BOUNDED WEAK SOLUTIONS TO A MATRIX DRIFT-DIFFUSION MODEL FOR SPIN-COHERENT ELECTRON TRANSPORT IN SEMICONDUCTORS

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Abstract. The global-in-time existence and uniqueness of bounded weak solutions to a spinorial matrix drift-diffusion model for semiconductors is proved. Developing the electron density matrix in the Pauli basis, the coefficients (charge density and spin-vector density) satisfy a parabolic 4×4 cross-diffusion system. The key idea of the existence proof is to work with different variables: the spin-up and spin-down densities as well as the parallel and perpendicular components of the spin-vector density with respect to the magnetization. In these variables, the diffusion matrix becomes diagonal. The proofs of the L^∞ estimates are based on Stampacchia truncation as well as Moser- and Alikakos-type iteration arguments. The monotonicity of the entropy (or free energy) is also proved. Numerical experiments in one space dimension using a finite-volume discretization indicate that the entropy decays exponentially fast to the equilibrium state.

1. Introduction

The aim of this work is to analyze a spinorial matrix drift-diffusion model. The evolution of the (Hermitian) electron density matrix $N \in \mathbb{C}^{2\times 2}$ and the current density matrix $J \in \mathbb{C}^{2\times 2}$ is governed by the matrix equations

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

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

where $[A,B] = AB - BA$ is the commutator for matrices A and B. The scaled physical parameters are the strength of the pseudo-exchange field $\gamma > 0$, the (normalized) direction of the magnetization $\vec{m} = (m_1, m_2, m_3) \in \mathbb{R}^3$, the spin-flip relaxation time $\tau > 0$, and the space-dependent diffusion coefficient $D = D(x) \in (0,\infty)$. In the analytic part of this paper, we assume that the magnetization vector $\vec{m}$ is constant. Furthermore, $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the triple of the Pauli matrices (see [17, Formula (1)]), σ_0 is the identity matrix in $\mathbb{C}^{2\times 2}$,

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Date: December 7, 2013.

2000 *Mathematics Subject Classification.* 35K51, 82D37.

Key words and phrases. Spinor drift-diffusion equations, semiconductors, bounded weak solutions, Stampacchia truncation, Moser iteration, Alikakos iteration.

The authors acknowledge partial support from the Austrian-French Project Amadée of the Austrian Exchange Service (ÖAD). The first and last authors have been partially supported by the Austrian Science Fund (FWF), grants P20214, P22108, I395, and W1245. The authors thank Stefan Possanner for helpful advices.

$\mathrm{tr}(N)$ denotes the trace of the matrix N, and $P = \sigma_0 + p\vec{m}\cdot\vec{\sigma}$, where $p = p(x) \in [0,1)$ represents the spin polarization of the scattering rates. The product $\vec{m}\cdot\vec{\sigma}$ is defined as the matrix $m_1\sigma_1 + m_2\sigma_2 + m_3\sigma_3$. System (1)-(2) is solved in the bounded cylinder $\Omega \times [0,T) \subset \mathbb{R}^3 \times [0,\infty)$, supplemented with the boundary and initial conditions

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

The electric potential V is given by the Poisson equation

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

where $\lambda_D > 0$ is the scaled Debye length and $C(x)$ the doping profile [13].

Equations (1)-(2) describe the time evolution of the density matrix of the electrons, coupling the charge and spin degrees of freedom. The coupling is linear in the polarization p of the scattering states. The commutator $[N, \vec{m}\cdot\vec{\sigma}]$ in (1) models the precession of the spin polarization on the macroscopic level. Furthermore, the right-hand side in (1) describes the relaxation of the spin density to an equilibrium density due to so-called spin-flip processes.

The above model was derived in [17] from a matrix Boltzmann equation involving the precession of the spin polarization in the diffusion limit. In this derivation, the scattering operator is assumed to consist of a (dominant) symmetric collision operator from the Stone model and a spin-flip operator with the relaxation time $\tau > 0$. Generally, D is a diffusion matrix in $\mathbb{R}^{3\times 3}$. However, under the assumption that the scattering rate in the Stone model is smooth and invariant under isometric transformations, Proposition 1 in [15] shows that D is a multiple of the identity matrix with a positive factor which is identified with the positive number D.

1.1. **State of the art.** In the mathematical literature, various spinorial diffusion models have been investigated. El Hajj [6] derived from a linear spinor Boltzmann equation a two-component drift-diffusion model assuming strong spin-orbit coupling (yielding (9)-(10) below). Two-component models are well known in the physical community [7, Formulas (II.39)-(II.40)]. They are parabolic equations which are only weakly coupled through spin-flip interaction terms. The existence, uniqueness, and boundedness of weak solutions to such models (for spin-polarized electrons and holes) was proved by Glitzky in two space dimensions [11]. In three space dimensions, the well-posedness of the stationary system was shown in [9].

El Hajj derived in [6] also a spin-vector drift-diffusion model assuming that the spin-orbit coupling is moderate compared to the mean free path. Mathematically, the model consists of matrix-valued linear parabolic equations which are strongly coupled. The strong coupling usually makes the analysis very difficult since standard tools like maximum principles and regularity theory generally do not apply. In [6], the scattering rates are supposed to be scalar quantities. Possanner and Negulescu [17] assumed that the scattering rates are positive definite Hermitian matrices, which yields spin-dependent mean free paths and hence more general model equations, which are analyzed in this paper.

Spinorial semiconductor models beyond drift-diffusion have been also investigated. For instance, Ben Abdallah and El Hajj [4] derived spinorial energy-transport and spin-vector drift-diffusion models with Fermi-Dirac statistics. Quantum drift-diffusion equations for a lateral superlattice with Rashba spin-orbit interaction were deduced by Bonilla et al. [3, 5] and numerically solved by Possanner et al. [16].

Because of the strong coupling of the model equations and the quadratic-type nonlinearity of the drift term, there are no analytical results available for spin-vector drift-diffusion systems like (1)-(4), at least up to our knowledge. In this work, we provide for the first time analytical results for the above spin-vector model.

1.2. **Various formulations.** The key idea of the analysis is to work with different variables.

1. Charge and spin-vector densities: It turns out that the analysis of (1)-(2) is easier, when we develop N and J in the Pauli basis $(\sigma_0,\ldots,\sigma_3)$ via $N=\frac{1}{2}n_0\sigma_0+\vec{n}\cdot\vec{\sigma}$ and $J=\frac{1}{2}j_0\sigma_0+\vec{j}\cdot\vec{\sigma}$, where n_0 is the electron charge density and $\vec{n}$ the spin-vector density. These quantities are real since N is Hermitian and positive semi-definite. Setting $\vec{n}=(n_1,n_2,n_3)$ and $\vec{j}=(j_1,j_2,j_3)$, system (1)-(2) can be written equivalently as [17, Remark 1]

$$\partial_t n_0 - \operatorname{div}\left(\frac{D}{\eta^2}(J_0 - 2p\vec{J}\cdot\vec{m})\right) = 0, \tag{5}$$

$$\partial_t n_k - \operatorname{div}\left(\frac{D}{\eta^2}\Big(\eta J_k + (1-\eta)(\vec{J}\cdot\vec{m})m_k - \frac{p}{2}J_0 m_k\Big)\right) - 2\gamma(\vec{n}\times\vec{m})_k = -\frac{n_k}{\tau}, \tag{6}$$

$$J_0 = \nabla n_0 + n_0\nabla V, \quad \vec{J} = (J_1,J_2,J_3) = \nabla\vec{n} + \vec{n}\nabla V, \quad x\in\Omega,\ t>0, \tag{7}$$

where $k=1,2,3$, $\eta=\sqrt{1-p^2}$ (which is generally space dependent), and $(j_0,\vec{j})$ and $(J_0,\vec{J})$ are related by

$$j_0 = -\frac{D}{\eta^2}(J_0 - 2p\vec{J}\cdot\vec{m}), \quad j_k = -\frac{D}{\eta^2}\left(\eta J_k + (1-\eta)(\vec{J}\cdot\vec{m})m_k - \frac{p}{2}J_0 m_k\right).$$

The boundary and initial data is given by

$$n_0 = n_D, \quad \vec{n} = 0 \quad \text{on } \partial\Omega,\ t>0, \quad n_0(0) = n_0^0, \quad \vec{n}(0) = \vec{n}^0 \quad \text{in } \Omega, \tag{8}$$

where $N^0=\frac{1}{2}n_0^0\sigma_0+\vec{n}^0\cdot\vec{\sigma}$. System (4)-(6) is strongly coupled due to the cross-diffusion terms in n_0 and $\vec{n}$ with linear diffusion coefficients. Note that any solution $(n_0,\vec{n})$ to (5)-(8) defines a solution N to (1)-(3).

2. Spin-up and spin-down densities: The coupling becomes weaker by working in the spin-up and spin-down densities $n_\pm=\frac{1}{2}n_0\pm\vec{n}\cdot\vec{m}$. Indeed, multiplying (6) by $\vec{m}$, some terms cancel, and combining the resulting expression with (5), we find that (n_+,n_-) solves

$$\partial_t n_+ - \operatorname{div}\big(D(1+p)(\nabla n_+ + n_+\nabla V)\big) = \frac{1}{2\tau}(n_- - n_+), \tag{9}$$

$$\partial_t n_- - \operatorname{div}\big(D(1-p)(\nabla n_- + n_-\nabla V)\big) = \frac{1}{2\tau}(n_+ - n_-), \quad x\in\Omega,\ t>0, \tag{10}$$

$$n_+ = n_- = \frac{1}{2}n_D \quad \text{on } \partial\Omega,\ t>0, \quad n_\pm(0) = \frac{1}{2}n_0^0 \pm \vec{n}^0\cdot\vec{m} \quad \text{in } \Omega. \tag{11}$$

This formulation is only possible if the magnetization $\vec{m}$ is constant. Its advantage is that the above system is only coupled in the source terms (and through the electric potential) such that we can apply a maximum principle. Note, however, that it is *not* equivalent to (5)-(7) since we are losing the information on the complete spin-vector density $\vec{n}$. Thus, this model contains less information than the full model (5)-(7), but it is easier to analyze mathematically. In fact, drift-diffusion equations similar to (9)-(10) have been thoroughly investigated in, e.g., [10].

3. Parallel and perpendicular densities: For the proof of the boundedness of $\vec{n}$, we employ a third formulation, the decomposition in the parallel and perpendipular components of $\vec{n}$ with respect to $\vec{m}$. For this, let $\vec{n}_\parallel = (\vec{n}\cdot\vec{m})\vec{m}$ and $\vec{n}_\perp = \vec{n} - (\vec{n}\cdot\vec{m})\vec{m}$. Then an elementary computation, using that $\vec{m}$ is constant, shows that $(\vec{n}_\parallel, \vec{n}_\perp)$ solves

$$\partial_t \vec{n}_\parallel - \operatorname{div}\left(\frac{D}{\eta^2}\Big((\vec{J}\cdot\vec{m})\vec{m} - \frac{p}{2}J_0\vec{m}\Big)\right) = -\frac{\vec{n}_\parallel}{\tau}, \tag{12}$$

$$\partial_t \vec{n}_\perp - \operatorname{div}\left(\frac{D}{\eta^2}(\nabla\vec{n}_\perp + \vec{n}_\perp\nabla V)\right) - 2\gamma(\vec{n}_\perp\times\vec{m}) = -\frac{\vec{n}_\perp}{\tau}. \tag{13}$$

The second equation depends on $\vec{n}_\perp$ only, which makes possible the application of a maximum principle.

1.3. **Main results.** Our first result is the global-in-time existence of weak solutions to (1)-(4) (or equivalently, (4)-(8)) under the assumption that the diffusion coefficient D and the spin polarization p are constant. We introduce the space

$$W^{1,2}(0,T;H_0^1,L^2) = H^1(0,T;H^{-1}(\Omega)) \cap L^2(0,T;H_0^1(\Omega)).$$

Recall that $\vec{m}$ is assumed to be a constant vector.

Theorem 1 (Existence of bounded weak solutions I)**.** *Let $T>0$ and let $\Omega\subset\mathbb{R}^3$ be a bounded domain with $\partial\Omega\in C^{1,1}$. Furthermore, let λ_D, γ, $D>0$, $0\le p<1$, and $\vec{m}\in\mathbb{R}^3$ with $|\vec{m}|=1$. The data satisfies $C\in L^\infty(\Omega)$ and*

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

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

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

In particular, n_0 and $\vec{n}\cdot\vec{m}$ are bounded uniformly in $t>0$. If additionally $|\vec{n}^0|\in L^\infty(\Omega)$, then $|\vec{n}|\in L^\infty(0,T;L^\infty(\Omega))$.

For simplicity, the boundary data is assumed to be independent of time. The general situation can also be treated but is more technical; see, e.g., [18]. The proof of the theorem is based on the Leray-Schauder fixed-point theorem. The key idea is to employ the variables

$(n_0, \vec{n}\cdot\vec{m})$ for the ellipticity argument. More precisely, consider the main part of the differential operator in its weak formulation (Equation (5) is divided by four),

$$I = \frac{D}{\eta^2}\int_\Omega \Big(\frac{1}{4}\nabla n_0\cdot\nabla\phi_0 - \frac{p}{2}\nabla(\vec{n}\cdot\vec{m})\cdot\nabla\phi_0 + \eta\nabla\vec{n} : \nabla\vec{\phi} + (1-\eta)\nabla(\vec{n}\cdot\vec{m})\cdot\nabla(\vec{\phi}\cdot\vec{m}) - \frac{p}{2}\nabla n_0\cdot\nabla(\vec{\phi}\cdot\vec{m})\Big)dx,$$

where $(\phi_0, \vec{\phi})$ is some test function. Then, choosing $\phi_0 = n_0$, $\vec{\phi} = \vec{n}$ and using $\eta(1-\eta/2)\|\nabla\vec{n}\|^2 \geq \eta(1-\eta/2)|\nabla\vec{n}\cdot\vec{m}|^2$, the above integral can be estimated by

$$\begin{aligned} I &= \frac{D}{\eta^2}\int_\Omega \Big(\frac{1}{4}|\nabla n_0|^2 - p\nabla(\vec{n}\cdot\vec{m})\cdot\nabla n_0 \\ &\quad + \eta\Big(1-\frac{\eta}{2}\Big)\|\nabla\vec{n}\|^2 + \frac{\eta^2}{2}\|\nabla\vec{n}\|^2 + (1-\eta)|\nabla(\vec{n}\cdot\vec{m})|^2\Big)dx \\ &\geq \frac{D}{\eta^2}\int_\Omega \begin{pmatrix}\nabla n_0 \\ \nabla(\vec{n}\cdot\vec{m})\end{pmatrix}^\top \begin{pmatrix} 1/4 & -p/2 \\ -p/2 & 1-\eta^2/2\end{pmatrix}\begin{pmatrix}\nabla n_0 \\ \nabla(\vec{n}\cdot\vec{m})\end{pmatrix} dx + \frac{D}{2}\int_\Omega \|\nabla\vec{n}\|^2 dx. \end{aligned} \tag{14}$$

The 2×2 matrix on the right-hand side is positive definite (see the discussion after (25)), which allows us to apply the Lax-Milgram lemma. Although the matrix is positive definite in the variables $(n_0, \vec{n}\cdot\vec{m})$ only, we achieve gradient estimates also for $\vec{n}$. This is the key estimate. Note that the assumption that $\vec{m}$ is constant is crucial here.

