2}n_0 T$ and $H_2 = \int_{\mathbb{R}^d} n_0 \log(n_0 T^{-3/2})dx$, up to a constant. This function corresponds to the entropy of the semiclassical energy-transport model [13, Chapter 6].

To show that equation (2.14) reduces to equation (2.16), we may employ expression (5.1) but we prefer to proceed in a slightly different way. We observe that the Pauli matrices are traceless and we employ the formula $(\vec{c}\cdot\vec{\sigma})(\vec{M}\cdot\vec{\sigma}) = (\vec{c}\cdot\vec{M})\sigma_0 + i(\vec{c}\times\vec{M})\cdot\vec{\sigma}$ (see [18, (7)]) to infer that

$$\begin{aligned} H_2 &= \frac{1}{2}\operatorname{tr}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}(M_0 + \vec{M}\cdot\vec{\sigma})\left(a_0\sigma_0 + (c_0\sigma_0 + \vec{c}\cdot\vec{\sigma})\frac{|k|^2}{2}\right)dkdx \\ &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\left(a_0 M_0 + c_0 M_0 \frac{|k|^2}{2} + \vec{c}\cdot\vec{M}\frac{|k|^2}{2}\right)dkdx \\ &= \int_{\mathbb{R}^3}\big(a_0 n_0 + c_0 W_0 + \vec{c}\cdot\vec{W}\big)dx. \end{aligned}$$

The Lagrange multiplier a_0 can be written in the following way, using the first equation in (4.11) and (4.20):

$$a_0 = \log\frac{K}{(2\pi)^{3/2}} = \frac{5}{2}\log n_0 - \frac{5}{2}\log(W_+^{3/5} + W_-^{3/5}) + \log(2\cdot 3^{3/2}(2\pi)^{-3/2}).$$

Observing that $\int_{\mathbb{R}^3} n_0 dx$ is constant in time, it holds that, up to a constant,

$$\int_{\mathbb{R}^3} a_0 n_0 dx = \frac{5}{2}\int_{\mathbb{R}^3} n_0 \log\frac{n_0}{W_+^{3/5} + W_-^{3/5}}dx.$$

By the second equation in (4.11), we have $c_0 \pm |\vec{c}| = -1/\theta_\pm$, which yields

$$c_0 = -\frac{1}{2}\left(\frac{1}{\theta_+} + \frac{1}{\theta_-}\right), \quad |\vec{c}| = \frac{1}{2}\left(\frac{1}{\theta_+} - \frac{1}{\theta_-}\right).$$

Furthermore, employing the third equation in (4.11) and (4.19), we have $\vec{c}/|\vec{c}| = \vec{\gamma} = \vec{W}/|\vec{W}|$ which shows that $\vec{c}\cdot\vec{W} = |\vec{c}||\vec{W}|$. Thus, replacing $\theta_\pm$ by the expression in equation (4.21),

$$2(c_0 W_0 + \vec{c}\cdot\vec{W}) = -\left(\frac{1}{\theta_+} + \frac{1}{\theta_-}\right)W_0 + \left(\frac{1}{\theta_+} - \frac{1}{\theta_-}\right)|\vec{W}|$$

$$
\begin{aligned}
&= -\frac{3n_0 W_0}{W_+^{3/5}+W_-^{3/5}}\left(\frac{1}{W_+^{2/5}}+\frac{1}{W_-^{2/5}}\right)+\frac{3n_0|\vec{W}|}{W_+^{3/5}+W_-^{3/5}}\left(\frac{1}{W_+^{2/5}}-\frac{1}{W_-^{2/5}}\right)\\
&= -\frac{3n_0}{W_+^{3/5}+W_-^{3/5}}\left(\frac{W_0+|\vec{W}|}{W_+^{2/5}}+\frac{W_0-|\vec{W}|}{W_-^{2/5}}\right)=-3n_0.
\end{aligned}
$$

Neglecting this contribution as well as the constant in the expression for a_0, this shows the claim.

We show now that the entropy (2.16) is nonincreasing in time and that it provides some gradient estimates.

Proposition 5.2 (Entropy inequality for system (5.5)). *The entropy* (2.16)*, considered as a function of time, is nonincreasing along (smooth) solutions* $(n_0,T,\vec{W})$ *to equation* (5.5) *in* $\mathbb{R}^3$*, where* $W_\pm = W_0 \pm |\vec{W}|$ *and* $W_0=\frac{3}{2}n_0T$*. Furthermore, it holds*

$$
\frac{dH_2}{dt}+c\int_{\mathbb{R}^3}\left(|\nabla\sqrt{W_+}|^2+|\nabla\sqrt{W_-}|^2+T|\nabla\sqrt{n_0}|^2+W_0^{-1}|(\nabla\vec{W})^\top|^2\right)dx\le 0, \tag{5.6}
$$

where $c>0$ *is a constant and* $(\nabla\vec{W})^\top=(\mathbb{I}-|\vec{W}|^{-2}\vec{W}\otimes\vec{W})\nabla\vec{W}$.

Proof. First, we perform some auxiliary computations:

$$
\begin{aligned}
\frac{\partial}{\partial n_0}\left(\frac{5}{2}n_0\log\frac{n_0}{W_+^{3/5}+W_-^{3/5}}\right)&=\frac{5}{2}\left(\log n_0-\log(W_+^{3/5}+W_-^{3/5})+1\right),\\
\frac{\partial}{\partial W_0}\left(\frac{5}{2}n_0\log\frac{n_0}{W_+^{3/5}+W_-^{3/5}}\right)&=-\frac{3}{2}n_0\frac{W_+^{-2/5}+W_-^{-2/5}}{W_+^{3/5}+W_-^{3/5}},\\
\frac{\partial}{\partial \vec{W}}\left(\frac{5}{2}n_0\log\frac{n_0}{W_+^{3/5}+W_-^{3/5}}\right)&=-\frac{3}{2}n_0\frac{W_+^{-2/5}-W_-^{-2/5}}{W_+^{3/5}+W_-^{3/5}}\frac{\vec{W}}{|\vec{W}|}.
\end{aligned}
$$

Using these expressions and equation (5.5), it follows that

$$
\begin{aligned}
\frac{dH_2}{dt}&=\int_{\mathbb{R}^3}\left\{\frac{5}{2}\left(\log n_0-\log(W_+^{3/5}+W_-^{3/5})+1\right)\partial_t n_0\right.\\
&\quad\left.-\frac{3}{2}n_0\frac{W_+^{-2/5}+W_-^{-2/5}}{W_+^{3/5}+W_-^{3/5}}\partial_t W_0-\frac{3}{2}n_0\frac{W_+^{-2/5}-W_-^{-2/5}}{W_+^{3/5}+W_-^{3/5}}\frac{\vec{W}}{|\vec{W}|}\cdot\partial_t\vec{W}\right\}dx\\
&=-\frac{5}{3}\int_{\mathbb{R}^3}\nabla\log\frac{n_0}{W_+^{3/5}+W_-^{3/5}}\cdot\nabla W_0\,dx\\
&\quad+\frac{5}{12}\int_{\mathbb{R}^3}\nabla\frac{n_0(W_+^{-2/5}+W_-^{-2/5})}{W_+^{3/5}+W_-^{3/5}}\cdot\nabla\left(\frac{W_+^{3/5}+W_-^{3/5}}{n_0}(W_+^{7/5}+W_-^{7/5})\right)dx\\
&\quad+\frac{5}{12}\int_{\mathbb{R}^3}\nabla\left(\frac{n_0(W_+^{-2/5}-W_-^{-2/5})}{W_+^{3/5}+W_-^{3/5}}\frac{\vec{W}}{|\vec{W}|}\right)\\
&\qquad\times\nabla\left(\frac{W_+^{3/5}+W_-^{3/5}}{n_0}(W_+^{7/5}-W_-^{7/5})\frac{\vec{W}}{|\vec{W}|}\right)dx\\
&\quad+\frac{3}{2\tau_{\rm sf}}\int_{\mathbb{R}^3}\frac{n_0(W_+^{-2/5}-W_-^{-2/5})}{W_+^{3/5}+W_-^{3/5}}|\vec{W}|\,dx.
\end{aligned}
$$

