



Large-time asymptotics for a matrix spin drift-diffusion model [☆]

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ABSTRACT

The large-time asymptotics of the density matrix solving a drift-diffusion-Poisson model for the spin-polarized electron transport in semiconductors is proved. The equations are analyzed in a bounded domain with initial and Dirichlet boundary conditions. If the relaxation time is sufficiently small and the boundary data is close to the equilibrium state, the density matrix converges exponentially fast to the spinless near-equilibrium steady state. The proof is based on a reformulation of the matrix-valued cross-diffusion equations using spin-up and spin-down densities as well as the perpendicular component of the spin-vector density, which removes the cross-diffusion terms. Key elements of the proof are time-uniform positive lower and upper bounds for the spin-up and spin-down densities, derived from the De Giorgi–Moser iteration method, and estimates of the relative free energy for the spin-up and spin-down densities.

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1. Introduction

Semiconductor lasers and transistor devices may be improved by taking into account spin-polarized electron injection. The corresponding semiconductor models should include the spin effects in an accurate way. A widely used model are the two-component spin drift-diffusion equations [15], which can be derived for strong spin-orbit coupling from the spinorial Boltzmann equation in the diffusion limit [13], describing the dynamics of the spin-up and spin-down electrons. When the spin-orbit coupling is only moderate, the diffusion limit in the spinorial Boltzmann equation leads to a matrix spin drift-diffusion model for the electron density matrix [13,33]. This model contains much more information than the two-component model, but the strong coupling between the four spin components makes the mathematical analysis very challenging. The existence of global weak solutions was shown in [25]. In this paper, we investigate the large-time asymptotics of the density matrix towards a near-equilibrium steady state.

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1.1. Model equations

We assume that the dynamics of the (Hermitian) density matrix $N(x, t) \in \mathbb{C}^{2 \times 2}$, the current density matrix $J(x, t) \in \mathbb{C}^{2 \times 2}$, and the electric potential $V(x, t)$ is given by the (scaled) matrix equations

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

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

$$-\lambda^2 \Delta V = \operatorname{tr}(N) - g(x) \quad \text{in } \Omega, \quad t > 0, \quad (3)$$

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 precession vector $\vec{\mu} = (\mu_1, \mu_2, \mu_3) \in \mathbb{R}^3$, the spin-flip relaxation time $\tau > 0$, the diffusion constant $D > 0$, the Debye length $\lambda > 0$, and the doping concentration $g(x)$. Equation (3) is the Poisson equation for the electric potential [24]. The precession vector plays the role of the local direction of the magnetization in the ferromagnet, and we assume that it is constant. This assumption is crucial for our analysis. Furthermore, $P = \sigma_0 + p\vec{\mu} \cdot \vec{\sigma} = \sigma_0 + p(\mu_1\sigma_1 + \mu_2\sigma_2 + \mu_3\sigma_3)$ is the matrix of spin polarization of the scattering rates, $p \in [0, 1]$ represents the spin polarization, σ_0 is the unit matrix in $\mathbb{R}^{2 \times 2}$, and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices, defined by

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

The number i is the complex unit, and $\operatorname{tr}(N)$ denotes the trace of the matrix N . Since the Pauli matrices are traceless, $\operatorname{tr}(N)$ only contains the σ_0 -component of N , which is the charge density. The commutator $[N, \vec{\mu} \cdot \vec{\sigma}]$ models the precession of the spin polarization. The right-hand side in (1) describes the spin-flip relaxation of the spin density to the (spinless) equilibrium state.

Equations (1)–(3) are solved in the bounded domain $\Omega \subset \mathbb{R}^3$ with time $t > 0$ and are supplemented with the boundary and initial conditions

$$N = \frac{1}{2} n_D \sigma_0, \quad V = V_D \quad \text{on } \partial\Omega, \quad t > 0, \quad N(0) = N^0 \quad \text{in } \Omega. \quad (4)$$

This means that no spin effects occur on the boundary. For simplicity, we choose time-independent boundary data; see [40] for boundary data depending on time. Mixed Dirichlet–Neumann boundary conditions may be also considered as long as they allow for $W^{2,q_0}(\Omega)$ elliptic regularity results, which restricts the geometry of $\partial\Omega$. Therefore, we have chosen pure Dirichlet boundary data as in [25].

The density matrix N can be expressed in terms of the Pauli matrix according to $N = \frac{1}{2} n_0 \sigma_0 + \vec{n} \cdot \vec{\sigma}$ and $\vec{n} = (n_1, n_2, n_3)$ is called the spin-vector density. Model (1)–(2), written in the four variables n_0, \dots, n_3 , is a cross-diffusion system with the constant diffusion matrix

$$\frac{D}{1-p^2} \begin{pmatrix} 1 & & & -p\vec{\mu}^\top \\ -p\vec{\mu} & \eta \mathbb{I} & + (1-\eta)\vec{\mu} \otimes \vec{\mu} \end{pmatrix} \in \mathbb{R}^{4 \times 4},$$

where \mathbb{I} is the unit matrix in $\mathbb{R}^{3 \times 3}$. Although this matrix is symmetric and positive definite, the strong coupling complicates the analysis of system (1)–(2), because maximum principle arguments and other standard tools cannot be (easily) applied.