The positivity and boundedness of n_0 is proved by applying a Stampacchia truncation argument to system (9)-(10) in the variables $n_\pm = \frac{1}{2}n_0 \pm \vec{n}\cdot\vec{m}$. The boundedness of $\vec{n}$ does not follow from this argument. The idea is to prove the boundedness of $\vec{n}_\perp = \vec{n} - (\vec{n}\cdot\vec{m})\vec{m}$, since it satisfies the decoupled drift-diffusion equation (13). Then, because of $\vec{n}\cdot\vec{m}\in L^\infty$, we infer that $|\vec{n}|\in L^\infty$. A standard Stampacchia truncation method cannot be employed here since the term $\vec{n}\times\vec{m}$ mixes the components of $\vec{n}$. Therefore, we use a Moser-type iteration method, i.e., we derive L^q estimates for $\vec{n}_\perp$ uniform in $q<\infty$ and pass to the limit $q\to\infty$.

For nonconstant diffusion coefficients $D(x)$ and spin polarizations $p(x)$, we are able to prove the existence of solutions with given electric potential only. The reason is that our proof is based on a truncation in the Poisson equation (see Section 2) and not in the drift term as was done in, e.g. [10]. This truncation yields $W^{1,\infty}$ regularity for the potential, but we lose the monotonicity of the nonlocal quadratic drift term. We assume that there exists $\delta_0 > 0$ such that

$$D, p\in L^\infty(\Omega), \quad D(x)\geq\delta_0>0,\ 0\leq p(x)\leq 1-\delta_0 \quad \text{for } x\in\Omega. \tag{15}$$

Theorem 2 (Existence of bounded weak solutions II)**.** *Let $|\nabla V|\in L^\infty(0,\infty;L^\infty(\Omega))$ be given and let the assumptions of Theorem 1 on the parameters and data hold with the exception that $D(x)$ and $p(x)$ satisfy (15). Then there exists a unique solution to (1)-(3) such that $N = \frac{1}{2}n_0\sigma_0 + \vec{n}\cdot\vec{\sigma}$ satisfies for any $T>0$, n_0, $n_k\in W^{1,2}(0,T;H_0^1,L^2)$ ($k=1,2,3$). Furthermore,*

$$0\leq \frac{1}{2}n_0 \pm \vec{n}\cdot\vec{m}\in L^\infty(0,\infty;L^\infty(\Omega)).$$

If additionally $|\vec{n}^0| \in L^\infty(\Omega)$*, then* $|\vec{n}| \in L^\infty(0,T;L^\infty(\Omega))$.

The well-posedness follows from an abstract existence result since the system is linear. The difficulty is to show the L^∞ bounds. Here, we employ a variant of Alikakos' iteration technique, modified by Kowalczyk [14] (see Lemma 6 in the appendix).

Our second result is the existence of an entropy (more precisely, free energy) for the spinorial drift-diffusion system. This result holds also for nonconstant diffusion coefficients $D(x)$ and spin polarizations $p(x)$. The entropy is formulated in terms of the solution to (9)-(10):

$$H_0(t) = \int_\Omega \left(h(n_+) + h(n_-) + \frac{\lambda_D^2}{2}|\nabla(V-V_D)|^2 \right) dx, \tag{16}$$
$$h(n_\pm) = \int_{n_D/2}^{n_\pm} (\log s - \log(n_D/2))ds.$$

The first two terms in the definition of $H_0(t)$ describe the internal energy of the two spin components and the last term is the electric energy, relative to the boundary values. From the results on the standard drift-diffusion model (see, e.g., [10]), it is not surprising that the entropy H_0 is nonincreasing in time if the initial data are in thermal equilibrium. We say that $(n_{\rm th}, V_{\rm th})$ is a thermal equilibrium state if $n_{\rm th} = \rho\exp(-V_{\rm th})$ for some constant $\rho > 0$ and $V_{\rm th}$ is the unique solution to

$$-\lambda_D^2\Delta V_{\rm th} = \rho e^{-V_{\rm th}} - C(x) \quad \text{in } \Omega, \quad V_{\rm th} = V_D \quad \text{on } \partial\Omega.$$

For given (n_D, V_D), defined on $\partial\Omega$ and satisfying $\log(n_D/2) + V_D = c \in \mathbb{R}$ on $\partial\Omega$, we extend these functions to Ω by setting $n_D = n_{\rm th}$, $V_D = V_{\rm th}$ and $\rho = 2\exp(c)$. Then $\log(n_D/2) + V_D = c$ in Ω. The following result holds.

Proposition 3 (Monotonicity of H_0)**.** *Let* (15) *hold,* $\log(n_D/2) + V_D = \text{const.}$ *in* Ω*, and* $n_D \in W^{1,\infty}(\Omega)$ *with* $n_D \ge n_* > 0$ *in* Ω*. Let* (n_+, n_-, V) *be a weak solution to* (4), (9)-(11) *in the sense of Theorem 1. Then* $t \mapsto H_0(t)$ *is nonincreasing for* $t > 0$.

Using the techniques of [10], it is possible to infer the exponential decay of $(n_+(t), n_-(t))$ to equilibrium as $t \to \infty$. Since the proof is very similar to that of [10], we omit it. However, we give a numerical example which illustrates the exponential decay.

One may ask if the quantum or von-Neumann entropy (or free energy)

$$H_Q(t) = \int_\Omega \Big({\rm tr}[N(\log N - \log N_D - 1) + N_D] + \frac{\lambda_D^2}{2}|\nabla(V-V_D)|^2 \Big) dx, \tag{17}$$

where $N_D = \frac{1}{2}n_D\sigma_0$ (see (3)), is also nonincreasing in time. Since the eigenvalues of $\log N$ are given by $\frac{1}{2}n_0 \pm |\vec{n}|$, we need to suppose that $\frac{1}{2}n_0 > |\vec{n}|$ to have well-posedness of the expression $\log N$. Because of the drift-diffusion structure of (1) such a functional would be a natural candidate for an entropy. However, we will show that this may be not the case. In fact, a formal computation (detailed in Remark 4) shows that

$$\frac{dH_Q}{dt} = -\int_\Omega Dn_0 \sum_{j=1}^3 {\rm tr}\left[N\big(\partial_j(\log N + V\sigma_0)P^{-1/2}\big)^2 \right] dx - \frac{1}{\tau}\int_\Omega |\vec{n}| \log\frac{\frac{1}{2}n_0 + |\vec{n}|}{\frac{1}{2}n_0 - |\vec{n}|} dx. \tag{18}$$

While the second integral is nonnegative, this may be not true for the first one. We show in Remark 5 that the integrand of the first integral may be negative for certain values of the variables.

In the special case $\vec{m} = (0,0,1)^\top$ and $\vec{n}_0 = (0,0,n_3^0)^\top$, which we assume in our numerical simulations in Section 4, the spin-vector density only depends on the third component, $\vec{n}(t) = (0,0,n_3(t))^\top$ for all $t > 0$. In this situation, H_Q is nonincreasing. This can be seen by writing H_Q equivalently as

$$\begin{aligned} H_Q(t) = \int_\Omega \Big(&(\tfrac{1}{2}n_0 + |\vec{n}|)\big(\log(\tfrac{1}{2}n_0 + |\vec{n}|) - 1\big) + (\tfrac{1}{2}n_0 - |\vec{n}|)\big(\log(\tfrac{1}{2}n_0 - |\vec{n}|) - 1\big) \\ &+ n_D - n_0 \log(\tfrac{1}{2}n_D) + \frac{\lambda_D^2}{2}|\nabla(V - V_D)|^2\Big)dx, \end{aligned}$$

This formulation follows from spectral theory and the fact that the eigenvalues of N are given by $\frac{1}{2}n_0 \pm |\vec{n}|$ [17, Section 2]. We recall that for any continuous function $f : \mathbb{R} \to \mathbb{R}$ and any Hermitian matrix A with (real) eigenvalues λ_j, it holds that $\mathrm{tr}[f(A)] = \sum_j f(\lambda_j)$. Now, $\frac{1}{2}n_0 \pm |\vec{n}| = \frac{1}{2}n_0 \pm n_3 = n_\pm$, and consequently, H_Q coincides with H_0, which is monotone by Proposition 3.

The paper is organized as follows. Theorems 1 and 2 are proved in Section 2. Proposition 3 and formula (18) are shown in Section 3. Some numerical results for a one-dimensional ballistic diode in a multilayer structure using a finite-volume scheme are presented in Section 4. The appendix is concerned with the proof of a general boundedness result needed for the proof of Theorem 2.

2. Existence of solutions

2.1. **Proof of Theorem 1.** The existence proof is based on the Leray-Schauder fixed-point theorem and a truncation argument. It is divided into several steps.

Step 1: Reformulation. We introduce the variable $w_0 = n_0 - n_D(x)$ whose trace vanishes on $\partial\Omega$. Then equations (5)-(7) are equivalent to

$$\frac{1}{4}\partial_t w_0 - \frac{D}{4\eta^2}\mathrm{div}(J_w - 2p\vec{J}\cdot\vec{m}) = \frac{D}{4\eta^2}\mathrm{div}(\nabla n_D + n_D\nabla V), \tag{19}$$

$$\begin{aligned} \partial_t n_k - \frac{D}{\eta^2}\mathrm{div}\Big(\eta J_k + (1-\eta)(\vec{J}\cdot\vec{m})m_k - \frac{p}{2}J_w m_k\Big) - 2\gamma(\vec{n}\times\vec{m})_k \\ = -\frac{n_k}{\tau} - \frac{Dp}{2\eta^2}\mathrm{div}\big((\nabla n_D + n_D\nabla V)m_k\big), \quad k = 1,2,3, \end{aligned} \tag{20}$$

where $J_w = \nabla w_0 + w_0\nabla V$. The boundary and initial conditions are given by

$$w_0 = n_k = 0 \quad \text{on } \partial\Omega,\ k = 1,2,3, \quad w_0(\cdot,0) = n_0^0 - n_D,\ \vec{n}(0) = \vec{n}^0 \quad \text{in } \Omega. \tag{21}$$

Step 2: Definition of the fixed-point operator. The idea is to fix a density $(\rho_0, \vec{\rho})$, to solve the Poisson equation including ρ_0 on its right-hand side, and finally to solve a linearized version of (19)-(20) for the density $(w_0, \vec{w})$, where $\vec{w} = (w_1, w_2, w_3)$. The fixed-point operator is then defined by the mapping $(\rho_0, \vec{\rho}) \mapsto V \mapsto (w_0, \vec{w})$. More precisely, let

$\rho = (\rho_0, \vec{\rho}) \in L^2(0,T;L^2(\Omega))^4$ and $\delta \in [0,1]$ be given and introduce the truncation $[x] = \max\{0, \min\{x, 2M\}\}$ for $x \in \mathbb{R}$, where

$$M = \max\Big\{ \sup_{\partial\Omega} n_D,\ \sup_{\Omega}\Big(\frac{1}{2}n_0^0 + |\vec{n}^0 \cdot \vec{m}|\Big),\ \sup_{\Omega} C\Big\}.$$

Let $V(t) \in H^1(\Omega)$ be the unique solution to

$$-\lambda^2 \Delta V(t) = [\rho_0(t) + n_D] - C(x) \quad \text{in } \Omega, \quad V(t) = V_D \quad \text{on } \partial\Omega. \tag{22}$$

Then $t \mapsto V(t)$ is Bochner measurable and $V \in L^2(0,T;H^1(\Omega))$. In fact, by elliptic regularity and $\partial\Omega \in C^{1,1}$, $V(t) \in W^{2,q_0}(\Omega)$ for $q_0 > 3$. Since the right-hand side of (22) is an element of $L^\infty(0,T;L^\infty(\Omega))$, $V \in L^\infty(0,T;W^{2,q_0}(\Omega))$. This implies, because of the Sobolev embedding $W^{2,q_0}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$ in dimensions $d \le 3$, that $|\nabla V| \in L^\infty(0,T;L^\infty(\Omega))$.