Setting $\lambda:=n_0/(W_+^{3/5}+W_-^{3/5})$, we can rewrite dH_2/dt as follows:

$$
\begin{aligned}
\frac{dH_2}{dt} &= -\frac{5}{3}\int_{\mathbb{R}^3}\lambda^{-1}\nabla\lambda\cdot\nabla W_0 dx \\
&\quad + \frac{5}{12}\int_{\mathbb{R}^3}\nabla\big(\lambda(W_+^{-2/5}+W_-^{-2/5})\big)\cdot\nabla\big(\lambda^{-1}(W_+^{7/5}+W_-^{7/5})\big)dx \\
&\quad + \frac{5}{12}\int_{\mathbb{R}^3}\nabla\bigg(\lambda(W_+^{-2/5}-W_-^{-2/5})\frac{\vec{W}}{|\vec{W}|}\bigg)\cdot\nabla\bigg(\lambda^{-1}(W_+^{7/5}-W_-^{7/5})\frac{\vec{W}}{|\vec{W}|}\bigg)dx \\
&\quad + \frac{3}{2\tau_{\rm sf}}\int_{\mathbb{R}^3}\lambda|\vec{W}|(W_+^{-2/5}-W_-^{-2/5})dx \\
&= I_1+I_2+I_3+I_4.
\end{aligned}
$$

Using $W_0=\frac{1}{2}(W_++W_-)$, the first integral becomes

$$
I_1 = -\frac{5}{6}\int_{\mathbb{R}^3}\sum_{s=\pm}\frac{\nabla\lambda}{\lambda}\cdot\nabla W_s dx.
$$

By the product rule, the third integral I_3 is computed as

$$
\begin{aligned}
I_3 &= \frac{5}{12}\int_{\mathbb{R}^3}\nabla\big(\lambda(W_+^{-2/5}-W_-^{-2/5})\big)\cdot\nabla\big(\lambda^{-1}(W_+^{7/5}-W_-^{7/5})\big)dx \\
&\quad + \frac{5}{12}\int_{\mathbb{R}^3}\lambda(W_+^{-2/5}-W_-^{-2/5})\lambda^{-1}(W_+^{7/5}-W_-^{7/5})\bigg|\nabla\frac{\vec{W}}{|\vec{W}|}\bigg|^2 dx,
\end{aligned}
$$

where the mixed terms vanish since $\nabla(\vec{W}/|\vec{W}|)\cdot(\vec{W}/|\vec{W}|)=0$ (which is a consequence of $\nabla|\vec{W}/|\vec{W}||^2=0$). Expanding the products in the first integral on the right-hand side and in I_2, some terms cancel, and we end up with

$$
\begin{aligned}
I_2+I_3 &= \frac{5}{6}\int_{\mathbb{R}^3}\big(\nabla(\lambda W_+^{-2/5})\cdot\nabla(\lambda^{-1}W_+^{7/5})+\nabla(\lambda W_-^{-2/5})\cdot\nabla(\lambda^{-1}W_-^{7/5})\big)dx \\
&\quad + \frac{5}{12}\int_{\mathbb{R}^3}(W_+^{-2/5}-W_-^{-2/5})(W_+^{7/5}-W_-^{7/5})\bigg|\nabla\frac{\vec{W}}{|\vec{W}|}\bigg|^2 dx \\
&= \frac{5}{6}\int_{\mathbb{R}^3}\sum_{s=\pm}\bigg(-\frac{14}{25}\frac{|\nabla W_s|^2}{W_s}+\frac{9}{5}\frac{\nabla\lambda}{\lambda}\cdot\nabla W_s-\frac{W_s}{\lambda^2}|\nabla\lambda|^2\bigg)dx \\
&\quad + \frac{5}{12}\int_{\mathbb{R}^3}(W_+^{-2/5}-W_-^{-2/5})(W_+^{7/5}-W_-^{7/5})\bigg|\nabla\frac{\vec{W}}{|\vec{W}|}\bigg|^2 dx.
\end{aligned}
$$

Finally, the fourth integral is nonpositive since $0\le W_-\le W_+$, i.e. $I_4\le 0$. Combining these results, we find that

$$
\begin{aligned}
\frac{dH_2}{dt} &\le -\frac{5}{6}\int_{\mathbb{R}^3}\sum_{s=\pm}\bigg(\frac{14}{25}\bigg|\frac{\nabla W_s}{\sqrt{W_s}}\bigg|^2-\frac{4}{5}\frac{\nabla W_s}{\sqrt{W_s}}\cdot\frac{\sqrt{W_s}}{\lambda}\nabla\lambda+\bigg|\frac{\sqrt{W_s}}{\lambda}\nabla\lambda\bigg|^2\bigg)dx \\
&\quad - \frac{5}{12}\int_{\mathbb{R}^3}(W_-^{-2/5}-W_+^{-2/5})(W_+^{7/5}-W_-^{7/5})\bigg|\nabla\frac{\vec{W}}{|\vec{W}|}\bigg|^2 dx \\
&= J_1+J_2. \qquad (5.7)
\end{aligned}
$$

First, we consider the first integral J_1. The quadratic form in J_1 is positive definite and the eigenvalues of the associated matrix are larger than $1/5$, so

$$\begin{aligned} J_1 &\le -\frac{1}{5}\int_{\mathbb{R}^3}\left(|\nabla\sqrt{W_+}|^2+|\nabla\sqrt{W_-}|^2+(W_++W_-)\left|\frac{\nabla\lambda}{\lambda}\right|^2\right)dx \\ &\le -\frac{1}{5}\int_{\mathbb{R}^3}\left(|\nabla\sqrt{W_+}|^2+|\nabla\sqrt{W_-}|^2+2\varepsilon W_0\left|\frac{\nabla\lambda}{\lambda}\right|^2\right)dx, \end{aligned} \tag{5.8}$$

where we replaced W_++W_- by $2W_0$ and introduced some $\varepsilon\in(0,1)$. The last term can be reformulated in terms of $W_0=\frac{1}{2}(W_++W_-)$ and $n_0=(W_+^{3/5}+W_-^{3/5})\lambda$, using the elementary inequalities $(a-b)^2\ge\frac{1}{2}a^2-b^2$ and $-(a+b)^2\ge-2(a^2+b^2)$:

$$\begin{aligned} W_0\left|\frac{\nabla\lambda}{\lambda}\right|^2 &= W_0\left|\frac{\nabla n_0}{n_0}-\frac{3}{5}\frac{W_+^{-2/5}\nabla W_+}{W_+^{3/5}+W_-^{3/5}}-\frac{3}{5}\frac{W_-^{-2/5}\nabla W_-}{W_+^{3/5}+W_-^{3/5}}\right|^2 \\ &\ge \frac{1}{2}W_0\left|\frac{\nabla n_0}{n_0}\right|^2-\frac{18}{25}W_0\left(\frac{W_+^{-4/5}|\nabla W_+|^2}{(W_+^{3/5}+W_-^{3/5})^2}+\frac{W_-^{-4/5}|\nabla W_-|^2}{(W_+^{3/5}+W_-^{3/5})^2}\right). \end{aligned}$$

Employing $W_+^{3/5}+W_-^{3/5}\ge(W_++W_-)^{3/5}=(2W_0)^{3/5}$ and $W_\pm^{1/5}\le(2W_0)^{1/5}$, we can estimate as follows:

$$\begin{aligned} W_0\left|\frac{\nabla\lambda}{\lambda}\right|^2 &\ge \frac{1}{2}W_0\left|\frac{\nabla n_0}{n_0}\right|^2-\frac{18}{25}W_0\left(\frac{4W_+^{1/5}|\nabla\sqrt{W_+}|^2}{(2W_0)^{6/5}}+\frac{4W_-^{1/5}|\nabla W_-|^2}{(2W_0)^{6/5}}\right) \\ &= \frac{1}{2}W_0\left|\frac{\nabla n_0}{n_0}\right|^2-\frac{18}{25}\frac{2^{4/5}}{W_0^{1/5}}\left(W_+^{1/5}|\nabla\sqrt{W_+}|^2+W_-^{1/5}|\nabla\sqrt{W_-}|^2\right) \\ &\ge \frac{1}{2}W_0\left|\frac{\nabla n_0}{n_0}\right|^2-\frac{36}{25}\left(|\nabla\sqrt{W_+}|^2+|\nabla\sqrt{W_-}|^2\right). \end{aligned}$$

Then, with the relation $W_0=\frac{3}{2}n_0T$,

$$W_0\left|\frac{\nabla\lambda}{\lambda}\right|^2\ge 3T|\nabla\sqrt{n_0}|^2-\frac{36}{25}\left(|\nabla\sqrt{W_+}|^2+|\nabla\sqrt{W_-}|^2\right).$$

Inserting this expression into estimate (5.8) and choosing $\varepsilon>0$ sufficiently small, we arrive at

$$J_1\le -c\int_{\mathbb{R}^3}\left(|\nabla\sqrt{W_+}|^2+|\nabla\sqrt{W_-}|^2+T|\nabla\sqrt{n_0}|^2\right)dx \tag{5.9}$$

for some number $0<c<1/5$.