The spin polarization matrix couples the charge and spin components of the electrons. By comparison of the coefficients of σ_0 [33], we see that the electron charge density n_0 satisfies

$$\partial_t n_0 - D_p \operatorname{div} j_0 = 0, \quad j_0 = \nabla n_0 + n_0 \nabla V - 2p(\nabla \vec{n} + \vec{n} \nabla V) \cdot \vec{\mu},$$

where $D_p = D/(1 - p^2)$. If $p = 0$, we recover the classical Van-Roosbroeck drift-diffusion equations [28,37]:

$$\partial_t n_0 - D \operatorname{div} j_0 = 0, \quad j_0 = \nabla n_0 + n_0 \nabla V, \quad (5)$$

coupled with the Poisson equation (3). The boundary conditions are $n_0 = n_D$ and $V = V_D$ on $\partial\Omega$ and the initial condition is $n_0(0) = n_0^0$ in Ω , where $N^0 = \frac{1}{2}n_0^0\sigma_0 + \vec{n}^0 \cdot \vec{\sigma}$. Another special case is given by the two-component spin drift-diffusion model. The spin-up and spin-down densities $n_{\pm} = \frac{1}{2}n_0 \pm \vec{n} \cdot \vec{\mu}$, respectively, satisfy the equations

$$\partial_t n_+ - \operatorname{div} (D_+(\nabla n_+ + n_+ \nabla V)) = \frac{1}{2\tau}(n_- - n_+), \quad (6)$$

$$\partial_t n_- - \operatorname{div} (D_-(\nabla n_- + n_- \nabla V)) = \frac{1}{2\tau}(n_+ - n_-), \quad (7)$$

$$n_{\pm} = \frac{n_D}{2}, \quad V = V_D \quad \text{on } \partial\Omega, \quad n_{\pm}(0) = \frac{1}{2}n_0^0 \pm \vec{n}^0 \cdot \vec{\mu} \quad \text{in } \Omega, \quad (8)$$

where $D_{\pm} = D/(1 \pm p)$. These equations are weakly coupled through the relaxation term.

Model (1)–(2) was derived in [33] from a matrix Boltzmann equation in the diffusion limit. The scattering operator in the Boltzmann model is assumed to consist of a dominant collision operator from the Stone model and a spin-flip relaxation operator. When the scattering rate in the Stone model is smooth and invariant under isometric transformations, the diffusion D can be identified with a positive number [34, Prop. 1].

1.2. State of the art

The first result on the global existence of solutions to the Van-Roosbroeck equations (5) (for electrons and positively charged holes) was proved by Mock [29]. He showed in [30] that the solution decays exponentially fast to the equilibrium state provided that the initial data is sufficiently close to the equilibrium. These results were generalized under physically more realistic assumptions on the boundary by Gajewski [16] and Gajewski and Gröger [17,18]. Further large-time asymptotics can be found in [4] for the whole-space problem and in [8], where the diffusion constant was replaced by a diffusion matrix. Moreover, in [12], the stability of the solutions in Wasserstein spaces was investigated.

Convergence rates of the whole-space solutions to their self-similar profile were investigated intensively in the literature. In [9], the relative free energy allowed the authors to prove the self-similar asymptotics in the $L^1(\mathbb{R}^d)$ norm. The results were improved in [26], showing optimal $L^p(\mathbb{R}^d)$ decay estimates. The asymptotic profile to drift-diffusion-Poisson equations with fractional diffusion was analyzed in [32,38].

Concerning drift-diffusion models for the spin-polarized electron transport, there are only few mathematical results. The stationary two-component drift-diffusion model (6)–(7) was analyzed in [22], while the transient equations were investigated in [21]. In particular, Glitzky proved in [21] the exponential decay to equilibrium. An existence analysis for a diffusion model for the spin accumulation with fixed electron current but non-constant magnetization was proved in [35] in one space dimension and in [19,20] for three space dimensions.

Also quantum spin diffusion models have been considered. For instance, in [40], the large-time asymptotics for a simple spin drift-diffusion system for quantum electron transport in graphene was studied. A more general quantum spin drift-diffusion model was derived in [5], with numerical experiments in [6]. Numerical simulations for diffusion models for the spin accumulation, coupled with the Landau–Lifshitz–Gilbert equation, can be found in [1,36]. For spin transport models in superlattices, we refer, for instance, to [10].

The existence of global weak solutions to the matrix spin drift-diffusion model (1)–(4) was shown in [25] with constant precession vector and in [39] with non-constant precession vector but assuming velocity saturation. Under the condition that the (thermal) equilibrium density is sufficiently small, the exponential decay to equilibrium was proved in [39]. An implicit Euler finite-volume scheme that preserves some of the features of the continuous model was analyzed in [11]. The numerical results of [11] indicate that the relative free energy is decaying with exponential rate, but no analytical proof was given.