Next, we define the bilinear form $a(\cdot,\cdot;t) : H_0^1(\Omega)^4 \times H_0^1(\Omega)^4 \to \mathbb{R}$ for all $w = (w_0, \vec{w}) = (w_0, w_1, w_2, w_3)$, $\phi = (\phi_0, \vec{\phi}) = (\phi_0, \phi_1, \phi_2, \phi_3) \in H_0^1(\Omega)^4$ by

$$a(w,\phi;t) = a_0(w,\phi) + a_V(w,\phi;t) + a_1(w,\phi) + a_2(w,\phi), \tag{23}$$

where

$$\begin{aligned} a_0(w,\phi) &= \frac{D}{\eta^2}\int_\Omega \Big(\frac{1}{4}\nabla w_0 \cdot \nabla\phi_0 + \eta\nabla\vec{w} : \nabla\vec{\phi} + (1-\eta)\nabla(\vec{w}\cdot\vec{m})\cdot\nabla(\vec{\phi}\cdot\vec{m}) \\ &\quad - \frac{p}{2}\nabla(\vec{w}\cdot\vec{m})\cdot\nabla\phi_0 - \frac{p}{2}\nabla w_0 \cdot \nabla(\vec{\phi}\cdot\vec{m})\Big)dx, \\ a_V(w,\phi;t) &= \frac{D\delta}{\eta^2}\int_\Omega \nabla V(t)\cdot\Big(\frac{1}{4}w_0\nabla\phi_0 + \eta\nabla\vec{\phi}\cdot\vec{w} + (1-\eta)(\vec{w}\cdot\vec{m})\nabla(\vec{\phi}\cdot\vec{m}) \\ &\quad - \frac{p}{2}(\vec{w}\cdot\vec{m})\nabla\phi_0 - \frac{p}{2}w_0\nabla(\vec{\phi}\cdot\vec{m})\Big)dx, \\ a_1(w,\phi) &= -2\gamma\delta\int_\Omega (\vec{w}\times\vec{m})\cdot\vec{\phi}dx, \\ a_2(w,\phi) &= \frac{1}{\tau}\int_\Omega \vec{w}\cdot\vec{\phi}dx, \end{aligned}$$

and $\nabla\vec{w} : \nabla\vec{\phi} = \sum_{k=1}^3 \nabla w_k \cdot \nabla\phi_k$, and the linear mapping $F(\cdot;t) : H_0^1(\Omega)^4 \to \mathbb{R}$ by

$$F(\phi;t) = -\frac{D\delta}{4\eta^2}\int_\Omega (\nabla n_D + n_D\nabla V)\cdot\nabla\phi_0 + \frac{D\delta p}{2\eta^2}\int_\Omega (\nabla n_D + n_D\nabla V)\cdot\nabla(\vec{\phi}\cdot\vec{m})dx.$$

Then the weak formulation of (19)-(21) (for $\delta = 1$) reads as

$$\frac{d}{dt}\int_\Omega w(t)\cdot\phi dx + a(w,\phi;t) = F(\phi;t) \quad \text{for } \phi \in H_0^1(\Omega),\ t > 0. \tag{24}$$

Since $|\nabla V| \in L^\infty(0,T;L^\infty(\Omega))$, an elementary estimation shows that a and F are bounded in the sense

$$a(w,\phi;t) \le K_0\|w\|_{H_0^1(\Omega)}\|\phi\|_{H_0^1(\Omega)}, \quad |F(\phi;t)| \le K_0\|\phi\|_{H_0^1(\Omega)}$$

for all w, $\phi \in H_0^1(\Omega)^4$, where $K_0 > 0$ depends on the $L^\infty(0,T;L^\infty(\Omega))$ norm of ∇V (and hence on M) but is independent of $t > 0$. We claim that a satisfies an abstract Gårding inequality, i.e., there exist K_1, $K_2 > 0$ such that for all $w \in H_0^1(\Omega)^4$,

$$a(w,w) \geq K_1\|w\|^2_{H_0^1(\Omega)} - K_2\|w\|^2_{L^2(\Omega)}.$$

To this end, we estimate the forms a_0, a_V, a_1, and a_2. The first form equals

$$\begin{aligned} a_0(w,w) = \frac{D}{\eta^2}\int_\Omega \Big(\frac{1}{4}|\nabla w_0|^2 + \frac{\eta^2}{2}\|\nabla\vec{w}\|^2 + \eta\Big(1-\frac{\eta}{2}\Big)\|\nabla\vec{w}\|^2 \\ + (1-\eta)|\nabla(\vec{w}\cdot\vec{m})|^2 - p\nabla w_0\cdot\nabla(\vec{w}\cdot\vec{m})\Big)dx. \end{aligned}$$

Estimate (14) in the introduction shows that

$$a_0(w,w) \geq \frac{D}{\eta^2}\int_\Omega \begin{pmatrix}\nabla w_0 \\ \nabla\vec{w}\cdot\vec{m}\end{pmatrix}^\top \begin{pmatrix} 1/4 & -p/2 \\ -p/2 & 1-\eta^2/2\end{pmatrix}\begin{pmatrix}\nabla w_0 \\ \nabla\vec{w}\cdot\vec{m}\end{pmatrix} dx + \frac{D}{2}\int_\Omega \|\nabla\vec{w}\|^2 dx. \tag{25}$$

The above symmetric matrix is positive definite because its eigenvalues

$$\lambda_\pm = \frac{1}{8}(5-2\eta^2) \pm \frac{1}{8}\sqrt{(5-2\eta^2)^2 - 8\eta^2}$$

are real (since $\eta \leq 1$) and positive (since $\eta > 0$). This leads to

$$a_0(w,w;t) \geq \frac{D}{\eta^2}\int_\Omega \Big(\lambda_-|\nabla w_0|^2 + \lambda_-|\nabla(\vec{w}\cdot\vec{m})|^2 + \frac{\eta^2}{2}\|\nabla\vec{w}\|^2\Big)dx \geq K_1\|w\|^2_{H_0^1(\Omega)},$$

where $K_1 = \min\{\lambda_-, \eta^2/2\}$.

In order to estimate the second form $a_V(w,w)$, we employ the Poisson equation:

$$\begin{aligned} a_V(w,w) &= \frac{D\delta}{2\eta^2}\int_\Omega \nabla V\cdot\nabla\Big(\frac{1}{4}w_0^2 + \eta|\vec{w}|^2 + (1-\eta)(\vec{w}\cdot\vec{m})^2 - pw_0(\vec{w}\cdot\vec{m})\Big)dx \\ &= \frac{D\delta}{2\eta^2\lambda_D^2}\int_\Omega ([\rho_0 + n_D] - C(x))\Big(\frac{1}{4}w_0^2 + \eta|\vec{w}|^2 + (1-\eta)(\vec{w}\cdot\vec{m})^2 - pw_0(\vec{w}\cdot\vec{m})\Big)dx. \end{aligned}$$

Observing that

$$\begin{aligned} &\frac{1}{4}w_0^2 + \eta|\vec{w}|^2 + (1-\eta)(\vec{w}\cdot\vec{m})^2 - pw_0(\vec{w}\cdot\vec{m}) \\ &\qquad = \Big(\frac{1}{2}w_0 - p\vec{w}\cdot\vec{m}\Big)^2 + \eta\big(|\vec{w}|^2 - (\vec{w}\cdot\vec{m})^2\big) + \eta^2(\vec{w}\cdot\vec{m})^2 \geq 0 \end{aligned}$$

and employing the Cauchy-Schwarz inequality, it follows that

$$\begin{aligned} a_V(w,w) &\geq -\frac{D}{2\eta^2\lambda_D^2}\int_\Omega |C(x)|\Big(\frac{1}{4}w_0^2 + \eta|\vec{w}|^2 + (1-\eta)(\vec{w}\cdot\vec{m})^2 - pw_0(\vec{w}\cdot\vec{m})\Big)dx \\ &\geq -K_2\|w\|^2_{L^2(\Omega)}, \end{aligned}$$

where K_2 depends on $\|C\|_{L^\infty(\Omega)}$ and the parameters D, p, and λ_D but not on M or ρ. Finally, the third form vanishes, $a_1(w,w) = 0$, and the fourth form is nonnegative, $a_2(w,w) \geq 0$. This shows the claim.

By Corollary 23.26 in [19], there exists a unique solution $w \in W^{1,2}(0,T;H_0^1,L^2)^4$ to (24) satisfying $w(0) = (n_0^0 - n_D, \vec{n}^0)$. This defines the fixed-point operator $S : L^2(0,T;L^2(\Omega))^4 \times [0,1] \to L^2(0,T;L^2(\Omega))^4$, $S(\rho,\delta) = w$. By construction, $S(\rho,0) = 0$. Furthermore, standard arguments show that S is continuous. By the Aubin lemma, the space $W^{1,2}(0,T;H_0^1, L^2)^4$ embeddes compactly into $L^2(0,T;L^2(\Omega))^4$. Consequently, S is compact. It remains to prove some uniform estimates for all fixed points of $S(\cdot,\delta)$ in $L^2(0,T;L^2(\Omega))^4$. Let $w \in W^{1,2}(0,T;H_0^1,L^2)^4$ be such a fixed point. Employing $w = (w_0,\vec{w})$ as a test function in (24), the above estimates show that

$$\begin{aligned}\frac{1}{2}\|w(\cdot,T)\|_{L^2(\Omega)}^2 + K_1\|w\|_{L^2(0,T;H_0^1(\Omega))}^2 &\le K_2\|w\|_{L^2(0,T;L^2(\Omega))}^2 + K_0\|w\|_{L^2(0,T;H_0^1(\Omega))} \\ &\le K_2\|w\|_{L^2(0,T;L^2(\Omega))}^2 + \frac{K_1}{2}\|w\|_{L^2(0,T;H_0^1(\Omega))}^2 + \frac{K_0^2}{2K_1}.\end{aligned}$$

Absorbing the second summand on the right-hand side by the corresponding term on the left-hand side and applying Gronwall's lemma, we achieve the bound $\|w\|_{L^2(0,T;L^2(\Omega))} \le K$ for some $K > 0$ uniform in ρ and δ. By the Leray-Schauder fixed-point theorem, there exists a fixed point of $S(\cdot,1)$, i.e. a solution to (19)-(22) with $[\rho(t) + n_D]$ replaced by $[w(t) + n_D]$.

Step 3: Lower and upper bounds. We show that $0 \le n_0 := w + n_D \le 2M$ in $\Omega \times (0,T)$ which allows us to remove the truncation in the Poisson equation. For this, we consider the variables $n_\pm = \frac{1}{2}n_0 \pm \vec{n}\cdot\vec{m}$. We claim that $n_\pm \ge 0$. Indeed, with the test functions $[n_\pm]^- = \min\{0,n_\pm\}$, which satisfy $[n_\pm]^- = 0$ on $\partial\Omega$ and $[n_\pm(0)]^- = 0$, in the weak formulation of (9) and (10), respectively, it follows from $n_\pm\nabla V\cdot\nabla[n_\pm]^- = [n_\pm]^-\nabla V\cdot\nabla[n_\pm]^- = \frac{1}{2}\nabla V\cdot\nabla([n_\pm]^-)^2$ that

$$\begin{aligned}&\frac{1}{2}\int_\Omega([n_\pm(t)]^-)^2dx + D(1\pm p)\int_0^t\int_\Omega|\nabla[n_\pm]^-|^2dx\,ds \\ &\quad= -D(1\pm p)\int_0^t\int_\Omega[n_\pm]^-\nabla V\cdot\nabla[n_\pm]^-dx\,ds \mp \frac{1}{2\tau}\int_0^t\int_\Omega(n_+-n_-)[n_\pm]^-dx\,ds \\ &\quad= -\frac{D(1\pm p)}{2\lambda_D^2}\int_0^t\int_\Omega([n_0]-C(x))([n_\pm]^-)^2dx\,ds \mp \frac{1}{2\tau}\int_0^t\int_\Omega(n_+-n_-)[n_\pm]^-dx\,ds.\end{aligned}$$

In the last step we have integrated by parts and employed the Poisson equation. We add both equations and neglect the integrals involving $|\nabla[n_\pm]^-|^2$ to obtain

$$\begin{aligned}&\frac{1}{2}\int_\Omega\big(([n_+(t)]^-)^2 + ([n_-(t)]^-)^2\big)dx \\ &\quad\le -\frac{D}{2\lambda_D^2}\int_0^t\int_\Omega([n_0]-C(x))\big((1+p)([n_+]^-)^2 + (1-p)([n_-]^-)^2\big)dx\,ds \\ &\qquad - \frac{1}{2\tau}\int_0^t\int_\Omega(n_+-n_-)([n_+]^- - [n_-]^-)dx\,ds \\ &\quad\le \frac{D}{2\lambda_D^2}\|C\|_{L^\infty(\Omega)}\int_0^t\int_\Omega\big(([n_+]^-)^2 + ([n_+]^-)^2\big)dx\,ds,\end{aligned}$$

using the fact that $x \mapsto [x]^-$ is nondecreasing. Gronwall's lemma shows that $[n_\pm(t)]^- = 0$ in Ω for any $t > 0$ and hence, $n_\pm \geq 0$ in $\Omega \times (0,T)$.

For the proof of the upper bound, we employ the test function $[n_\pm - M]^+ = \max\{0, n_\pm - M\}$, which is admissible since $M \geq \frac{1}{2}\sup_{\Omega\times(0,T)} n_D$, and which satisfies $[n_\pm(0) - M]^- = 0$, in (9) and (10), respectively, and add both equations:

$$
\begin{aligned}
&\frac{1}{2}\int_\Omega \big([n_+(t) - M]^{+2} + [n_-(t) - M]^{+2}\big)dx \\
&\qquad + D\int_0^t\int_\Omega \big((1+p)|\nabla[n_+ - M]^+|^2 + (1-p)|\nabla[n_- - M]^+|^2\big)dx\,ds \\
&\quad = -D\int_0^t\int_\Omega \big((1+p)(n_+ - M)\nabla V\cdot\nabla[n_+ - M]^+ \\
&\qquad + (1-p)(n_- - M)\nabla V\cdot\nabla[n_- - M]^+\big)dx\,ds \\
&\qquad - DM\int_0^t\int_\Omega \nabla V\cdot\big((1+p)\nabla[n_+ - M]^+ + (1-p)\nabla[n_- - M]^+\big)dx\,ds \\
&\qquad - \frac{1}{2\tau}\int_0^t\int_\Omega (n_+ - n_-)\big([n_+ - M]^+ - [n_- - M]^+\big)dx\,ds.
\end{aligned}
$$

Observing that $(n_\pm - M)\nabla V\cdot\nabla[n_\pm - M]^+ = \frac{1}{2}\nabla V\cdot\nabla([n_\pm - M]^+)^2$, integrating by parts, and employing the Poisson equation, we find that

$$
\begin{aligned}
&\frac{1}{2}\int_\Omega \big(([n_+(t) - M]^+)^2 + ([n_-(t) - M]^+)^2\big)dx \\
&\quad \leq -\frac{D}{2\lambda_D^2}\int_0^t\int_\Omega ([n_0] - C(x))\big((1+p)([n_+ - M]^+)^2 + (1-p)([n_- - M]^+)^2\big)dx\,ds \\
&\qquad - \frac{DM}{\lambda_D^2}\int_0^t\int_\Omega ([n_0] - C(x))\big((1+p)[n_+ - M]^+ + (1-p)[n_- - M]^+\big)dx\,ds.
\end{aligned}
$$

The last integral is nonnegative since $[n_0] - C(x) = [n_+ + n_-] - C(x) \geq 0$ on $\{n_\pm \geq M\}$ by definition of M. Then Gronwall's lemma gives $[n_\pm - M]^+ = 0$ and $n_\pm \leq M$ in $\Omega\times(0,T)$. We have shown that $n_0 = n_+ + n_- \leq 2M$, $\vec{n}\cdot\vec{m} = \frac{1}{2}(n_+ - n_-) \leq \frac{1}{2}n_+ \leq \frac{1}{2}M$, and $\vec{n}\cdot\vec{m} \geq -\frac{1}{2}n_- \geq -\frac{1}{2}M$. Thus, we can remove the truncation in the Poisson equation, since $[n_0] = n_0$.