Next, we estimate the second integral J_2 in estimate (5.7). By the mean-value theorem, there exist ξ, $\eta\in[W_-,W_+]$ such that

$$\begin{aligned} (W_-^{-2/5}-W_+^{-2/5})(W_+^{7/5}-W_-^{7/5}) &= (W_+W_-)^{-2/5}(W_+^{2/5}-W_-^{2/5})(W_+^{7/5}-W_-^{7/5}) \\ &= \frac{14}{25}(W_+W_-)^{-2/5}\xi^{-3/5}\eta^{2/5}(W_+-W_-)^2\ge\frac{14}{25}W_+^{-1}(W_+-W_-)^2\ge\frac{28}{25}\frac{|\vec{W}|^2}{W_0}, \end{aligned}$$

where we used that $W_+\le 2W_0$ and $W_+-W_-=2|\vec{W}|$. Consequently,

$$J_2\ge\frac{28}{25}\int_{\mathbb{R}^3}\frac{|\vec{W}|^2}{W_0}\left|\nabla\frac{\vec{W}}{|\vec{W}|}\right|^2dx=\frac{28}{25}\int_{\mathbb{R}^3}\frac{1}{W_0}\left|\left(\mathbb{I}-\frac{\vec{W}\otimes\vec{W}}{|\vec{W}|^2}\right)\nabla\vec{W}\right|^2dx.$$

Combining this inequality and estimate (5.9) with estimate (5.7), the result follows. ∎

5.3. Entropy inequality for the third model. We show that there exists an entropy for the third model (2.10)–(2.12) ($\vec{a}=\lambda\vec{c}$) for vanishing electric fields, i.e.

$$\partial_t n_\pm - \Delta(n_\pm T_\pm) = \mp\frac{1}{2\tau_{\rm sf}}(n_+ - n_-) \mp \frac{1}{2}(n_+T_+ - n_-T_-)|\nabla\vec{s}|^2, \tag{5.10}$$

$$\frac{3}{2}\partial_t(n_\pm T_\pm) - \frac{5}{2}\Delta(n_\pm T_\pm^2) = \mp\frac{3}{4\tau_{\rm sf}}(n_+T_+ - n_-T_-) \mp \frac{5}{4}(n_+T_+^2 - n_-T_-^2)|\nabla\vec{s}|^2, \tag{5.11}$$

$$\partial_t\vec{s} - \frac{n_+T_+ - n_-T_-}{n_+ - n_-}\vec{s}\times(\Delta\vec{s}\times\vec{s}) = 2\frac{\nabla(n_+T_+ - n_-T_-)}{n_+ - n_-}\cdot\nabla\vec{s} - \vec{\Omega}_{\rm e}\times\vec{s}, \tag{5.12}$$

where $x\in\mathbb{R}^3$, $t>0$. As in Section 5.2, we make first explicit the entropy functional (2.14), where the Maxwellian is given by its Pauli components (4.23). A computation shows that $M_\pm = n_\pm g_{T_\pm}(k)\sigma_0$, so equation (5.1) yields immediately entropy (2.17).

PROPOSITION 5.3 (Entropy inequality for system (5.10)–(5.12)). *The entropy* (2.17)*, considered as a function of time, is nonincreasing along (smooth) solutions* $(n_\pm, T_\pm, \vec{s})$ *to system* (5.10)–(5.12) *in* $\mathbb{R}^3$*, and there exists a number* $c>0$ *such that*

$$\frac{dH_3}{dt} + c\int_{\mathbb{R}^3}\sum_{s=\pm}\left(T_s|\nabla\sqrt{n_s}|^2 + n_s|\nabla\sqrt{T_s}|^2\right)dx \le 0.$$

Proof. Before computing the derivative dH_3/dt, let us consider the semiclassical energy-transport system

$$\partial_t n = \Delta(nT), \quad \frac{3}{2}\partial_t(nT) = \frac{5}{2}\Delta(nT^2) \quad \text{in } \mathbb{R}^3,$$

which is known to dissipate the entropy $H_0 = \int_{\mathbb{R}^3} n\log(nT^{-3/2})dx$. Indeed, a computation shows that

$$\begin{aligned}\frac{dH_0}{dt} &= -\int_{\mathbb{R}^3}\left(\nabla(nT)\cdot\nabla(nT^{-3/2}) - \frac{5}{2}\nabla\frac{1}{T}\cdot\nabla(nT^2)\right)dx \\ &= -4\int_{\mathbb{R}^3}\left(|\sqrt{T}\nabla\sqrt{n}|^2 + 2\sqrt{T}\nabla\sqrt{n}\cdot\sqrt{n}\nabla\sqrt{T} + \frac{7}{2}|\sqrt{n}\sqrt{T}|^2\right)dx.\end{aligned}$$

The quadratic form in the variables $\sqrt{T}\nabla\sqrt{n}$ and $\sqrt{n}\nabla\sqrt{T}$ is positive definite and the eigenvalues of the associated matrix are larger than 1/2, so

$$\frac{dH_0}{dt} + 2\int_{\mathbb{R}^3}\left(|\sqrt{T}\nabla\sqrt{n}|^2 + |\sqrt{n}\nabla\sqrt{T}|^2\right)dx \le 0.$$

The similarity in structure between H_3 and H_0 as well as between the spin and semiclassical energy-transport system allows us to deduce that, for some number $c>0$,

$$\begin{aligned}&\frac{dH_3}{dt} + c\int_{\mathbb{R}^3}\sum_{s=\pm}\left(T_s|\nabla\sqrt{n_s}|^2 + n_s|\nabla T_s|^2\right)dx \\ &\le -\frac{1}{2\tau_{\rm sf}}\int_{\mathbb{R}^3}\left(\log\frac{n_+T_+^{-3/2}}{n_-T_-^{-3/2}}(n_+ - n_-) + \frac{3}{2}\frac{T_+ - T_-}{T_+T_-}(n_+T_+ - n_-T_-)\right)dx \\ &\quad - \frac{1}{2}\int_{\mathbb{R}^3}\left(\log\frac{n_+T_+^{-3/2}}{n_-T_-^{-3/2}}(n_+T_+ - n_-T_-) + \frac{5}{2}\frac{T_+ - T_-}{T_+T_-}(n_+T_+^2 - n_-T_-^2)\right)|\vec{s}|^2dx = I_1 + I_2.\end{aligned}$$

We claim that $I_1 \le 0$ and $I_2 \le 0$ which concludes the proof.

First, we prove that $I_1 \le 0$. It holds that

$$\begin{aligned} I_1 &= -\frac{1}{2\tau_{\rm sf}}\int_{\mathbb{R}^3}(n_+ - n_-)(\log n_+ - \log n_-)dx \\ &\quad - \frac{3}{4\tau_{\rm sf}}\int_{\mathbb{R}^3}\left(-(n_+ - n_-)\log\frac{T_+}{T_-} + \frac{T_+ - T_-}{T_+T_-}(n_+T_+ - n_-T_-)\right)dx \\ &\le -\frac{3}{4\tau_{\rm sf}}\int_{\mathbb{R}^3}\left(-(n_+ - n_-)\log\frac{T_+}{T_-} + \frac{T_+ - T_-}{T_+T_-}(n_+T_+ - n_-T_-)\right)dx. \end{aligned}$$

Because of $T_- \le T_+$ and $n_- \ge 0$, we have $n_+T_+ - n_-T_- \ge (n_+ - n_-)T_+$ which shows that

$$\begin{aligned} I_1 e &- \frac{3}{4\tau_{\rm sf}}\int_{\mathbb{R}^3}\left(-(n_+ - n_-)\log\frac{T_+}{T_-} + \frac{1}{T_-}(n_+ - n_-)(T_+ - T_-)\right)dx \\ &= -\frac{3}{4\tau_{\rm sf}}\int_{\mathbb{R}^3}(n_+ - n_-)\left(\frac{T_+}{T_-} - 1 - \log\frac{T_+}{T_-}\right)dx \le 0. \end{aligned}$$

In a similar way as above, we find that $n_+T_+^2 - n_-T_-^2 \ge (n_+T_+ - n_-T_-)T_+$ and

$$\begin{aligned} I_2 &= -\frac{1}{2}\int_{\mathbb{R}^3}(n_+T_+ - n_-T_-)(\log(n_+T_+) - \log(n_-T_-))dx \\ &\quad - \frac{5}{4}\int_{\mathbb{R}^3}\left(-(n_+T_+ - n_-T_-)\log\frac{T_+}{T_-} + \frac{T_+ - T_-}{T_+T_-}(n_+T_+^2 - n_-T_-^2)\right)|\vec{s}|^2 dx \\ &\le -\frac{5}{4}\int_{\mathbb{R}^3}\left(-(n_+T_+ - n_-T_-)\log\frac{T_+}{T_-} + \frac{1}{T_-}(n_+T_+ - n_-T_-)(T_+ - T_-)\right)|\vec{s}|^2 dx \\ &= -\frac{5}{4}\int_{\mathbb{R}^3}(n_+T_+ - n_-T_-)\left(\frac{T_+}{T_-} - 1 - \log\frac{T_+}{T_-}\right)dx \le 0. \end{aligned}$$

This finishes the proof. ∎

6. Existence analysis of the second model

We show the existence of weak solutions to a time-discrete version of the second model in the formulation (4.12)–(4.14) for vanishing electric field. Replacing $W_0 = \frac{3}{2}n_0T$ and Z_0, $\vec{Z}$ by expressions (4.15), (4.16), respectively, we obtain system (2.19)–(2.21). We recall that $h > 0$ is the time step size, $(n_0, W_0, \vec{W})$ are the unknowns, and $(n_0^0, W_0^0, \vec{W}^0)$ are the moments at the previous time step (supposed to be given).