Step 4: Uniqueness of solutions. Let (w, V) and (w^*, V^*) with $w = (w_0, \vec{w})$ and $w^* = (w_0^*, \vec{w}^*)$ be two weak solutions to (22) and (24). Taking the difference of the equations (24) for w and w^*, respectively, and employing the admissible test function $w - w^*$, we obtain

$$
\begin{aligned}
&\frac{1}{2}\|(w - w^*)(T)\|_{L^2(\Omega)}^2 + \int_0^T \big(a(w, w - w^*; t) - a^*(w^*, w - w^*; t)\big)dt \\
&\quad = \int_0^T (F(w - w^*; t) - F^*(w - w^*; t))dt,
\end{aligned}
$$

where a^* and F^* denote the forms with V replaced by V^*. The Cauchy-Schwarz and Young inequalities and the elliptic estimate $\|\nabla(V-V^*)\|_{L^2(\Omega)} \le K\|w_0-w_0^*\|_{L^2(\Omega)}$ yield

$$\begin{aligned}\int_0^T (F(w-w^*;t) - F^*(w-w^*;t))dt &= -\frac{D}{4\eta^2}\int_0^T\int_\Omega n_D\nabla(V-V^*)\cdot\nabla(w_0-w_0^*)dx\,dt \\ &\quad + \frac{Dp}{2\eta^2}\int_0^T\int_\Omega n_D\nabla(V-V^*)\cdot\nabla((\vec{w}-\vec{w}^*)\cdot\vec{m})dx\,dt \\ &\le \varepsilon\|\nabla(w-w^*)\|^2_{L^2(0,T;L^2(\Omega))} + K(\varepsilon)\|w_0-w_0^*\|^2_{L^2(0,T;L^2(\Omega))},\end{aligned}$$

where here and in the following, $K>0$ denotes a generic constant and $\varepsilon>0$.

Next, we consider the difference $a(w,w-w^*;t) - a^*(w^*,w-w^*;t)$. As in Step 2, we find that

$$\begin{aligned}&\int_0^T a_0(w-w^*,w-w^*)dt \ge K\int_0^T\int_\Omega\big(|\nabla(w_0-w_0^*)|^2 + \|\nabla(\vec{w}-\vec{w}^*)\|^2\big)dx\,dt, \\ &\int_0^T a_1(w-w^*,w-w^*)dt = 0, \\ &\int_0^T a_2(w-w^*,w-w^*)dt = \frac{1}{\tau}\int_0^T\int_\Omega|\vec{w}-\vec{w}^*|^2dx\,dt \ge 0.\end{aligned}$$

The remaining difference involving the electric potentials becomes

$$\begin{aligned}&\int_0^T\big(a_V(w,w-w^*;t) - a_{V^*}(w^*,w-w^*;t)\big)dt \\ &\quad= \frac{D}{2\eta^2}\int_0^T\int_\Omega\nabla V\cdot\nabla\Big(\frac14(w_0-w_0^*)^2 + \eta|\vec{w}-\vec{w}^*|^2 + (1-\eta)((\vec{w}-\vec{w}^*)\cdot\vec{m})^2 \\ &\quad\quad - \frac{p}{2}(w_0-w_0^*)(\vec{w}-\vec{w}^*)\cdot\vec{m}\Big)dx\,dt \\ &\quad\quad + \frac{D}{\eta^2}\int_0^T\int_\Omega\nabla(V-V^*)\cdot\Big(\frac14 w_0^*\nabla(w_0-w_0^*) + \eta\vec{w}^*\nabla(\vec{w}-\vec{w}^*) \\ &\quad\quad + (1-\eta)(\vec{w}^*\cdot\vec{m})\nabla((\vec{w}-\vec{w}^*)\cdot\vec{m}) \\ &\quad\quad - \frac{p}{2}(\vec{w}^*\cdot\vec{m})\nabla(w_0-w_0^*) - \frac{p}{2}w_0^*\nabla((\vec{w}-\vec{w}^*)\cdot\vec{m})\Big)dx\,dt.\end{aligned}$$

Integrating by parts in the first integral on the right-hand side and employing the Poisson equation shows that the first integral can be estimated from above by

$$K\big(\|w_0-w_0^*\|^2_{L^2(0,T;L^2(\Omega))} + \|\vec{w}-\vec{w}^*\|^2_{L^2(0,T;L^2(\Omega))} + \|(\vec{w}-\vec{w}^*)\cdot\vec{m}\|^2_{L^2(0,T;L^2(\Omega))}\big),$$

where $K>0$ depends on the $L^\infty(0,T;L^\infty(\Omega))$ norm of w_0. We take into account the L^∞ norms of w_0^* and $\vec{w}^*\cdot\vec{m}$ to estimate the second integral from above by

$$\begin{aligned}&K\|\nabla(V-V^*)\|_{L^2(0,T;L^2(\Omega))}\big(\|\nabla(w_0-w_0^*)\|_{L^2(0,T;L^2(\Omega))} + \|(\vec{w}-\vec{w}^*)\cdot\vec{m}\|_{L^2(0,T;L^2(\Omega))}\big) \\ &\quad + \|\nabla(V-V^*)\|_{L^2(0,T;L^6(\Omega))}\|\vec{w}\|_{L^\infty(0,T;L^2(\Omega))}\|\vec{w}-\vec{w}^*\|_{L^2(0,T;L^3(\Omega))}.\end{aligned} \tag{26}$$

By elliptic regularity and Sobolev embedding, it follows that

$$\|\nabla(V-V^*)\|_{L^6(\Omega)} \le K\|V-V^*\|_{H^2(\Omega)} \le K\|w_0-w_0^*\|_{L^2(\Omega)}.$$

Furthermore, by the Gagliardo-Nirenberg inequality,

$$\|\vec{w}-\vec{w}^*\|_{L^2(0,T;L^3(\Omega))} \le K\|\vec{w}-\vec{w}^*\|^{1/2}_{L^2(0,T;L^2(\Omega))}\|\nabla(\vec{w}-\vec{w}^*)\|^{1/2}_{L^2(0,T;L^2(\Omega))}.$$

Putting together these estimates and using Young's inequality as well as the embedding $W^{1,2}(0,T;H_0^1,L^2) \hookrightarrow L^\infty(0,T;L^2(\Omega))$, we obtain for any $\varepsilon>0$,

$$\begin{aligned}
&\|\nabla(V-V^*)\|_{L^2(0,T;L^6(\Omega))}\|\vec{w}\|_{L^\infty(0,T;L^2(\Omega))}\|\vec{w}-\vec{w}^*\|_{L^2(0,T;L^3(\Omega))} \\
&\quad\le K\|w_0-w_0^*\|_{L^2(0,T;L^2(\Omega))}\|\vec{w}-\vec{w}^*\|^{1/2}_{L^2(0,T;L^2(\Omega))}\|\nabla(\vec{w}-\vec{w}^*)\|^{1/2}_{L^2(0,T;L^2(\Omega))} \\
&\quad\le \varepsilon\|\nabla(\vec{w}-\vec{w}^*)\|^2_{L^2(0,T;L^2(\Omega))} + K(\varepsilon)\|w_0-w_0^*\|^2_{L^2(\Omega)} + K(\varepsilon)\|\vec{w}-\vec{w}^*\|^2_{L^2(0,T;L^2(\Omega))}.
\end{aligned}$$

Hence, (26) can be estimated from above by

$$\varepsilon\|\nabla(\vec{w}-\vec{w}^*)\|^2_{L^2(0,T;L^2(\Omega))} + K(\varepsilon)\|w_0-w_0^*\|^2_{L^2(\Omega)} + K(\varepsilon)\|\vec{w}-\vec{w}^*\|^2_{L^2(0,T;L^2(\Omega))}.$$

Summarizing the above estimates, we infer that

$$\begin{aligned}
&\|(w-w^*)(T)\|^2_{L^2(\Omega)} + K\int_0^T \big(\|\nabla(w_0-w_0^*)\|^2_{L^2(\Omega)} + \|\nabla(\vec{w}-\vec{w}^*)\|^2_{L^2(\Omega)}\big)dt \\
&\quad\le \varepsilon\int_0^T \|\nabla(\vec{w}-\vec{w}^*)\|^2_{L^2(\Omega)}dt + K(\varepsilon)\int_0^T \big(\|w_0-w_0^*\|^2_{L^2(\Omega)} + \|\vec{w}-\vec{w}^*\|^2_{L^2(\Omega)}\big)dt.
\end{aligned}$$

Thus, choosing $\varepsilon>0$ sufficiently small and employing Gronwall's lemma, we infer that $w=w^*$ in Ω, $t>0$.

Step 5: L^∞ bound for $\vec{n}$. Let $q\ge 1$. Since $|\vec{n}_\perp|^q\vec{n}_\perp$ is not an admissible test function, we need to regularize. For this, set $g_\varepsilon(y)=y^q/(1+\varepsilon y^q)$ and $G_\varepsilon(y)=\int_0^y g_\varepsilon(z)dz$ for $y\ge 0$ and $\varepsilon>0$. Then $g_\varepsilon(|\vec{n}_\perp|^2)\vec{n}_\perp$ is an admissible test function in the weak formulation of (13) (since $\vec{n}=0$ on $\partial\Omega$):

$$\begin{aligned}
&\int_0^t \langle\partial_t\vec{n}_\perp, g_\varepsilon(|\vec{n}_\perp|^2)\vec{n}_\perp\rangle ds + \frac{D}{\eta}\int_0^t\int_\Omega(\nabla\vec{n}_\perp+\nabla V\vec{n}_\perp):\nabla(g_\varepsilon(|\vec{n}_\perp|^2)\vec{n}_\perp)dx\,ds \\
&\quad= 2\gamma\int_0^t\int_\Omega g_\varepsilon(|\vec{n}_\perp|^2)(\vec{n}_\perp\times\vec{m})\cdot\vec{n}_\perp dx\,ds - \frac{1}{\tau}\int_0^t\int_\Omega g_\varepsilon(|\vec{n}_\perp|^2)|\vec{n}_\perp|^2dx\,ds \le 0, \qquad (27)
\end{aligned}$$

since the first integral on the right-hand side vanishes and the second one is nonnegative. Here, $\langle\cdot,\cdot\rangle$ denotes the dual product between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. Taking into account a variant of Prop. 23.20 in [19], the first integral on the left-hand side of (27) equals

$$\langle\partial_t\vec{n}_\perp, g_\varepsilon(|\vec{n}_\perp|^2)\vec{n}_\perp\rangle = \frac{1}{2}\frac{d}{dt}\int_\Omega G_\varepsilon(|\vec{n}_\perp|^2)dx.$$

Setting $F_\varepsilon(y)=\int_0^y g_\varepsilon'(z)zdz$ and employing the Poisson equation (4), the second integral in (27) can be estimated as

$$\frac{D}{\eta}\int_0^t\int_\Omega\Big(\frac{1}{4}g_\varepsilon'(|\vec{n}_\perp|^2)\big|\nabla(|\vec{n}_\perp|^2)\big|^2 + g_\varepsilon(|\vec{n}_\perp|^2)\|\nabla\vec{n}_\perp\|^2$$

$$
\begin{aligned}
&\quad + g_\varepsilon'(|\vec{n}_\perp|^2)|\vec{n}_\perp|^2\nabla(|\vec{n}_\perp|^2)\cdot\nabla V + \frac{1}{2}g_\varepsilon(|\vec{n}_\perp|^2)\nabla(|\vec{n}_\perp|^2)\cdot\nabla V\Big)dx\,ds \\
&\ge \frac{D}{2\eta}\int_0^t\int_\Omega \nabla\big(2F_\varepsilon(|\vec{n}_\perp|^2) + G_\varepsilon(|\vec{n}_\perp|^2)\big)\cdot\nabla V dx\,ds \\
&= \frac{D}{2\eta\lambda_D^2}\int_0^t\int_\Omega \big(2F_\varepsilon(|\vec{n}_\perp|^2) + G_\varepsilon(|\vec{n}_\perp|^2)\big)(n_0 - C(x))dx\,ds \\
&\ge -\frac{D}{2\eta\lambda_D^2}\|C\|_{L^\infty(\Omega)}\int_0^t\int_\Omega \big(2F_\varepsilon(|\vec{n}_\perp|^2) + G_\varepsilon(|\vec{n}_\perp|^2)\big)dx\,ds.
\end{aligned}
$$

We have proved that

$$
\frac{d}{dt}\int_\Omega G_\varepsilon(|\vec{n}_\perp|^2)dx \le \frac{D}{\eta\lambda_D^2}\|C\|_{L^\infty(\Omega)}\int_0^t\int_\Omega \big(2F_\varepsilon(|\vec{n}_\perp|^2) + G_\varepsilon(|\vec{n}_\perp|^2)\big)dx\,ds.
$$

Elementary estimations show that $F_\varepsilon(y) \le qG_\varepsilon(y)$ for all $y \ge 0$, yielding

$$
\frac{d}{dt}\int_\Omega G_\varepsilon(|\vec{n}_\perp|^2)dx \le K(2q+1)\int_\Omega G_\varepsilon(|\vec{n}_\perp|^2)dx, \quad K = \frac{D}{\eta\lambda_D^2}\|C\|_{L^\infty(\Omega)}.
$$

Then Gronwall's lemma and the assumption $|\vec{n}_\perp(0)| \in L^\infty(\Omega)$ give for all $t > 0$,

$$
\int_\Omega G_\varepsilon(|\vec{n}_\perp(t)|^2)dx \le e^{K(2q+1)t}\int_\Omega G_\varepsilon(|\vec{n}_\perp(0)|^2)dx \le e^{K(2q+1)t}\int_\Omega |\vec{n}_\perp(0)|^{2q}dx.
$$

By dominated convergence, we can pass to the limit $\varepsilon \to 0$. Then, taking the $2q$-th root,

$$
\|\vec{n}_\perp(t)\|_{L^{2q}(\Omega)} \le e^{2Kt}\|\vec{n}_\perp(0)\|_{L^{2q}(\Omega)}, \quad t > 0.
$$

The right-hand side is bounded uniformly in $q < \infty$. Therefore, the limit $q \to \infty$ leads to

$$
\|\vec{n}_\perp(t)\|_{L^\infty(\Omega)} \le e^{2Kt}\|\vec{n}_\perp(0)\|_{L^\infty(\Omega)}, \quad t > 0,
$$

which ends the proof.

2.2. **Proof of Theorem 2.** Since for given V, system (5)-(7) is linear, we only need to prove the coercivity of the bilinear form (23) in order to prove the existence of a weak solution to (24). Compared to the proof of Theorem 1, the quotient D/η^2 depends on the spatial variables and we cannot employ the Poisson equation to estimate the form $a_V(w,w;t)$. Instead, we use the Cauchy-Schwarz inequality to obtain for all $\varepsilon > 0$,

$$
a_V(w,w;t) \ge \varepsilon\|w\|_{H_0^1(\Omega)}^2 - K(\varepsilon)\|w\|_{L^2(\Omega)}^2.
$$

The constant $K(\varepsilon) > 0$ depends on the L^∞ norm of ∇V. Thus, the existence and uniqueness of a weak solution follows from Corollary 23.26 in [19]. The nonnegativity of $n_\pm$ and hence of n_0 is shown as in the proof of Theorem 1.

The main difficulty of the proof of Theorem 2 is to derive the L^∞ bounds. To this end, we employ Lemma 6 in the appendix, which is based on the iterative technique of Alikakos [1], modified by Kowalczyk [14]. First, we note that the entropy estimate from Proposition 3 implies that $n_\pm \in L^\infty(0,T;L^1(\Omega))$. The proposition is proved for special boundary data.

However, the proof also shows that for general boundary data, the entropy is bounded on each interval $(0,T)$.

Next, let $k = \|n_+(0)\|_{L^\infty(\Omega)} + \|n_-(0)\|_{L^\infty(\Omega)}$. $0 < k < L$, $q \geq 1$, and set $[n_+]_L = \min\{n_+, L\}$. Then $\phi(n_+) = (([n_+]_L - k)^+)^q$ is an admissibible test function in the weak formulation of (9). Since $\phi(n_+(0)) = 0$ by construction and

$$\Phi(n_+) = \int_0^{n_+} \phi(y)dy \geq \frac{1}{q+1}(([n_+]_L - k)^+)^{q+1},$$

it follows that

$$\int_0^t \langle \partial_t n_+, \phi(n_+)\rangle ds = \int_\Omega \big(\Phi(n_+(t)) - \Phi(n_+(0))\big)dx \geq \frac{1}{q+1}\int_\Omega (([n_+(t)]_L - k)^+)^{q+1}dx.$$

Therefore, setting $D_0(x) = D(x)(1+p(x))$, we infer from (9) that

$$\begin{aligned}\frac{1}{q+1}&\int_\Omega (([n_+(t)]_L - k)^+)^{q+1}dx + q\int_0^t\int_\Omega (([n_+]_L - k)^+)^{q-1}|\nabla n_+|^2 dx\,ds \\ &= -q\int_0^t\int_\Omega D_0(x)(n_+ - k)(([n_+]_L - k)^+)^{q-1}\nabla V\cdot\nabla([n_+(t)]_L - k)^+ dx\,ds \\ &\quad - kq\int_0^t\int_\Omega D_0(x)(([n_+]_L - k)^+)^{q-1}\nabla V\cdot\nabla([n_+]_L - k)^+ dx\,ds \\ &\quad - \frac{1}{\tau}\int_0^t\int_\Omega (n_+ - n_-)(([n_+]_L - k)^+)^q dx\,ds.\end{aligned}$$

Since $n_+ - k = ([n_+]_L - k)^+$ and $\nabla n_+ = \nabla([n_+(t)]_L - k)^+$ in $\{k < n_+ < L\}$, this can be written as

$$\begin{aligned}&\int_\Omega (([n_+(t)]_L - k)^+)^{q+1}dx + \frac{4q}{q+1}\int_0^t\int_\Omega |\nabla(([n_+]_L - k)^+)^{(q+1)/2}|^2 dx\,ds \\ &= -2q\int_0^t\int_\Omega D_0(x)(([n_+]_L - k)^+)^{(q+1)/2}\nabla V\cdot\nabla(([n_+]_L - k)^+)^{(q+1)/2}dx\,ds \\ &\quad - 2kq\int_0^t\int_\Omega D_0(x)(([n_+]_L - k)^+)^{(q-1)/2}\nabla V\cdot\nabla(([n_+]_L - k)^+)^{(q+1)/2}dx\,ds \\ &\quad - \frac{1}{\tau}\int_0^t\int_\Omega (n_+ - n_-)(([n_+]_L - k)^+)^q dx\,ds.\end{aligned}$$

Employing the Cauchy-Schwarz inequality and absorbing the gradient terms by the second integral on the left-hand side, we conclude that

$$\begin{aligned}&\int_\Omega (([n_+(t)]_L - k)^+)^{q+1}dx + \frac{2q}{q+1}\int_0^t\int_\Omega |\nabla(([n_+]_L - k)^+)^{(q+1)/2}|^2 dx\,ds \\ &\quad \leq q(q+1)K_1\int_0^t\int_\Omega (([n_+]_L - k)^+)^{q+1}dx\,ds \\ &\qquad + q(q+1)k^2K_1\int_0^t\int_\Omega (([n_+]_L - k)^+)^{q-1}dx\,ds\end{aligned}$$

$$- \frac{1}{\tau}\int_0^t\int_\Omega (n_+ - n_-)(([n_+]_L - k)^+)^q dx\,ds.$$

where $K_1 = \|D(1+p)\|^2_{L^\infty(\Omega)}\|\nabla V\|^2_{L^\infty(0,T;L^\infty(\Omega))}$. We apply Young's inequality in the form $z^{q-1} \le ((q-1)/(q+1))z^{p+1} + 2/(q+1)$ to the second integral on the right-hand side to find that

$$\begin{aligned}\int_\Omega (([n_+(t)]_L - k)^+)^{q+1}dx + \frac{2q}{q+1}\int_0^t\int_\Omega |\nabla(([n_+]_L-k)^+)^{(q+1)/2}|^2 dx\,ds \\ \le q(q+1)(1+k^2)K_1\int_0^t\int_\Omega (([n_+]_L-k)^+)^{q+1}dx\,ds + 2qk^2K_1T\mathrm{meas}(\Omega) \\ - \frac{1}{\tau}\int_0^t\int_\Omega (n_+ - n_-)(([n_+]_L - k)^+)^q dx\,ds.\end{aligned}$$

A similar inequality can be derived by n_-. Adding both inequalities and observing that

$$-\frac{1}{\tau}\int_0^t\int_\Omega (n_+ - n_-)\big((([n_+]_L-k)^+)^q - (([n_+]_L-k)^+)^q\big)dx\,ds \le 0,$$

it follows that

$$\begin{aligned}\int_\Omega \sum_{j=\pm}(([n_j(t)]_L - k)^+)^{q+1}dx + \frac{2q}{q+1}\int_0^t\int_\Omega \sum_{j=\pm}|\nabla(([n_j]_L-k)^+)^{(q+1)/2}|^2 dx\,ds \\ \le q(q+1)K_2\int_0^t\int_\Omega \sum_{j=\pm}(([n_j]_L-k)^+)^{q+1}dx\,ds + qK_3.\end{aligned}$$

where $K_2 = (1+k^2)K_1$ and $K_3 = 2k^2K_1T\mathrm{meas}(\Omega)$. By the Gronwall lemma,

$$2^{-q}\bigg(\sum_{j=\pm}\|([n_j(t)]_L - k)^+\|_{L^{q+1}(\Omega)}\bigg)^{q+1} \le \sum_{j=\pm}\|([n_j(t)]_L-k)^+\|^{q+1}_{L^{q+1}(\Omega)} \le qK_3e^{K_2q(q+1)t}.$$

Since the right-hand side does not depend on $L > 0$, we can perform the limit $L \to \infty$:

$$\|(n_+(t)-k)^+\|_{L^{q+1}(\Omega)} + \|(n_-(t)-k)^+\|_{L^{q+1}(\Omega)} \le 2(qK_3)^{1/(q+1)}e^{K_2qt}.$$

This shows that $n_+, n_- \in L^\infty(0,T;L^q(\Omega))$ for all $q < \infty$. Unfortunately, we cannot perform the limit $q \to \infty$. In order to derive an L^∞ bound, we derive recursive inequalities. The idea is to exploit the gradient term via the Gagliardo-Nirenberg inequality.

Since

$$\begin{aligned}\partial_t n_+ - \mathrm{div}(D_0(x)\nabla n_+) &= -\mathrm{div}(D_0(x)n_+\nabla V) - \frac{n_+ - n_-}{\tau} \\ &\in L^\infty(0,T;(W^{1,q/(q-1)}(\Omega))') \quad \text{for all } q < \infty,\end{aligned}$$

maximal regularity [2] implies that $n_+ \in L^q(0,T;W^{1,q}(\Omega))$. This proves, together with the regularity $n_+ \in L^\infty(0,T;L^q(\Omega))$ for all $q < \infty$, that $n_+^q \in L^2(0,T;H^1(\Omega))$. Hence

$n_+^q - n_D^q \in L^2(0,T;H_0^1(\Omega))$ is an admissible test function in (9). Estimating as above, we arrive at

$$\begin{aligned} \frac{d}{dt}\int_\Omega (n_+^{q+1}+n_-^{q+1})dx + \frac{2q}{q+1}\int_\Omega \big(|\nabla n_+^{(q+1)/2}|^2 + |\nabla n_-^{(q+1)/2}|^2\big)dx \\ \le q(q+1)K_2\int_\Omega (n_+^{q+1}+n_-^{q+1})dx + qK_4, \end{aligned}$$

where $K_4 > 0$ depends on the boundary data n_D. Lemma 6 in the appendix shows that $n_+(t)$, $n_-(t)$ are bounded in $L^\infty(\Omega)$ uniformly in $t > 0$. We infer that $n_0 = n_+ + n_-$ and $\vec{n}\cdot\vec{m} = \frac{1}{2}(n_+ - n_-)$ are uniformly bounded in $L^\infty(\Omega)$.

It remains to prove the boundedness of $\vec{n}$ which follows if we have shown the boundedness of $\vec{n}_\perp$. An estimation as in Step 5 of the proof of Theorem 1 shows that $|\vec{n}_\perp| \in L^\infty(0,T;L^q(\Omega))$ for all $q < \infty$. Then the Alikakos iteration technique, applied to (13), shows that $|\vec{n}_\perp| \in L^\infty(0,T;L^\infty(\Omega))$.

3. Monotonicity of the entropy

In this section, we prove Proposition 3 and formula (18).

Proof of Proposition 3. The idea is to employ $(\log(n_+/\widetilde{n}_D)+V-V_D, \log(n_-/\widetilde{n}_D)+V-V_D)$ as a test function in (9)-(10), where $\widetilde{n}_D = \frac{1}{2}n_D$. Since the logarithm may be undefined, we need to regularize. We set

$$\begin{aligned} H_\delta(t) &= \int_\Omega \left(h_\delta(n_+) + h_\delta(n_-) + \frac{\lambda_D^2}{2}|\nabla(V-V_D)|^2\right)dx, \quad \delta > 0, \\ h_\delta(n_\pm) &= \int_{\widetilde{n}_D}^{n_\pm} \big(\log(s+\delta) - \log(\widetilde{n}_D+\delta)\big)ds \\ &= (n_\pm+\delta)(\log(n_\pm+\delta)-1) - (\widetilde{n}_D+\delta)(\log(\widetilde{n}_D+\delta)-1). \end{aligned}$$

Then the pointwise convergence $h_\delta(n_\pm) \to n_\pm(\log n_\pm - 1) - \widetilde{n}_D(\log\widetilde{n}_D - 1)$ as $\delta \to 0$ holds. Since $n_\pm = \frac{1}{2}n_D = \widetilde{n}_D$ on $\partial\Omega$ and $-\lambda_D^2\partial_t\Delta V = \partial_t(n_+ + n_-) \in L^2(0,T;H^{-1}(\Omega))$, we can differentiate H_δ to obtain

$$\begin{aligned} \frac{dH_\delta}{dt} &= \langle\partial_t n_+, \log(n_+ + \delta) - \log(\widetilde{n}_D+\delta)\rangle + \langle\partial_t n_-, \log(n_- + \delta) - \log(\widetilde{n}_D+\delta)\rangle \\ &\quad + \lambda_D^2\langle\partial_t\nabla V, \nabla(V-V_D)\rangle, \end{aligned}$$

where $\langle\cdot,\cdot\rangle$ is the duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. Observing that

$$\lambda_D^2\langle\partial_t\nabla V, \nabla(V-V_D)\rangle = -\lambda_D^2\langle\partial_t\Delta V, V-V_D\rangle = \langle\partial_t(n_+ + n_-), V-V_D\rangle,$$

it follows that

$$\begin{aligned} \frac{dH_\delta}{dt} &= \langle\partial_t n_+, \log(n_+ + \delta) + V - \log(\widetilde{n}_D+\delta) - V_D\rangle \\ &\quad + \langle\partial_t n_-, \log(n_- + \delta) + V - \log(\widetilde{n}_D+\delta) - V_D\rangle \\ &= I_1 + I_2. \end{aligned}$$