THEOREM 6.1 (Existence for the time-discrete second model). *Let $\mathcal{D} \subset \mathbb{R}^d$ ($d \le 3$) be a bounded domain and let n_0^0, $W_0^0 \in L^2(\mathcal{D})$, n_0^D, $W_0^D \in H^1(\mathcal{D}) \cap L^\infty(\mathcal{D})$, $\vec{W}^D \in H^1(\mathcal{D};\mathbb{R}^3) \cap L^\infty(\mathcal{D};\mathbb{R}^3)$, $\vec{W}^0 \in L^2(\mathcal{D};\mathbb{R}^3)$ satisfy $\sup_{\partial\mathcal{D}}|\vec{W}^D|/W_0^D < 1$ and*

$$n_0^0 > 0,\ W_0^0 > 0 \quad \textit{in } \mathcal{D}, \quad \inf_{\mathcal{D}}\frac{W_0^0}{n_0^0} > 0, \quad \sup_{\mathcal{D}}\frac{|\vec{W}^0|}{W_0^0} < 1.$$

Then there exists a solution $(n_0, W_0, \vec{W}) \in H^1(\mathcal{D};\mathbb{R}^5)$ to system (2.19)–(2.22) such that

$$n_0 > 0,\ W_0 > 0 \quad \textit{in } \mathcal{D}, \quad \inf_{\mathcal{D}}\frac{W_0}{n_0} > 0, \quad \sup_{\mathcal{D}}\frac{|\vec{W}|}{W_0} < 1.$$

Proof. The proof is inspired by the techniques employed in [21]. The idea is to introduce new variables to make the differential operator linear and to truncate the nonlinearities. We proceed in several steps.

Step 1: new variables. Let $W_\pm = W_0 \pm |\vec{W}|$. We define

$$u := \frac{2}{3}W_0, \quad v_0 := \frac{5}{18n_0}(W_+^{3/5} + W_-^{3/5})(W_+^{7/5} + W_-^{7/5}),$$
$$\vec{v} := \frac{5}{18n_0}(W_+^{3/5} + W_-^{3/5})(W_+^{7/5} - W_-^{7/5})\frac{\vec{W}}{|\vec{W}|}.$$

Observe that $\sup_{\partial\mathcal{D}}|\vec{W}^D|/W_0^D < 1$ implies that $\inf_{\partial\mathcal{D}} W_\pm > 0$ and $\sup_{\partial\mathcal{D}}|\vec{v}|/v_0 < 1$. Furthermore,

$$|\vec{v}| = \frac{5}{18n_0}(W_+^{3/5} + W_-^{3/5})(W_+^{7/5} - W_-^{7/5}), \quad \frac{\vec{v}}{|\vec{v}|} = \frac{\vec{W}}{|\vec{W}|},$$
$$v_\pm := v_0 \pm |\vec{v}| = \frac{5}{9n_0}(W_+^{3/5} + W_-^{3/5})W_\pm^{7/5}.$$

This shows that $v_+/v_- = (W_+/W_-)^{7/5}$ or equivalently, $W_+/W_- = (v_+/v_-)^{5/7}$. We rewrite the variables in terms of $v_\pm$, observing that $v_+ + v_- = 2v_0$:

$$v_0 = \frac{5}{18}\frac{W_-^2}{n_0}\left(1 + \left(\frac{v_+}{v_-}\right)^{3/7}\right)\left(1 + \frac{v_+}{v_-}\right) = \frac{5}{18}\frac{W_+^2}{n_0}\left(1 + \left(\frac{v_-}{v_+}\right)^{3/7}\right)\left(1 + \frac{v_-}{v_+}\right),$$
$$W_\pm = \left(\frac{18}{5}n_0 v_0\right)^{1/2} v_\pm^{5/7}(v_+^{3/7} + v_-^{3/7})^{-1/2}(v_+ + v_-)^{-1/2}$$
$$= \left(\frac{9}{5}n_0\right)^{1/2} v_\pm^{5/7}(v_+^{3/7} + v_-^{3/7})^{-1/2}$$
$$u = \frac{1}{3}(W_+ + W_-) = \left(\frac{2}{5}n_0 v_0\right)^{1/2}(v_+^{5/7} + v_-^{5/7})(v_+^{3/7} + v_-^{3/7})^{-1/2}(v_+ + v_-)^{1/2}$$
$$= \left(\frac{n_0}{5}\right)^{1/2}(v_+^{5/7} + v_-^{5/7})(v_+^{3/7} + v_-^{3/7})^{-1/2}. \tag{6.1}$$

Solving the last expression for n_0 yields

$$n_0 = 5u^2\frac{v_+^{3/7} + v_-^{3/7}}{(v_+^{5/7} + v_-^{5/7})^2}, \tag{6.2}$$

and inserting this equation into (6.1) gives $W_\pm = 3uv_\pm^{5/7}/(v_+^{5/7} + v_-^{5/7})$. Because of $\vec{v}/|\vec{v}| = \vec{W}/|\vec{W}|$, it follows that

$$W_0 = \frac{1}{2}(W_+ + W_-) = \frac{3}{2}u, \quad \vec{W} = \frac{3}{2}u\frac{v_+^{5/7} - v_-^{5/7}}{v_+^{5/7} + v_-^{5/7}}\frac{\vec{v}}{|\vec{v}|}. \tag{6.3}$$

We infer that system (2.19)–(2.21) can be written as

$$n_0(u, v_0, \vec{v}) - h\Delta u = n_0^0, \tag{6.4}$$
$$W_0(u, v_0, \vec{v}) - h\Delta v_0 = W_0^0, \tag{6.5}$$

$$\left(1+\frac{h}{\tau_{\rm sf}}\right)\vec{W}(u,v_0,\vec{v})-h\Delta\vec{v}=\vec{W}^0 \quad \text{in } \mathcal{D}, \tag{6.6}$$

where $n_0(u,v_0,\vec{v})$, $W_0(u,v_0,\vec{v})$, and $\vec{W}(u,v_0,\vec{v})$ are given by equations (6.2)–(6.3).

Step 2: truncation. We introduce for $\varepsilon>0$ the truncation operator

$$[f]_\varepsilon := \begin{cases} 0 & \text{for } f\le 0,\\ f & \text{for } 0<f\le 1/\varepsilon,\\ 1/\varepsilon & \text{for } f>1/\varepsilon,\end{cases}$$

and the auxiliary functions

$$\lambda(\xi,v_+,v_-) := \frac{5}{2}\xi\frac{(v_+^{3/7}+v_-^{3/7})(v_++v_-)}{(v_+^{5/7}+v_-^{5/7})^2},$$
$$\mu(\xi,v_+,v_-) := \frac{3}{2}\left(1+\frac{h}{\tau_{\rm sf}}\right)\xi\frac{v_+^{5/7}-v_-^{5/7}}{v_+^{5/7}+v_-^{5/7}}.$$

These definitions imply that

$$n_0(u,v_0,\vec{v})=\lambda(u/v_0,v_+,v_-)u, \quad \vec{W}(u,v_0,\vec{v})=\mu(u/v_0,v_+,v_-)v_0\frac{\vec{v}}{|\vec{v}|}.$$

We claim that the following estimate holds for λ and μ:

$$\frac{5}{2}\xi\le\lambda(\xi,v_+,v_-)\le 6\xi, \quad 0\le\mu(\xi,v_+,v_-)\le\frac{3}{2}\left(1+\frac{h}{\tau_{\rm sf}}\right)\xi \tag{6.7}$$

for all $\xi\ge 0$, $v_+\ge v_-\ge 0$. Indeed, the bounds for μ are obvious. In order to prove the upper bound for λ, we observe that

$$(v_+^{3/7}+v_-^{3/7})(v_++v_-)=v_+^{10/7}+v_-^{10/7}+v_+^{3/7}v_-+v_-^{3/7}v_+.$$

By Young's inequality,

$$v_+^{3/7}v_-\le\frac{3}{10}v_+^{10/7}+\frac{7}{10}v_-^{10/7}\le\frac{7}{10}\left(v_+^{10/7}+v_-^{10/7}\right),$$

and the same bound holds for $v_-^{3/7}v_+$ such that

$$(v_+^{3/7}+v_-^{3/7})(v_++v_-)\le\frac{12}{5}\left(v_+^{10/7}+v_-^{10/7}\right)\le\frac{12}{5}\left(v_+^{5/7}+v_-^{5/7}\right)^2.$$

Inserting this estimate into the definition of λ, the upper bound follows. The lower bound is equivalent to $(v_+^{3/7}+v_-^{3/7})(v_++v_-)\ge(v_+^{5/7}+v_-^{5/7})^2$ which follows from

$$\begin{aligned}\left(v_+^{5/7}+v_-^{5/7}\right)^2-\left(v_+^{3/7}+v_-^{3/7}\right)(v_++v_-) &= 2v_+^{5/7}v_-^{5/7}-v_+^{3/7}v_--v_-^{3/7}v_+\\ &= 2(v_+v_-)^{5/7}\left(1-\frac{1}{2}\left(\frac{v_-}{v_+}\right)^{2/7}-\frac{1}{2}\left(\frac{v_+}{v_-}\right)^{2/7}\right)\le 0.\end{aligned}$$

This completes the proof of estimate (6.7).

With the above truncation, we wish to prove the existence of a weak solution to

$$\lambda\big([u/v_0]_\varepsilon,v_+,v_-\big)u-h\Delta u=n_0^0, \tag{6.8}$$

$$\frac{3}{2}[u/v_0]_\varepsilon v_0 - h\Delta v_0 = W_0^0, \tag{6.9}$$

$$\mu\big([u/v_0]_\varepsilon, v_+, v_-\big) v_0 \frac{\vec{v}}{|\vec{v}|} - h\Delta\vec{v} = \vec{W}^0 \quad \text{in } \mathcal{D}, \tag{6.10}$$

where, slightly abusing the notation, $v_\pm$ is here defined by $v_\pm = \max\{0, v_0 \pm |\vec{v}|\}$. Since we will prove below that $v_0 \pm |\vec{v}| \geq 0$, this notation is consistent. The boundary conditions are

$$u = u^D := \frac{2}{3} W_0^D, \quad v_0 = v_0^D, \quad \vec{v} = \vec{v}^D \quad \text{on } \partial\mathcal{D}, \tag{6.11}$$

where

$$v_0^D := \frac{5}{18 n_0^D}((W_+^D)^{3/5} + (W_-^D)^{3/5})((W_+^D)^{7/5} + (W_-^D)^{7/5}),$$

$$\vec{v}^D := \frac{5}{18 n_0^D}((W_+^D)^{3/5} + (W_-^D)^{3/5})((W_+^D)^{7/5} - (W_-^D)^{7/5}) \frac{\vec{W}^D}{|\vec{W}^D|},$$

and $W_\pm^D := W_0^D \pm |\vec{W}^D|$.

Step 3: existence of solutions to the truncated problem. The existence of a solution to system (6.8)-(6.10) is shown using the Leray–Schauder fixed-point theorem. For this, we define the mapping $F: L^2(\mathcal{D};\mathbb{R}^5) \times [0,1] \to L^2(\mathcal{D};\mathbb{R}^5)$, $F(\rho, \nu_0, \vec{\nu}; \sigma) = (u/v_0, v_0, \vec{v})$, such that

$$\sigma\lambda\big([\rho]_\varepsilon, \nu_+, \nu_-\big) u - h\Delta u = n_0^0 \quad \text{in } \mathcal{D}, \quad u = u^D \quad \text{on } \partial\mathcal{D}, \tag{6.12}$$

$$\frac{3}{2}\sigma[\rho]_\varepsilon v_0 - h\Delta v_0 = W_0^0 \quad \text{in } \mathcal{D}, \quad v_0 = v_0^D \quad \text{on } \partial\mathcal{D}, \tag{6.13}$$

$$\sigma\mu\big([\rho]_\varepsilon, \nu_+, \nu_-\big) \nu_0 \frac{\vec{\nu}}{|\vec{\nu}|} - h\Delta\vec{v} = \vec{W}^0 \quad \text{in } \mathcal{D}, \quad \vec{v} = \vec{v}^D \quad \text{on } \partial\mathcal{D}, \tag{6.14}$$

where $\nu_\pm := \max\{0, \nu_0 \pm |\vec{\nu}|\}$. We first show that F is well defined, i.e. $u/v_0 \in L^2(\mathcal{D})$. Standard elliptic regularity implies that u, $v_0 \in H^2(D) \subset L^\infty(\mathcal{D})$ (here we use $d \leq 3$). By Stampacchia's truncation technique, we infer that u and v_0 are strictly positive (see, e.g., Step 2 in [21, Section 2]). We deduce that $u/v_0 \in H^1(\mathcal{D})$, and F is well defined. Since $\vec{v} \in H^2(\mathcal{D};\mathbb{R}^3)$ by elliptic regularity again, the range of F lies in $H^1(\mathcal{D};\mathbb{R}^5)$. Employing u, v_0, $\vec{v}$, respectively, as test functions in the weak formulation of system (6.12)–(6.14) and using the Poincaré inequality (note that $(u, v_0, \vec{v})$ are bounded functions), we obtain for some constant $C > 0$,

$$\|F(\rho, \nu_0, \vec{\nu}; \sigma)\|_{H^1(\mathcal{D};\mathbb{R}^5)} \leq C\big(\|(n_0^0, W_0^0, \vec{W}^0)\|_{L^2(\mathcal{D};\mathbb{R}^5)} + \|(\rho, \nu_0, \vec{\nu})\|_{L^2(\mathcal{D};\mathbb{R}^5)}\big).$$

Standard arguments show that F is continuous. Then the Sobolev embedding $H^1(\mathcal{D}) \hookrightarrow L^2(\mathcal{D})$ implies that F is compact. Moreover, $F(\cdot;0)$ is constant.

It remains to derive uniform a priori estimates for all fixed points of $F(\cdot;\sigma)$. Let $(\rho, \nu_0, \vec{\nu}) \in L^2(\mathcal{D};\mathbb{R}^5)$ be such a fixed point. Then $(\rho, \nu_0, \vec{\nu}) \in H^1(\mathcal{D};\mathbb{R}^5)$ and $u = \rho\nu_0$. Employing $u - u^D$, $v_0 - v_0^D$ as test functions in the weak formulation of system (6.12)–(6.13), respectively, and the Poincaré inequality, we find that

$$\|u\|_{H^1(\mathcal{D})} + \|v_0\|_{H^1(\mathcal{D})} \leq ch^{-1/2}\big(\|n_0^0\|_{L^2(\mathcal{D})} + \|W_0^0\|_{L^2(\mathcal{D})}\big),$$

where here and in the following, $c>0$ denotes a generic constant independent of the solutions (and of ε). Similarly, with the test function $\vec{v}-\vec{v}^D$ in the weak formulation of (6.14), using the nonnegativity of ν_0 and μ,

$$\|\vec{v}\|_{H^1(\mathcal{D})} \le Ch^{-1/2}\|\vec{W}^0\|_{L^2(\mathcal{D})}.$$

These estimates provides the uniform bound in $L^2(\mathcal{D};\mathbb{R}^5)$ for all fixed points of $F(\cdot,\sigma)$. By the Leray–Schauder fixed-point theorem, we infer the existence of a weak solution to system (6.8)–(6.10).

Step 4: removing the truncation. We prove that that there exists a positive lower bound for u/v_0 which is independent of ε. As a consequence, the truncation in system (6.8)–(6.10) can be removed for sufficiently small values of $\varepsilon>0$, giving a solution to system (2.19)–(2.21).