After inserting the evolution equation (9) for n_+, setting $J_+ = D_+(\nabla n_+ + n_+\nabla V)$ with $D_\pm = D(1\pm p)$, and integrating by parts, we find that the first term I_1 equals

$$I_1 = -\int_\Omega \big(J_+\cdot\nabla(\log(n_++\delta)+V) - J_+\cdot\nabla(\log(\widetilde{n}_D+\delta)+V_D)\big)dx$$
$$-\int_\Omega \frac{n_+-n_-}{\tau}\big(\log(n_++\delta)+V-\log(\widetilde{n}_D+\delta)-V_D\big)dx.$$

By Young's inequality, the first integral becomes

$$\int_\Omega\left(-\frac{J_+}{n_++\delta}\cdot(\nabla n_+ + (n_++\delta)\nabla V) + J_+\cdot\nabla(\log(\widetilde{n}_D+\delta)+V_D)\right)dx$$
$$= \int_\Omega\left(-\frac{|J_+|^2}{D_+(n_++\delta)} - \frac{\delta J_+\cdot\nabla V}{D_+(n_++\delta)} + J_+\cdot\nabla(\log(\widetilde{n}_D+\delta)+V_D)\right)dx$$
$$\le -\int_\Omega \frac{|J_+|^2}{2D_+(n_++\delta)}dx + \delta^2\int_\Omega\frac{|\nabla V|^2}{D_+(n_++\delta)}dx + \int_\Omega (n_++\delta)|\nabla(\log(\widetilde{n}_D+\delta)+V_D)|^2dx$$
$$\le -\int_\Omega \frac{|J_+|^2}{2D_+(n_++\delta)}dx + \delta\int_\Omega\frac{|\nabla V|^2}{D_+}dx + \int_\Omega (n_++\delta)|\nabla(\log(\widetilde{n}_D+\delta)+V_D)|^2dx.$$

The integral I_2 can be estimated in a similar way, eventually leading to

$$\frac{dH_\delta}{dt} \le -\int_\Omega\left(\frac{|J_+|^2}{2D_+(n_++\delta)} + \frac{|J_-|^2}{2D_-(n_-+\delta)}\right)dx + \delta\int_\Omega\left(\frac{1}{D_+}+\frac{1}{D_-}\right)|\nabla V|^2dx$$
$$+\int_\Omega\big((n_++\delta)+(n_-+\delta)\big)|\nabla(\log(\widetilde{n}_D+\delta)+V_D)|^2dx$$
$$-\int_\Omega\frac{n_+-n_-}{\tau}\big(\log(n_++\delta)-\log(n_-+\delta)\big)dx.$$

The last integral is nonnegative since $x\mapsto\log(x+\delta)$ is an increasing function. Therefore,

$$H_\delta(t) \le H_\delta(0) + \delta\int_0^t\int_\Omega\left(\frac{1}{D_+}+\frac{1}{D_-}\right)|\nabla V|^2dx\,dt$$
$$+\int_0^t\int_\Omega\big((n_++\delta)+(n_-+\delta)\big)|\nabla(\log(\widetilde{n}_D+\delta)+V_D)|^2dx\,ds. \tag{28}$$

Since $\log\widetilde{n}_D + V_D = \text{const.}$ and $n_D\ge n_*>0$, the gradient term in the last integral can be estimated by

$$|\nabla(\log(\widetilde{n}_D+\delta)+V_D)|^2 = \big|\nabla(\log\widetilde{n}_D+V_D)+\nabla(\log(\widetilde{n}_D+\delta)-\log\widetilde{n}_D)\big|^2$$
$$\le \frac{\delta^2|\nabla\widetilde{n}_D|^2}{\frac12 n_*(\frac12 n_*+\delta)},$$

and the right-hand side is bounded in $L^\infty(\Omega)$ uniformly in δ.

Therefore, the last two integrals in (28) can be bounded from above by a multiple of H_δ. Then Gronwall's lemma shows that H_δ is bounded uniformly in $\delta\in(0,1)$. By dominated convergence, we can pass to the limit $\delta \to 0$ in the integrals, leading to $H_\delta(t) \le H_0(0)$ for $t > 0$, where we used that $\nabla(\log \widetilde{n}_D + V_D) = 0$. This finishes the proof. $\square$

Remark 4. We prove formula (18). For this, we first observe that the formula $\partial_t \exp(A) = \exp(A)\partial_t A$ for any matrix A and the fact that the matrix logarithm of N is defined by the matrix A satisfying $\exp(A) = N$ imply that $\partial_t \log N = N^{-1}\partial_t N$ holds. We assume that $\log(n_D/2) + V_D = c \in \mathbb{R}$ in Ω (thermal equilibrium). Then $\log N_D + V_D\sigma_0 = c\sigma_0$ in Ω.

Now, using the Poisson equation (4), a formal computation leads to

$$\begin{aligned}
\frac{dH_Q}{dt} &= \int_\Omega \big(\operatorname{tr}[\partial_t N(\log N - \log N_D)] + \lambda_D^2 \partial_t \nabla V \cdot \nabla(V - V_D)\big) dx \\
&= \int_\Omega \big(\operatorname{tr}[\partial_t N(\log N - \log N_D)] dx + \partial_t(\operatorname{tr}(N) - C(x))(V - V_D)\big) dx \\
&= \int_\Omega \operatorname{tr}\big[\partial_t N(\log N - \log N_D + (V - V_D)\sigma_0)\big] dx.
\end{aligned}$$

Then, with the evolution equation (1) for N, an integration by parts, and the property $\log N_D + V_D\sigma_0 = c\sigma_0$ in Ω, we obtain

$$\begin{aligned}
\frac{dH_Q}{dt} &= -\int_\Omega \sum_{j=1}^3 D(x) \operatorname{tr}\big[P^{-1/2}(\partial_j N + N\partial_j V)P^{-1/2}\partial_j(\log N + V\sigma_0)\big] dx \\
&\quad - i\gamma \int_\Omega \operatorname{tr}\big[[N, \vec{m}\cdot\vec{\sigma}](\log N + V\sigma_0)\big] dx \\
&\quad + \frac{1}{\tau}\int_\Omega \operatorname{tr}\left[\left(\frac12 \operatorname{tr}(N)\sigma_0 - N\right)(\log N + V\sigma_0)\right] dx \\
&= I_1 + I_2 + I_3.
\end{aligned}$$

We compute the three integrals term by term. Employing the invariance of the trace under cyclic permutations and the commutativity relation $\log(N)N = N\log(N)$ gives

$$\operatorname{tr}\big[[N, \vec{m}\cdot\vec{\sigma}]\log N\big] = \operatorname{tr}\big[\vec{m}\cdot\vec{\sigma}\log(N)N - \vec{m}\cdot\vec{\sigma}N\log(N)\big] = 0,$$

which shows that $I_2 = 0$. For the integral I_3, the spectral property $\operatorname{tr}[f(A)] = \sum_j f(\lambda_j)$ for any continuous function f and any Hermitian matrix A with (real) eigenvalues λ_j, we have

$$\begin{aligned}
&\operatorname{tr}\left[\left(\frac12 \operatorname{tr}(N)\sigma_0 - N\right)(\log N + V\sigma_0)\right] = \frac12 \operatorname{tr}[N]\operatorname{tr}[\log N] - \operatorname{tr}[N\log N] \\
&\quad = \frac12 n_0\left(\log\left(\frac12 n_0 + |\vec{n}|\right) + \log\left(\frac12 n_0 - |\vec{n}|\right)\right) - \left(\frac12 n_0 + |\vec{n}|\right)\log\left(\frac12 n_0 + |\vec{n}|\right) \\
&\qquad - \left(\frac12 n_0 - |\vec{n}|\right)\log\left(\frac12 n_0 - |\vec{n}|\right) \\
&\quad = -|\vec{n}|\left(\log\left(\frac12 n_0 + |\vec{n}|\right) - \log\left(\frac12 n_0 - |\vec{n}|\right)\right) \le 0.
\end{aligned}$$

Hence, $I_3 \leq 0$. Finally, for the integral I_1, we employ the property $\partial_j N = N\partial_j \log N$ and the cyclicity of the trace:

$$\begin{aligned} I_1 &= -\int_\Omega D(x)\sum_{j=1}^3 \operatorname{tr}\big[N(\partial_j \log N + \partial_j V\sigma_0)P^{-1/2}\partial_j(\log N + V\sigma_0)P^{-1/2}\big]dx \\ &= -\int_\Omega D(x)\sum_{j=1}^3 \operatorname{tr}\big[N(\partial_j(\log N + V\sigma_0)P^{-1/2})^2\big]dx. \end{aligned}$$

This proves (18). □

Remark 5. We compute the trace of the matrix $N(\partial_j(\log N + V\sigma_0)P^{-1/2})^2$. The matrix $P^{-1/2}$ can be expanded into the Pauli basis. Indeed, using $P^{-1} = (1-p^2)^{-1}(\sigma_0 - p\vec{m}\cdot\vec{\sigma})$ and Lemma 2.3 in [17], we infer that

$$P^{-1/2} = p_+\sigma_0 - p_-\vec{m}\cdot\vec{\sigma}, \quad p_\pm = \frac{1}{2\sqrt{1-p^2}}\big(\sqrt{1+p} \pm \sqrt{1-p}\big).$$

The matrix $A := \partial_j(\log N + V\sigma_0) = a_0\sigma_0 + \vec{a}\cdot\vec{\sigma}$ can be also expanded. We observe that $N^{-1} = \beta(\frac{1}{2}n_0\sigma_0 - \vec{n}\cdot\vec{\sigma})$, where $\beta = 1/(\frac{1}{4}n_0^2 - |\vec{n}|^2)$. By Formula (8) in [17], we can write

$$(b_0\sigma_0 + \vec{b}\cdot\vec{\sigma})(c_0\sigma_0 + \vec{c}\cdot\vec{\sigma}) = (b_0c_0 + \vec{b}\cdot\vec{c})\sigma_0 + (b_0\vec{c} + c_0\vec{b} + i\vec{b}\times\vec{c})\cdot\vec{\sigma}.$$

With this identity, we find that

$$\begin{aligned} \partial_j \log N &= N^{-1}\partial_j N \\ &= \beta\left(\frac{1}{4}n_0\partial_j n_0 - \vec{n}\cdot\partial_j\vec{n}\right)\sigma_0 + \frac{\beta}{2}(n_0\partial_j\vec{n} - \partial_j n_0\vec{n})\cdot\vec{\sigma} - i\beta(\vec{n}\times\partial_j\vec{n})\cdot\vec{\sigma}. \end{aligned}$$

Consequently,

$$a_0 = \frac{\beta}{2}\partial_j\left(\frac{n_0^2}{4} - |\vec{n}|^2\right) + \partial_j V, \quad \vec{a} = \frac{\beta}{2}(n_0\partial_j\vec{n} - \partial_j n_0\vec{n}) - i\beta(\vec{n}\times\partial_j\vec{n}).$$

In particular, $\vec{a}$ is generally a complex vector. We write $\vec{a} = \vec{a}_1 + i\vec{a}_2$ with real vectors $\vec{a}_1$ and $\vec{a}_2$.

With these preparations, we calculate

$$\begin{aligned} (AP^{-1/2})^2 &= \big[(a_0p_+ - p_-\vec{a}\cdot\vec{m})\sigma_0 + (p_+\vec{a} - a_0p_-\vec{m} - ip_-(\vec{a}\times\vec{m}))\cdot\vec{\sigma}\big]^2 \\ &= \big[(a_0p_+ - p_-\vec{a}\cdot\vec{m})^2 + (p_+\vec{a} - a_0p_-\vec{m} - ip_-(\vec{a}\times\vec{m}))^2\big]\sigma_0 \\ &\quad + 2(a_0p_+ - p_-\vec{a}\cdot\vec{m})(p_+\vec{a} - a_0p_-\vec{m} - ip_-(\vec{a}\times\vec{m}))\cdot\vec{\sigma} \\ &= \big[(a_0p_+ - p_-\vec{a}\cdot\vec{m})^2 + (p_+\vec{a} - a_0p_-\vec{m})^2 \\ &\quad - 2ip_-(p_+\vec{a} - a_0p_-\vec{m})\cdot(\vec{a}\times\vec{m}) - p_-^2(\vec{a}\times\vec{m})^2\big]\sigma_0 \\ &\quad + 2(a_0p_+ - p_-\vec{a}\cdot\vec{m})(p_+\vec{a} - a_0p_-\vec{m} - ip_-(\vec{a}\times\vec{m}))\cdot\vec{\sigma}. \end{aligned}$$

Since $\vec{a}\cdot(\vec{a}\times\vec{m}) = \vec{m}\cdot(\vec{a}\times\vec{m}) = 0$, the right-hand side simplifies slightly:

$$(AP^{-1/2})^2 = \big[(a_0p_+ - p_-\vec{a}\cdot\vec{m})^2 + (p_+\vec{a} - a_0p_-\vec{m})^2 - p_-^2(\vec{a}\times\vec{m})^2\big]\sigma_0$$

$$+ 2(a_0p_+ - p_-\vec{a}\cdot\vec{m})(p_+\vec{a} - a_0p_-\vec{m} - ip_-(\vec{a}\times\vec{m}))\cdot\vec{\sigma}.$$

After multiplication by $N = \frac{1}{2}n_0\sigma_0 + \vec{n}\cdot\vec{\sigma}$, it follows that

$$\begin{aligned} N(AP^{-1/2})^2 &= \tfrac{1}{2}n_0\big((a_0p_+ - p_-\vec{a}\cdot\vec{m})^2 + (p_+\vec{a} - a_0p_-\vec{m})^2 - p_-^2(\vec{a}\times\vec{m})^2\big)\sigma_0 \\ &\quad + 2(a_0p_+ - p_-\vec{a}\cdot\vec{m})\vec{n}\cdot(p_+\vec{a} - a_0p_-\vec{m} - ip_-(\vec{a}\times\vec{m}))\sigma_0 + \vec{B}\cdot\vec{\sigma}, \end{aligned}$$

for some vector $\vec{B}$ which disappears after taking the trace (since σ_j is traceless):

$$\begin{aligned} \operatorname{tr}\big[N(AP^{-1/2})^2\big] &= n_0\big((a_0p_+ - p_-\vec{a}\cdot\vec{m})^2 + (p_+\vec{a} - a_0p_-\vec{m})^2 - p_-^2(\vec{a}\times\vec{m})^2\big) \\ &\quad + 4(a_0p_+ - p_-\vec{a}\cdot\vec{m})\vec{n}\cdot(p_+\vec{a} - a_0p_-\vec{m} - ip_-(\vec{a}\times\vec{m})). \end{aligned}$$

Since dH_Q/dt is real, the above trace is real too. Thus,

$$\begin{aligned} \operatorname{tr}\big[N(AP^{-1/2})^2\big] &= n_0(a_0p_+ - p_-\vec{a}_1\cdot\vec{m})^2 - n_0p_-^2(\vec{a}_2\cdot\vec{m})^2 + n_0(p_+\vec{a}_1 - a_0p_-\vec{m})^2 \\ &\quad - n_0p_+^2\vec{a}_2^2 - n_0p_-^2(\vec{a}_1\times\vec{m})^2 + n_0p_-^2(\vec{a}_2\times\vec{m})^2 \\ &\quad + 4(a_0p_+ - p_-\vec{a}_1\cdot\vec{m})\vec{n}\cdot(p_+\vec{a}_1 - a_0p_-\vec{m} + p_-(\vec{a}_2\times\vec{m})) \\ &\quad + 4p_-(\vec{a}_2\cdot\vec{m})\vec{n}\cdot(p_+\vec{a}_2 - p_-\vec{a}_1\times\vec{m}) \\ &= J_1 + J_2, \end{aligned}$$

where

$$\begin{aligned} J_1 &= n_0(a_0p_+ - p_-\vec{a}_1\cdot\vec{m})^2 + n_0(p_+\vec{a}_1 - a_0p_-\vec{m})^2 \\ &\quad + 4(a_0p_+ - p_-\vec{a}_1\cdot\vec{m})\vec{n}\cdot(p_+\vec{a}_1 - a_0p_-\vec{m}), \\ J_2 &= -n_0p_-^2(\vec{a}_2\cdot\vec{m})^2 - n_0p_+^2\vec{a}_2^2 - n_0p_-^2(\vec{a}_1\times\vec{m})^2 + n_0p_-^2(\vec{a}_2\times\vec{m})^2 \\ &\quad + 4p_+p_-a_0\vec{n}\cdot(\vec{a}_2\times\vec{m}) - 4p_-^2(\vec{a}_1\cdot\vec{m})\vec{n}\cdot(\vec{a}_2\times\vec{m}) \\ &\quad + 4p_+p_-(\vec{a}_2\cdot\vec{m})\vec{n}\cdot\vec{a}_2 - 4p_-^2(\vec{a}_2\cdot\vec{m})\vec{n}\cdot(\vec{a}_1\times\vec{m}). \end{aligned}$$

The term J_1 is nonnegative. Indeed, set $c_0 = a_0p_+ - p_-\vec{a}_1\cdot\vec{m}$ and $\vec{c} = p_+\vec{a}_1 - a_0p_-\vec{m}$. Then

$$J_1 = n_0c_0^2 + n_0\vec{c}^2 + 4c_0\vec{n}\cdot\vec{c} = n_0\left(c_0 + \frac{2}{n_0}\vec{n}\cdot\vec{c}\right)^2 + n_0\left(\vec{c}^2 - \frac{4}{n_0^2}(\vec{n}\cdot\vec{c})^2\right).$$

Since $\frac{1}{2}n_0 > |\vec{n}|$ by assumption, the Cauchy-Schwarz inequality shows that the last term is nonnegative and thus, $J_1 \geq 0$.

As $\vec{n}\cdot\vec{a}_2 = 0$, the last summand in J_2 vanishes. Because of $\vec{n}\cdot(\vec{a}_1\times\vec{m}) = \vec{m}\cdot(\vec{n}\times\vec{a}_1) = \frac{1}{2}\beta n_0\vec{m}\cdot(\vec{n}\times\partial_j\vec{n}) = -\frac{1}{2}n_0(\vec{a}_2\times\vec{m})$, the next to last summand in J_2 can be combined with the first summand, yielding

$$\begin{aligned} J_2 &= n_0p_-^2(\vec{a}_2\cdot\vec{m})^2 - n_0p_+^2\vec{a}_2^2 - n_0p_-^2(\vec{a}_1\times\vec{m})^2 + n_0p_-^2(\vec{a}_2\times\vec{m})^2 \\ &\quad + 4p_+p_-a_0\vec{n}\cdot(\vec{a}_2\times\vec{m}) - 4p_-^2(\vec{a}_1\cdot\vec{m})\vec{n}\cdot(\vec{a}_2\times\vec{m}). \end{aligned}$$

Employing $(\vec{a}_1\times\vec{m})^2 = \vec{a}_1^2 - (\vec{a}_1\cdot\vec{m})^2$, the third summand can be reformulated, and we end up with

$$J_2 = n_0p_-^2(\vec{a}_2\cdot\vec{m})^2 - n_0p_+^2\vec{a}_2^2 - n_0p_-^2\vec{a}_1^2 + 4p_+p_-a_0\vec{n}\cdot(\vec{a}_2\times\vec{m})$$

$$+ n_0 p_-^2 \left(\vec{a}_1 \cdot \vec{m} - \frac{2}{n_0} \vec{n} \cdot (\vec{a}_2 \times \vec{m}) \right)^2 + n_0 p_-^2 \left((\vec{a}_2 \times \vec{m})^2 - \frac{4}{n_0^2} (\vec{n} \cdot (\vec{a}_2 \times \vec{m}))^2 \right).$$

Arguing similarly as for J_1, we see that the last two summands are nonnegative.

Suppose that $\vec{n}$ is parallel to $\vec{c}$, $\vec{a}_2$ is parallel to $\vec{m}$, and $c_0 = 0$. Then, if $n_0 \gg 1$ and $|\vec{a}_2| \gg 1$, we obtain $J_1 \approx 0$ and $J_2 < 0$. Hence, $\mathrm{tr}[N(AP^{-1/2})^2]$ may be negative. ☐

4. Numerical simulations

In this section, we solve equations (4)-(8) numerically for a one-dimensional ballistic diode in a multilayer structure. The aim is twofold: First, we present simulations of the stationary state in order to compare our numerical results to those of [17] and to detail the differences between the numerical solutions with and without Poisson equation. Second, we show numerically that the entropy (16) decreases exponentially fast in time.

The multilayer consists of a ferromagnetic layer sandwiched between two nonmagnetic layers. More precisely, let $\Omega = (0, L)$. The nonmagnetic layers $(0, \ell_1)$ and (ℓ_2, L) are characterized by $\vec{m} = 0$, $p = 0$ and a high doping concentration, $C(x) = C_{\max}$ for $x \in (0, \ell_1) \cup (\ell_2, L)$, whereas the magnetic layer (ℓ_1, ℓ_2) features a nonvanishing magnetization, $\vec{m} = (0, 0, 1)^\top$ and $p > 0$, and a low doping, $C(x) = C_{\min}$ for $x \in (\ell_1, \ell_2)$. This multilayer structure was numerically solved in [17] but for constant electric fields only and without doping.

The boundary conditions read as

$$n_0(0, t) = n_0(L, t) = C_{\max}, \quad \vec{n}(0, t) = \vec{n}(L, t) = 0, \quad V(0, t) = 0, \; V(L, t) = U$$

for all $t > 0$, and the initial conditions are $n_0(x) = 1$, $\vec{n}(x) = 0$, and $V(x) = Ux/L$ for $x \in \Omega$ and for some $U > 0$. We choose $C_{\max} = 10^{21}\, m^{-3}$ and $C_{\min} = 0.4 \cdot 10^{19}\, m^{-3}$. This corresponds to an overall low-doping situation. With larger doping concentrations, we observed numerical problems in the Poisson equation due to the smallness of the scaled Debye length λ_D. This problem is well known and can be solved by employing more sophisticated numerical methods.

We choose the same physical parameters as in [17]: the diffusion coefficient $D = 10^{-3}\,\mathrm{m^2 s^{-1}}$, the thermal voltage $V_{\mathrm{th}} = 0.0259\,\mathrm{V}$, the spin-flip relaxation time $\tau = 10^{-12}\,\mathrm{s}$, the strength of the pseudo-exchange field $\gamma = 2\hbar/\tau$, and the applied potential $U = 1\,\mathrm{V}$. Typically, the spin-flip relaxation time is of the order of a few to 100 picoseconds [8]. The layers have the same length of $0.4\,\mu\mathrm{m}$ such that the device length equals $L = 1.2\,\mu\mathrm{m}$.

4.1. **Implementation.** The equations are discretized in time by the implicit Euler approximation and in space by a node-centered finite-volume method. This method is conservative and is able to deal with discontinuous coefficients. We choose a uniform grid of M points $x_i = i\triangle x$ with step size $\triangle x > 0$, containing the interface points ℓ_1 and ℓ_2, and uniform time steps $t_k = k\triangle t$ with step size $\triangle t > 0$. We also introduce the cell-center points $x_{i+1/2} = (i + 1/2)\triangle x$. Denoting by $n_{\ell,i}^k$ an approximation of $(\triangle x)^{-1} \int_{x_{i-1/2}}^{x_{i+1/2}} n_\ell(x, t_k) dx$ for $\ell = 0, 1, 2, 3$ (the index of the spin component), the discretization of (5)-(6) reads as follows:

$$\frac{1}{\triangle t}(n_{0,i}^k - n_{0,i}^{k-1}) + \frac{1}{\triangle x}(j_{0,i+1/2}^k - j_{0,i-1/2}^k) = 0, \tag{29}$$

$$\frac{1}{\triangle t}(n_{\ell,i}^k - n_{\ell,i}^{k-1}) + \frac{1}{\triangle x}(j_{\ell,i+1/2}^k - j_{\ell,i-1/2}^k) - \frac{2\gamma}{\hbar}(\vec{n}_i^k \times \vec{m}_i)_\ell + \frac{1}{\tau}n_{\ell,i}^k = 0, \tag{30}$$

where $\ell = 1,2,3$, $\vec{n}_i^k = (n_{1,i}^k, n_{2,i}^k, n_{3,i}^k)$, $\vec{m}_i = (m_{1,i}, m_{2,i}, m_{3,i}) = \vec{m}(x_i)$, and

$$j_{0,i+1/2}^k = -\frac{D}{\eta_{i+1/2}^2}\big(J_{0,i+1/2}^k - 2p_{i+1/2}\vec{J}_{i+1/2}^k \cdot \vec{m}_{i+1/2}\big),$$

$$j_{\ell,i+1/2}^k = -\frac{D}{\eta_{i+1/2}^2}\bigg(\eta_{i+1/2}J_{\ell,i+1/2}^k + (1-\eta_{i+1/2})(\vec{J}_{i+1/2}^k \cdot \vec{m}_{i+1/2})m_{\ell,i+1/2} - \frac{p_{i+1/2}}{2}J_{0,i+1/2}^k m_{\ell,i+1/2}\bigg),$$

$$J_{\ell,i+1/2}^k = \frac{1}{\triangle x}\bigg((n_{\ell,i+1}^k - n_{\ell,i}^k) + \frac{1}{2}(n_{\ell,i+1}^k + n_{\ell,i}^k)(V_{i+1}^k - V_i^k)\bigg), \quad \ell = 0,1,2,3.$$

where $\vec{J}_{i+1/2}^k = (J_{\ell,i+1/2}^k)_{\ell=1,2,3}$. The discrete electric potential V_i^k, which is scaled by the thermal voltage V_{th}, is obtained from the Poisson equation, discretized by central finite differences. The nonlinear discrete system is solved by the Gummel method, i.e., given $(n_{\ell,i}^{k-1}, V_i^{k-1})$ and setting $\rho_i = n_{0,i}^{k-1}\exp(-V_i^{k-1})$, we solve first the nonlinear system

$$-\lambda_D^2(V_{i+1}^k - 2V_i^k + V_{i-1}^k) = \rho_i e^{V_i^k} - C(x_i),$$

by Newton's method. Then, using the updated potential (V_i^k), the discrete system (29)-(30) is solved for $n_{\ell,i}^k$, and the procedure is iterated. For details on the Gummel method, we refer to [12]. We have chosen 60 grid points in each layer (i.e. $M = 180$) and the time step size $\triangle t = 0.005\tau$. These values are chosen in such a way that further refinement did not change the results.

4.2. **Numerical simulations.** We wish to compare the stationary numerical solutions to those presented in [17]. To this end, we compute the solution to the above numerical scheme for "large" time until the steady state is approximately reached. As in [17], we fix a linear potential (i.e. without Poisson equation). The (scaled) stationary charge density n_0 and spin-vector density $\vec{n} = (0,0,n_3)$ are presented in Figure 1. According to [17], the discontinuity of the spin polarization p at the interfaces is compensated by a decrease of n_0 in the ferromagnetic layer, leading to a non-equilibrium spin density $n_3 \neq 0$. Our numerical results correspond to those in [17, Figure 1] except for the values of the charge density n_0 in the right layer. Possanner and Negulescu found that n_0 is strictly smaller than the doping concentration and that there is a small boundary layer at $x = L$.

In order to understand this difference, we have implemented the scheme of [17], which consists of a standard Crank-Nicolson discretization in each of the layers, together with continuity conditions for n_0, $\vec{n}$, j_0, and $\vec{j} = (j_1, j_2, j_3)$ at the interfaces $x = \ell_1$ and $x = \ell_2$. The numerical result for n_0 is shown in Figure 2. This does not correspond exactly to

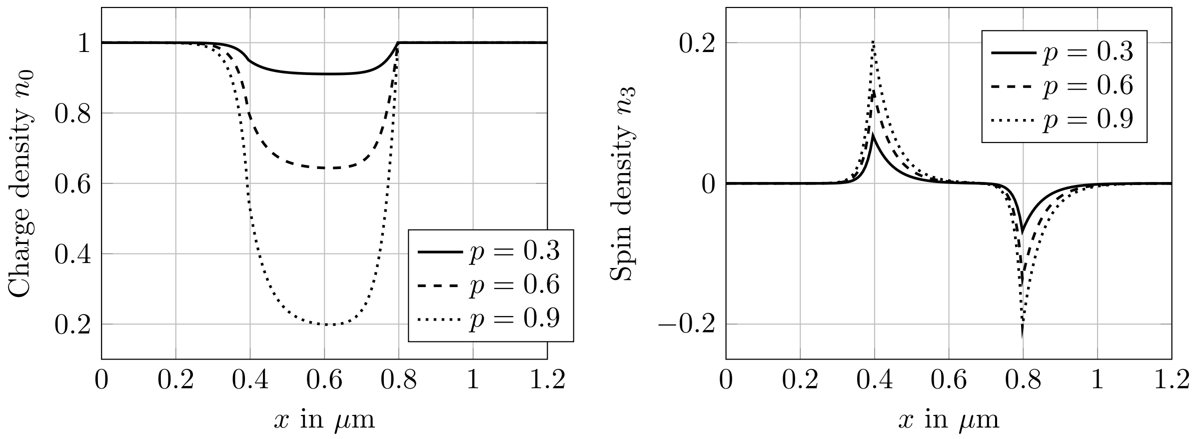

FIGURE 1. Charge density n_0 (left) and spin density n_3 (right) in the three-layer structure with linear potential and different spin polarizations p.

the outcome of [17] since our charge density is strictly *larger* than the doping in the right layer. Refining the mesh, however, we see that n_0 becomes closer to the doping and to the behavior shown in Figure 1 (left). This supports the validity of the numerical results computed from the finite-volume scheme.