We choose $\varepsilon := \min\{\inf_{\mathcal{D}}(W_0^0/n_0^0),(\sup_{\mathcal{D}}(u^D/v_0^D))^{-1}\}$, which is positive by assumption, and define $\phi(z)=\max\{0,z-1/\varepsilon\}$. We use the (admissible) test functions $v_0\phi(u/v_0)$, $u\phi(u/v_0)$ in (6.8), (6.9), respectively, and take the difference of the resulting equations:

$$\begin{aligned}
&\int_{\mathcal{D}}\Big(\lambda\big([u/v_0]_\varepsilon,v_+,v_-\big)-\frac{3}{2}[u/v_0]_\varepsilon\Big)uv_0\phi(u/v_0)dx \\
&\qquad + h\int_{\mathcal{D}}\big(\nabla(v_0\phi(u/v_0))\cdot\nabla u-\nabla(u\phi(u/v_0))\cdot\nabla v_0\big)dx \\
&= \int_{\mathcal{D}}(v_0n_0^0-uW_0^0)\phi(u/v_0)dx. \qquad (6.15)
\end{aligned}$$

By estimate (6.7), the first integral on the left-hand side can be estimated from below,

$$\int_{\mathcal{D}}\Big(\lambda\big([u/v_0]_\varepsilon,v_+,v_-\big)-\frac{3}{2}[u/v_0]_\varepsilon\Big)uv_0\phi(u/v_0)dx \ge \int_{\mathcal{D}}[u/v_0]_\varepsilon uv_0\phi(u/v_0)dx \ge 0.$$

The second integral on the left-hand side of equation (6.15) is nonnegative since

$$\begin{aligned}
&\int_{\mathcal{D}}\big(\nabla(v_0\phi(u/v_0))\cdot\nabla u-\nabla(u\phi(u/v_0))\cdot\nabla v_0\big)dx \\
&= \int_{\mathcal{D}}\big(v_0\nabla\phi(u/v_0)\cdot\nabla u-u\nabla\phi(u/v_0)\cdot\nabla v_0\big)dx \\
&= \int_{\mathcal{D}}(v_0\nabla u-u\nabla v_0)\cdot\nabla(u/v_0)\phi'(u/v_0)dx = \int_{\mathcal{D}}v_0^2|\nabla(u/v_0)|^2\phi'(u/v_0)dx \ge 0.
\end{aligned}$$

Finally, because of $\phi(u/v_0)=0$ if $v_0/u\ge\varepsilon$ and $\varepsilon\le W_0^0/n_0^0$, the integral on the right-hand side of equation (6.15) becomes

$$\begin{aligned}
\int_{\mathcal{D}}(v_0n_0^0-uW_0^0)\phi(u/v_0)dx &= \int_{\mathcal{D}}un_0^0\left(\frac{v_0}{u}-\frac{W_0^0}{n_0^0}\right)\phi(u/v_0)dx \\
&\le \int_{\mathcal{D}}un_0^0\left(\varepsilon-\frac{W_0^0}{n_0^0}\right)\phi(u/v_0)dx \le 0.
\end{aligned}$$

Therefore, equation (6.15) implies that

$$0 \le \int_{\mathcal{D}}uv_0\phi(u/v_0)dx \le 0,$$

from which we deduce that $\phi(u/v_0)=0$ a.e. in $\mathcal{D}$ and consequently, $u/v_0\le 1/\varepsilon$ a.e. in $\mathcal{D}$. Hence, $[u/v_0]_\varepsilon=u/v_0$ and we can remove the truncation in system (6.8)–(6.10).

Step 5: proof of $v_0>|\vec{v}|$ in $\mathcal{D}$. More precisely, we show that $(1-\delta)v_0-|\vec{v}|\ge 0$ for

$$0<\delta<\min\left\{1-\sup_{\mathcal{D}}\frac{|\vec{W}^0|}{W_0^0},1-\sup_{\mathcal{D}}\frac{|\vec{v}^D|}{v_0^D},\left(\frac{1}{6}\right)^{7/5}\right\}.$$

Note that such a choice is possible because of our assumptions. To prove the claim, we use $w:=\min\{0,(1-\delta)v_0-|\vec{v}|\}$ and $\vec{w}:=w\vec{v}/|\vec{v}|$ as test functions in the weak formulations of equations (6.9) and (6.10), respectively. Note that, since v_0 is strictly positive, $\vec{w}$ vanishes in a neighborhood of $\vec{v}=0$, so $\vec{w}\in H^1(\mathcal{D})$. By definition of δ, it holds that $w=0$ on $\partial\mathcal{D}$, so w, $\vec{w}\in H_0^1(\mathcal{D})$. We find that

$$\frac{3}{2}\int_{\mathcal{D}}uwdx+h\int_{\mathcal{D}}\nabla v_0\cdot\nabla wdx=\int_{\mathcal{D}}W_0^0wdx,$$

$$\frac{3}{2}\left(1+\frac{h}{\tau_{\rm sf}}\right)\int_{\mathcal{D}}\frac{v_+^{5/7}-v_-^{5/7}}{v_+^{5/7}+v_-^{5/7}}uwdx+h\int_{\mathcal{D}}\nabla\vec{v}\cdot\nabla\vec{w}dx=\int_{\mathcal{D}}\vec{W}^0\cdot\vec{w}dx.$$

We take the difference between the first equation, multiplied by $1-\delta$, and the second equation:

$$\int_{\mathcal{D}}\left((1-\delta)-\frac{3}{2}\left(1+\frac{h}{\tau_{\rm sf}}\right)\frac{v_+^{5/7}-v_-^{5/7}}{v_+^{5/7}+v_-^{5/7}}\right)uwdx+h\int_{\mathcal{D}}\big((1-\delta)\nabla v_0\cdot\nabla w-\nabla\vec{v}\cdot\nabla\vec{w}\big)dx$$
$$=\int_{\mathcal{D}}\left((1-\delta)W_0^0-\frac{\vec{v}}{|\vec{v}|}\cdot\vec{W}^0\right)wdx. \tag{6.16}$$

We deduce from the definition of δ that for any $z\ge 1-\delta$,

$$\frac{(1+z)^{5/7}-\max\{0,1-z\}^{5/7}}{(1+z)^{5/7}+\max\{0,1-z\}^{5/7}}=1-\frac{2\max\{0,1-z\}^{5/7}}{(1+z)^{5/7}+\max\{0,1-z\}^{5/7}}\ge 1-2\delta^{5/7}>\frac{2}{3}.$$

Thus, since $v_\pm=\max\{0,v_0\pm|\vec{v}|\}$ and taking $z=|\vec{v}|/v_0\ge 1-\delta$ on $\{w\le 0\}$, the first integral on the left-hand side of equation (6.16) is estimated as

$$\int_{\mathcal{D}}\left((1-\delta)-\frac{3}{2}\left(1+\frac{h}{\tau_{\rm sf}}\right)\frac{v_+^{5/7}-v_-^{5/7}}{v_+^{5/7}+v_-^{5/7}}\right)uwdx$$
$$\ge\int_{\mathcal{D}}\left(1-\frac{3}{2}\frac{(1+|\vec{v}|/v_0)^{5/7}-\max\{0,1-|\vec{v}|/v_0\}^{5/7}}{(1+|\vec{v}|/v_0)^{5/7}+\max\{0,1-|\vec{v}|/v_0\}^{5/7}}\right)uwdx$$
$$\ge -c_\delta\int_{\mathcal{D}}uwdx=-c_\delta\int_{\mathcal{D}}u\max\{0,(1-\delta)v_0-|\vec{v}|\}dx,$$

where $c_\delta=\frac{3}{2}(1-2\delta^{5/7})-1=\frac{1}{2}-3\delta^{5/7}>0$. The second integral on the left-hand side of equation (6.16) equals

$$\int_{\mathcal{D}}\left((1-\delta)\nabla v_0\cdot w-\nabla\vec{v}\cdot\nabla\left(w\frac{\vec{v}}{|\vec{v}|}\right)\right)dx$$
$$=\int_{\mathcal{D}}\left((1-\delta)\nabla v_0\cdot w-\nabla|\vec{v}|\cdot\nabla w-w\nabla\vec{v}\cdot\nabla\frac{\vec{v}}{|\vec{v}|}\right)dx$$

$$= \int_{\mathcal{D}} \left(|\nabla w|^2 - |\vec{v}| w \left| \nabla \frac{\vec{v}}{|\vec{v}|} \right|^2 \right) dx \geq 0,$$

using the fact that $w \leq 0$. Finally, by the definition of δ, the integral on the right-hand side of equation (6.16) is nonpositive,

$$\int_{\mathcal{D}} \left((1-\delta) W_0^0 - \frac{\vec{v}}{|\vec{v}|} \cdot \vec{W}^0 \right) w dx \leq \int_{\mathcal{D}} \left((1-\delta) W_0^0 - |\vec{W}^0| \right) w dx \leq 0.$$

Summarizing these estimates, equation (6.16) implies that

$$-c_\delta \int_{\mathcal{D}} u \min\{0, (1-\delta) v_0 - |\vec{v}|\} dx = -c_\delta \int_{\mathcal{D}} u w dx \leq 0$$

and hence, $(1-\delta) v_0 - |\vec{v}| \geq 0$ a.e. in $\mathcal{D}$, which proves the claim. ◻

7. Numerical experiments

We perform some numerical simulations using the first model (2.4)–(2.6) with the spin polarization matrix, We consider, as in [18], three- and five-layer structures that consist of alternating nonmagnetic and ferromagnetic layers. Multilayer structures are promising for applications in micro-sensor and high-frequency devices. In this paper, they serve to illustrate the solution behavior rather than to model practical devices.