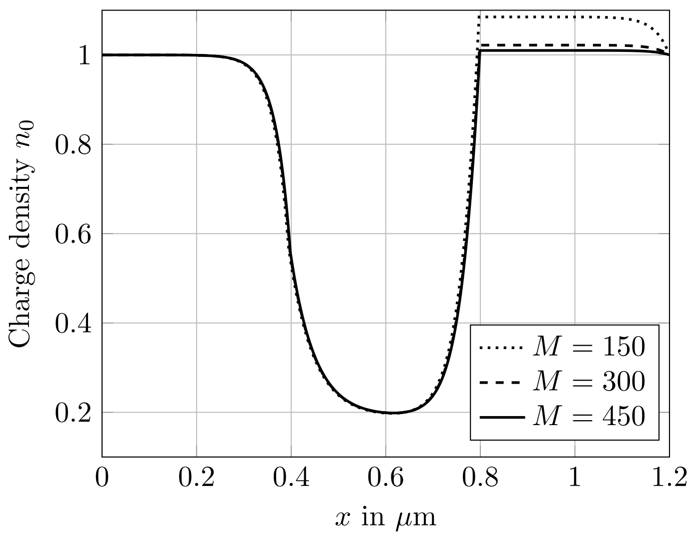

FIGURE 2. Charge density n_0 computed from the scheme in [17] (without Poisson equation) for different grid point numbers M.

Figure 3 illustrates the densities n_0 and n_3 calculated from the full model with self-consistent electric potential. Because of the rather small doping concentration and the large voltage, electrons drift to the right contact, leading to a significant decrease of the charge density in the right layer. For small values of the spin polarization p, the charge density is similar to the charge density computed with vanishing magnetization. When the spin polarization p increases, the charge density is reduced in the ferromagnetic layer and increases in the right nonmagnetic region. The self-consistent potential leads to a slight reduction of the peaks of the spin density, compared with Figure 1 (right).

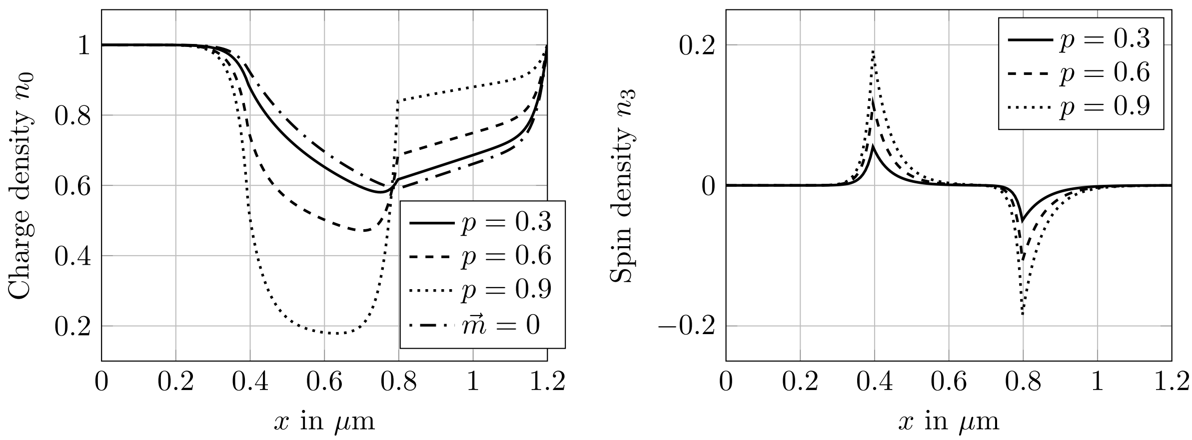

FIGURE 3. Charge density n_0 (left) and spin density n_3 (right) in the three-layer structure with self-consistent potential and different spin polarizations p.

Next, we consider a smaller device with length $L = 0.4\,\mu$m and a higher level of doping, $C_{\max} = 9 \cdot 10^{21}\,\mathrm{m}^{-3}$. With these parameters, the scaled Debye length is the same as in the previous case. As a consequence, the charge density without magnetization does not change. The influence of the spin polarization is similar as in the previous test case (see Figure 4), but the charge density is larger in the ferromagnetic layer due to the reduced size.

Our final example is concerned with a transient simulation. As initial data, we choose $V = 0$, $n_0 = 1$, and $\vec{n} = 0$. Figure 5 presents the time decay of the entropy (free energy) H_0, defined in (16). It turns out that $H_0(t)$ is decaying exponentially fast. For times $t > 270\,$ps, the equilibrium state is almost reached, and since we reached the computer precision of about 10^{-16}, we observe some oscillations in the values for H_0.

Appendix A. A boundedness result

We prove the following lemma which is an extension of a result due to Kowalczyk [14], based on the iteration technique of Alikakos [1].

Lemma 6. *Let $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) be a bounded domain and let $u_i \geq 0$, $u_i^{q/2} \in L^2(0,T;H^1(\Omega))$ for all $2 \leq q < \infty$, $i = 1,\ldots,n$. Suppose that there exist constants K_0, K_1, K_2 such that for all $q \geq 2$,*

$$\frac{d}{dt}\sum_{i=1}^n \int_\Omega u_i^{q+1}dx + K_0 \sum_{i=1}^n \int_\Omega |\nabla u_i^{(q+1)/2}|^2 dx \leq q(q+1)K_1 \sum_{i=1}^n \int_\Omega u_i^{q+1}dx + q(q+1)K_2. \tag{31}$$

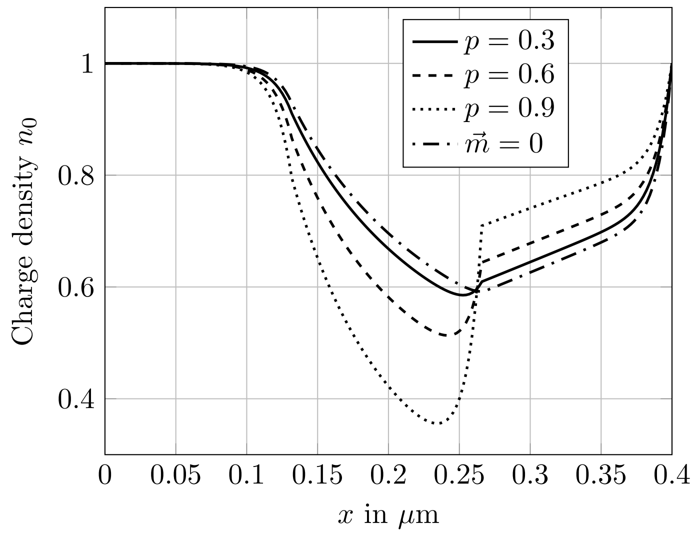

FIGURE 4. Charge density n_0 in the three-layer structure with self-consistent potential and smaller device length $L = 0.4\,\mu$m.

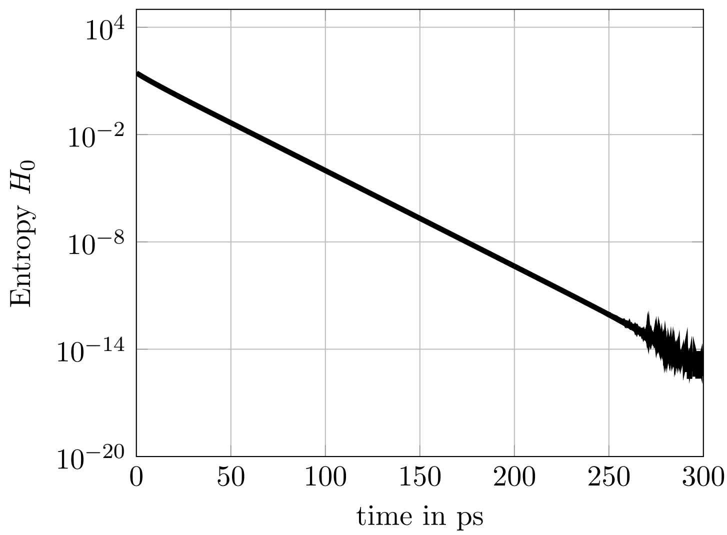

FIGURE 5. Semilogarithmic plot of the entropy $H_0(t)$ versus time.

Then for all $0 \le t \le T$,

$$\sum_{i=1}^n \|u_i(t)\|_{L^\infty(\Omega)} \le K^* \max\left\{1, \sum_{i=1}^n \|u_i\|_{L^\infty(0,T;L^1(\Omega))}, n\sum_{i=1}^n \|u_i(0)\|_{L^\infty(\Omega)}\right\},$$

where $K^* = 2^{7+2d}(1+\max\{K_1,K_2\})$.

Proof. Note that the proof does not follow directly from the Gronwall lemma and the limit $q \to \infty$ because of the quadratic term in q on the right-hand side. First, we estimate the

L^{q+1} norm of u_i. By the Gagliardo-Nirenberg inequality with $\theta = d/(d+2) < 1$ and the Young inequality $ab \le \theta\varepsilon a^{1/\theta} + (1-\theta)\varepsilon^{-\theta/(1-\theta)} b^{1/(1-\theta)}$ for $0 < \varepsilon < 1$, it follows that

$$\int_\Omega u_i^{q+1} dx = \|u_i^{(q+1)/2}\|_{L^2(\Omega)}^2 \le K_3 \|u_i^{(q+1)/2}\|_{H^1(\Omega)}^{2\theta} \|u_i^{(q+1)/2}\|_{L^1(\Omega)}^{2(1-\theta)}$$
$$\le \varepsilon\big(\|\nabla u_i^{(q+1)/2}\|_{L^2(\Omega)}^2 + \|u_i^{(q+1)/2}\|_{L^2(\Omega)}^2\big) + \frac{K_3^{1/(1-\theta)}}{\varepsilon^{\theta/(1-\theta)}} \|u_i^{(q+1)/2}\|_{L^1(\Omega)}^2.$$

Since $1/(1-\theta) = 1 + d/2$ and $\theta/(1-\theta) = d/2$, this gives

$$\int_\Omega u_i^{q+1} dx \le \frac{\varepsilon}{1-\varepsilon} \|\nabla u_i^{(q+1)/2}\|_{L^2(\Omega)}^2 + \frac{K_3^{1+d/2}}{\varepsilon^{d/2}(1-\varepsilon)} \|u_i^{(q+1)/2}\|_{L^1(\Omega)}^2.$$

We choose $\varepsilon > 0$ such that $(\varepsilon/(1-\varepsilon))(q(q+1)K_1 + (q+1)^{-1}) = K_0$ (then $\varepsilon = O(q^{-2})$ as $q \to \infty$). Hence, there exists a constant $K_4 > 0$ which is independent of q such that $K_3^{1+d/2}/(\varepsilon^{d/2}(1-\varepsilon)) \le K_4(q+1)^d$. Multiplying the above inequality by $q(q+1)K_1 + (q+1)^{-1}$, we conclude that

$$\big(q(q+1)K_1 + (q+1)^{-1}\big) \int_\Omega u_i^{q+1} dx$$
$$\le K_0 \|\nabla u_i^{(q+1)/2}\|_{L^2(\Omega)}^2 + K_4(q+1)^d \big(q(q+1)K_1 + (q+1)^{-1}\big) \|u_i^{(q+1)/2}\|_{L^1(\Omega)}^2.$$

We insert this estimate in (31):

$$\frac{d}{dt} \sum_{i=1}^n \int_\Omega u_i^{q+1} dx + \frac{1}{q+1} \sum_{i=1}^n \int_\Omega u_i^{q+1} dx$$
$$\le K_4(q+1)^d \big(q(q+1)K_1 + (q+1)^{-1}\big) \sum_{i=1}^n \|u_i^{(q+1)/2}\|_{L^1(\Omega)}^2 + q(q+1)K_2.$$

Setting $q = \lambda_m = 2^m - 1$ for $m \in \mathbb{N}$, $\varepsilon_m = 2^{-m}$, $a_m = 2^m(2^m - 1)\max\{K_1, K_2\}$, and $c_m = 2^{dm} K_4$, the above inequality can be written as

(32)
$$\frac{d}{dt} \sum_{i=1}^n \int_\Omega u_i^{\lambda_m+1} dx + \varepsilon_m \sum_{i=1}^n \int_\Omega u_i^{\lambda_m+1} dx \le (a_m + \varepsilon_m) c_m \left(\sum_{i=1}^n \sup_{t>0} \int_\Omega u_i^{\lambda_{m-1}+1} dx \right)^2 + a_m.$$

If $n = 1$, the result follows directly from Lemma 5.1 in [14]. An inspection of the proof of Lemma 5.1 shows that the conclusion still holds with a slightly different L^∞ bound which comes from the fact that

$$\sum_{i=1}^n \int_\Omega u_i(0)^{\lambda_k+1} dx \le n^{\lambda_k} \left(\sum_{i=1}^n \|u_i(0)\|_{L^{\lambda_k+1}(\Omega)} \right)^{\lambda_k+1}$$
$$\le \operatorname{meas}(\Omega) \left(n \sum_{i=1}^n \|u_i(0)\|_{L^\infty(\Omega)} \right)^{\lambda_k+1}.$$

This ends the proof. □

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