7.1. Numerical scheme. We solve equations (2.4)–(2.6) on the finite interval $[0,1]$ which is divided in m equal subintervals K of length $\triangle x = 1/m$. The finite-volume method is employed and the generic unknown u_K is an approximation of the integral $\int_K u dx$. The difference quotient $\mathrm{D}u_{K,\sigma}/(\triangle x) := (u_{K,\sigma} - u_K)/(\triangle x)$ approximates the gradient of u in the subinterval K, where $u_{K,\sigma}$ is the value in the neighboring element K' such that $\overline{K} \cap \overline{K'} = \{\sigma\}$. Then the flux $J_u = -(\nabla(uT) + u\nabla V)$ through the point σ can be approximated by

$$J_{u,K,\sigma} = -\frac{1}{\triangle x} \left(\mathrm{D}(uT)_{K,\sigma} + \frac{1}{2}(u_K + u_{K,\sigma}) \mathrm{D}V_{K,\sigma} \right). \tag{7.1}$$

Special care has to be taken for the discretization of the Joule heating term $\mathcal{J}_n \cdot \nabla V$. We suggest to approximate it according to

$$\int_K \mathcal{J}_n \cdot \nabla V dx \approx \frac{1}{2\triangle x} \sum_\sigma \triangle x \mathcal{J}_{n,K,\sigma} \mathrm{D}V_{K,\sigma},$$

where the sum is (here and in the following) over the two end points of the interval K. The values C_K, $\vec{\Omega}_K$, p_K are given by the integrals of $C(x)$, $\vec{\Omega}(x)$, $p(x)$ over K, respectively, and the values $\vec{\Omega}_\sigma$, p_σ are the arithmetic averages of $\vec{\Omega}$, p in the neighboring subintervals of the intersecting point σ, respectively. Finally, we set $\eta_\sigma = \sqrt{1-p_\sigma^2}$.

The stationary solution is computed as the limit $t_k = k\triangle t \to \infty$ from the implicit Euler finite-volume discretization of equations (2.4)–(2.6). We solve first the Poisson equation for the electric potential V^k with the charge density from the previous time step $k-1$, solve then the moment equations for $(n_0^k, W_0^k, \vec{n}^k)$, and update finally the temperature. Given $(n_{0,K}^{k-1}, \vec{n}_K^{k-1}, T_K^{k-1})$ and $W_{0,K}^{k-1} = \frac{3}{2} n_{0,K}^{k-1} T_K^{k-1}$, the numerical scheme reads as

$$-\frac{\lambda_D^2}{\triangle x} \sum_\sigma \mathrm{D}V_{K,\sigma}^k = \triangle x (n_{0,K}^{k-1} - C_K),$$

$$\frac{\triangle x}{\triangle t}(n_{0,K}^k - n_{0,K}^{k-1}) + \sum_\sigma \mathcal{J}_{n,K,\sigma}^k = 0,$$
$$\frac{\triangle x}{\triangle t}(W_{0,K}^k - W_{0,K}^{k-1}) + \sum_\sigma \mathcal{J}_{W,K,\sigma}^k + \frac{1}{2\triangle x}\sum_\sigma \triangle x \mathcal{J}_{n,K,\sigma}^k \mathrm{D}V_{K,\sigma}^k = 0,$$
$$\frac{\triangle x}{\triangle t}(\vec{n}_K^k - \vec{n}_K^{k-1}) + \sum_\sigma \vec{\mathcal{J}}_{K,\sigma}^k + \gamma \triangle x(\vec{\Omega}_K \times \vec{n}_K^k) = -\frac{\triangle x}{\tau_{\mathrm{sf}}}\vec{n}_K^k,$$
$$T_K^k = \frac{2}{3}\frac{W_{0,K}^k}{n_{0,K}^k},$$

and the discrete fluxes are defined by

$$\begin{aligned}
\mathcal{J}_{n,K,\sigma}^k &= -D_0\eta_\sigma^{-2}\big(J_{n,K,\sigma}^k - p_\sigma \vec{\Omega}_\sigma \cdot \vec{J}_{n,K,\sigma}^k\big),\\
\mathcal{J}_{W,K,\sigma}^k &= -\frac{5}{3}D_0\eta_\sigma^{-2}\big(J_{W,K,\sigma}^k - p\vec{\Omega}_\sigma \cdot \vec{J}_{W,K,\sigma}\big),\\
\vec{\mathcal{J}}_{K,\sigma}^k &= -D_0\eta_\sigma^{-2}\big(-p_\sigma\vec{\Omega}_\sigma J_{n,K,\sigma}^k + (1-\eta_\sigma)\vec{\Omega}_\sigma \otimes \vec{\Omega}_\sigma \cdot \vec{J}_{n,K,\sigma}^k + \eta_\sigma \vec{J}_{n,k,\sigma}^k\big),
\end{aligned}$$

and the fluxes $J_{n,K,\sigma}^k$, $\mathcal{J}_{W,K,\sigma}^k$, and $\vec{J}_{K,\sigma}^k$ are discretized according to equation (7.1) with the exception that the temperature and the densities in the drift term are explicit, i.e.

$$J_{u,K,\sigma}^k = -\frac{1}{\triangle x}\left(\mathrm{D}(u^k T^{k-1})_{K,\sigma} + \frac{1}{2}(u_K^{k-1} + u_{K,\sigma}^{k-1})\mathrm{D}V_{K,\sigma}^k\right).$$

Note that we have introduced the scaled diffusion coefficient D_0 and the parameter γ, which come from the scaling of the equations. The values are $D_0 \approx 6.9\cdot 10^{-4}$ and $\gamma = 4$. The scaled Debye length equals $\lambda_D \approx 1.2\cdot 10^{-4}$. We have chosen the (scaled) boundary conditions $n_0 = 1$, $\vec{n} = 0$, and $V = V_D$ at $x = 0,1$ with $V_D(0) = 0$ and $V_D(1) = U/U_T$. Here, $U_T = 0.026\,\mathrm{V}$ is the thermal voltage at room temperature.

The discrete linear system is solved for each time step k until the maximum norm of the difference between two consecutive solutions is smaller than a predefined threshold ($10^{-8}\ldots 10^{-10}$). This solution is considered as a steady state. The numerical parameters are $\triangle x = 0.003$, $\triangle t = 5\cdot 10^{-4}\ldots 10^{-3}$, and the (unscaled) physical parameters are $D = 10^{-3}\,\mathrm{m^2 s^{-1}}$ (diffusion coefficient), $\tau_{\mathrm{sf}} = 10^{-12}\,\mathrm{s}$, and $U = -1\,\mathrm{V}$ (applied bias).

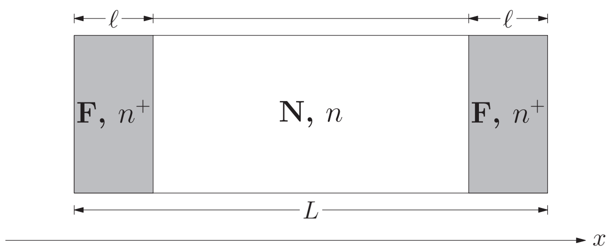

FIG. 7.1. *Geometry of the three-layer structure with ferromagnetic (***F***) highly doped (n^+) source and drain regions and nonmagnetic (***N***) lowly doped (n) channel region.*

7.2. Three-layer structure. As the first numerical experiment, we consider a three-layer structure which consists of a nonmagnetic layer sandwiched between two ferromagnetic layers; see Figure 7.1. This structure may be regarded as a diode with ferromagnetic source and drain regions. The length of the diode is $L = 1.2\,\mu\mathrm{m}$, the

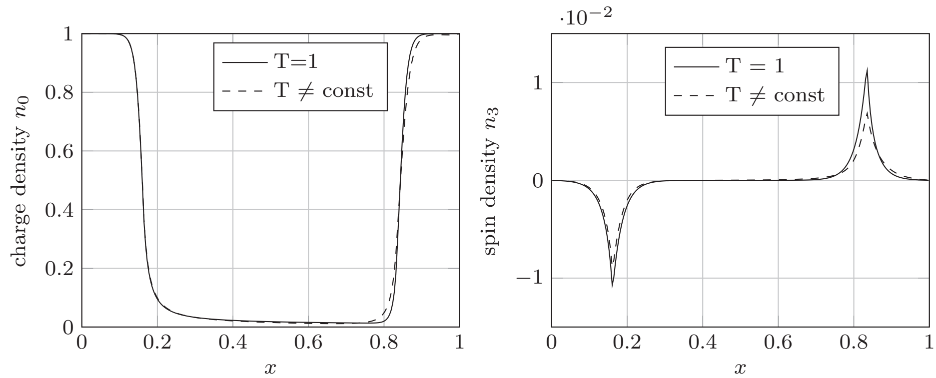

FIG. 7.2. *Charge density n_0 (left) and spin density n_3 (right) in the three-layer structure computed from the spin energy-transport model ($T \neq$ const.) and from the corresponding spin drift-diffusion model ($T=1$).*

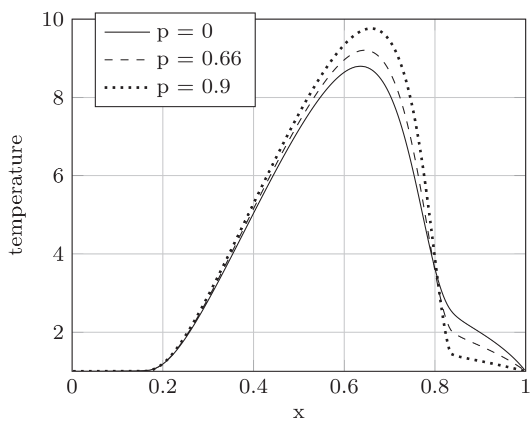

FIG. 7.3. *Temperature in the three-layer structure for various polarizations p.*

ferromagnetic layers have length $\ell = 0.2\,\mu$m, and the doping concentrations are $C = 10^{23}\,\mathrm{m}^{-3}$ in the highly doped regions and $C = 4\cdot 10^{20}\,\mathrm{m}^{-3}$ in the lowly doped region.

The local magnetization in the side regions is aligned with the z-axis (orthogonal to the diode), $\vec{\Omega}(x) = (0,0,1)^\top$ for $x \in [0,\ell] \cup [L-\ell, L]$ and $\vec{\Omega}(x) = 0$ else. The polarization in the ferromagnetic regions equals $p = 0.66$.

Figure 7.2 shows the stationary charge density n_0 (left panel) and the spin density $\vec{n} = (0,0,n_3)$ (right panel), compared with the solution to the corresponding spinorial drift-diffusion model (with constant temperature). As expected, the charge densities are similar with some small differences close to the junction of the drain region. The spin component n_3 exhibits some peaks around the junctions which can be explained by the discontinuity of $p(x)$ (and hence $\eta(x)$) at the junctions [18, Sec. 8.1]. The peaks are smaller in the energy-transport model which may be due to thermal diffusion.

The temperature for different values of the polarization p is illustrated in Figure 7.3. The case $p = 0$ corresponds to a nonmagnetic diode. The temperature maximum increases with p but the temperature decreases with p in the drain region. Possibly, higher values of p lead to stronger heat fluxes increasing the temperature in the channel region, while the highly doped drain region leads to a cooling.

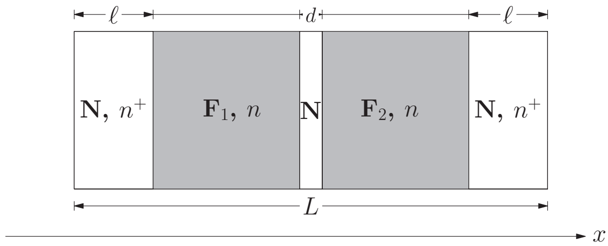

FIG. 7.4. *Geometry of the five-layer structure with ferromagnetic (* $\mathbf{F}_1$, $\mathbf{F}_2$*) lowly doped (n) regions and nonmagnetic (* **N** *) regions. The source and drain regions are highly doped (* n^* *), while the middle region is lowly doped.*

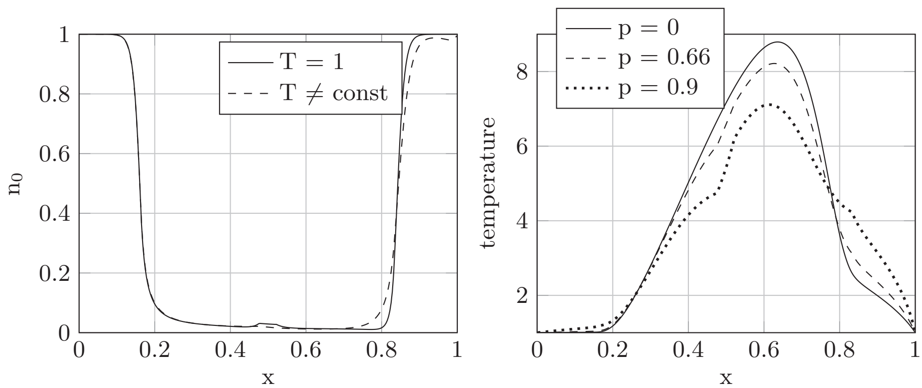

FIG. 7.5. *Charge density* n_0 *(left) and temperature* T *(right) in the five-layer structure.*

7.3. Five-layer structure. The five-layer structure is composed of two ferromagnetic layers sandwiched between two nonmagnetic layers and separated by a thin nonmagnetic layer in the middle of the structure; see Figure 7.4. The choice of the lengths L and ℓ and of the doping concentrations is as in Subsection 7.2. The middle region has the thickness $d = L/21 \approx 60\,\mathrm{nm}$. Again we take $p = 0.66$. The local magnetization is different in the two layers: $\vec{\Omega}(x) = (0,0,1)^\top$ for $x \in [L/6, 10L/21]$, $\vec{\Omega}(x) = (0,1,0)^\top$ for $x \in [11L/21, 5L/6]$, and $\vec{\Omega}(x) = 0$ else.

The effect of the temperature is now stronger than in the three-layer structure. The charge density n_0 and temperature T are presented in Figure 7.5. The interplay of the charge and spin densities in the nonmagnetic middle region causes a small hump in n_0 and a more significant increase before the drain junction, compared to Figure 7.2 (left). The hump is larger when the electric potential is a linear function and the temperature is constant; see Figure 3 in [18]. The temperature maximum decreases with p, opposite to the situation in the three-layer structure. Maybe this observation is related to the coupling mechanism of the $\mathbf{F}_1$ and $\mathbf{F}_2$ multilayers, which depends on the device temperature and may have counterintuitive effects [16]. Another explanation could be that in real devices, the spin-flip scattering should depend on the temperature, and the lack of this dependence in our model may lead to the observed effect. However, note that T is the electron temperature, which is usually only weakly coupled to the device temperature. We observe that the polarization strongly influences the temperature. When $p = 0$, we obtain the same curve as in Figure 7.3 since this describes the same nonmagnetic diode.

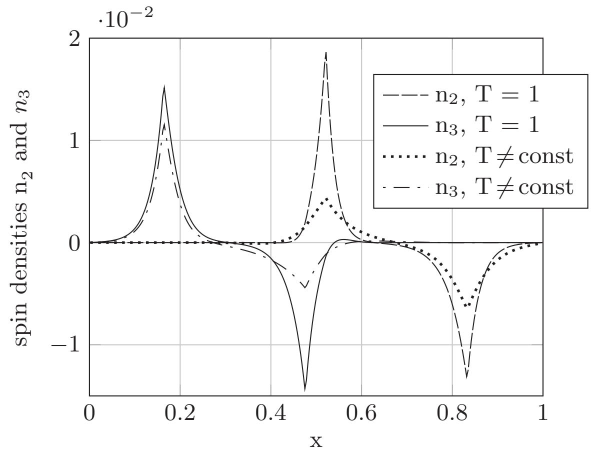

FIG. 7.6. *Spin density components n_2 and n_3 in the five-layer structure computed from the spin energy-transport model ($T \neq$ const.) and from the corresponding spin drift-diffusion model ($T=1$).*

In contrast to the three-layer structure, all components of the spin vector density are nonzero. This comes from the fact that the local magnetization in the $\mathbf{F}_1$-layer leads to a spin polarization in the z-direction, while the $\mathbf{F}_2$-layer causes a spin polarization in the y-direction. Furthermore, the component n_1 of the x-direction is relatively small. We present the components n_2 and n_3 in Figure 7.6. The peaks at the $\mathbf{F}/\mathbf{N}$ interfaces are a result of non-equilibrium spin polarization due to the discontinuity of p; see [18]. The temperature causes a significant smoothing of the peaks between the magnetic/nonmagnetic junctions.

8. Conclusion

We have derived several spin energy-transport models by formulating the general spin energy-transport system of [3] in terms of the Pauli components and applying some simplifying assumptions on the Lagrange multipliers in the Hermitian-valued Maxwellian. It turns out that if one of the spin components of the Lagrange multipliers is set to zero, the resulting spin energy-transport models are only weakly coupled. If both components are aligned, a more interesting model is derived, which contains a Landau–Lifshitz-type equation for the normalized spin vector density. Including a polarization matrix in the definition of the collision operator leads to a stronger mixing of the components.

The entropy (free energy) structure of all the models (without polarization matrix) is analyzed, and for one of the weakly coupled models, we proved the existence of weak solutions for a time-discrete version. Furthermore, we performed numerical simulations for one of these models including the polarization matrix.

The results show that the spin energy-transport models are much more complex than the spin drift-diffusion models, and only partial results on their structure could be achieved so far. Future work may be concerned with the analysis of the models with polarization matrix and the inclusion of temperature-dependent relaxation times as well as a coupling between the electron temperature and device temperature in the numerical simulations.

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