In this paper, we prove that the solution $(N(t), V(t))$ to (1)–(4) converges exponentially fast to a steady state $(\frac{1}{2}n_\infty\sigma_0, V_\infty)$, solving the stationary spinless drift-diffusion-Poisson equations

$$\operatorname{div}(\nabla n_\infty + n_\infty \nabla V_\infty) = 0, \quad -\lambda^2 \Delta V_\infty = n_\infty - g(x) \quad \text{in } \Omega \quad (9)$$

$$n_\infty = n_D, \quad V = V_D \quad \text{on } \partial\Omega, \quad (10)$$

under the condition that the boundary data is close to the (thermal) equilibrium state, defined by $\log n_D + V_D = 0$ on $\partial\Omega$. Compared to [39], where $\|n_\infty\|_{L^\infty(\Omega)} \ll 1$ is needed, our smallness assumption is physically reasonable; see the discussion in the following subsection.

1.3. Main result and key ideas

Our main result is as follows.

Theorem 1 (*Exponential time decay*). *Let $T > 0$ and let $\Omega \subset \mathbb{R}^3$ be a bounded domain with $\partial\Omega \in C^{1,1}$. Furthermore, let $0 < m_* < 1$, $\lambda > 0$, $\gamma > 0$, $D > 0$, $0 \leq p < 1$, $q_0 > 3$, and $\vec{\mu} \in \mathbb{R}^3$ with $|\vec{\mu}| = 1$. The data satisfies $g \in L^\infty(\Omega)$, $g \geq 0$ in Ω , and*

$$\begin{aligned} n_D, V_D &\in W^{2,q_0}(\Omega), \quad n_D \geq m_* > 0 \text{ on } \partial\Omega, \\ n_0^0, \vec{n}^0 \cdot \vec{\mu} &\in L^\infty(\Omega), \quad \frac{1}{2}n_0^0 \pm \vec{n}^0 \cdot \vec{\mu} \geq \frac{m_*}{2} > 0. \end{aligned}$$

Let $\phi_D := \log n_D + V_D$. Then there exist $\kappa > 0$, $C_0 > 0$, and $\delta > 0$ such that if $\|\phi_D\|_{W^{2,q_0}(\Omega)} \leq \delta$,

$$\|n_\pm(t) - \frac{1}{2}n_\infty\|_{L^2(\Omega)} + \|V(t) - V_\infty\|_{H^1(\Omega)} \leq C_0 e^{-\kappa t}, \quad t > 0,$$

where n_\pm are solutions to (6)–(8) and (n_∞, V_∞) is the weak solution to (9)–(10). Furthermore, there exists $\tau_0 > 0$ such that if $0 < \tau \leq \tau_0$ then

$$\|N(t) - \frac{1}{2}n_\infty\sigma_0\|_{L^2(\Omega; \mathbb{C}^{2 \times 2})} \leq C_0^* e^{-\kappa^* t}, \quad t > 0,$$

and $C_0, C_0^* > 0$ depend on the initial relative free energy $H(0)$ (see (12) below).

The smallness condition on ϕ_D means that the system is close to equilibrium, as $\phi_D = 0$ characterizes the (thermal) equilibrium state. Since the stationary drift-diffusion equations (9) may possess multiple solutions if ϕ_D is large in a certain sense [2,30], the condition on ϕ_D is not surprising. The smallness condition on the relaxation time, however, seems to be purely technical. It is needed to estimate the drift part when we derive $L^2(\Omega)$ bounds for the perpendicular component of \vec{n} . If an entropy structure exists for the equation for \vec{n} , we expect that this condition can be avoided but currently, such a structure is not clear; see [25, Remarks 3.1–3.2]. If the initial spin-vector density is parallel to the precession vector, we are able to remove the smallness condition on τ ; see Remark 9. We show in Remark 10 that, independently of the initial spin-vector density, the smallness condition is satisfied in a certain physical regime.

The analysis of the asymptotic behavior of the solutions to the Van-Roosbroeck drift-diffusion system (5) and the two-component system (6)–(7) is based on the observation that the relative free energy, consisting of the internal and electric energies, is a Lyapunov functional along the solutions and that the energy dissipation can be bounded from below in terms of the relative free energy itself. The strong coupling of (1)–(2) prohibits this approach. Indeed, we showed in [25, Section 3] that the relative free energy associated to (1)–(2), consisting of the von Neumann energy and the electric energy, is nonincreasing in time only in very particular cases.

Our idea is the observation that the matrix system (1)–(2) can be reformulated as drift-diffusion-type equations in terms of certain projections of the density matrix relative to the precession vector. This idea was already used in [25] for the existence analysis. The reformulation removes the cross-diffusion terms, which allows us to apply the techniques of Gajewski and Gröger [18] used for the Van-Roosbroeck model. This idea only works if the precession vector $\vec{\mu}$ is constant. A non-constant vector $\vec{\mu}$ (solving the Landau–Lifshitz–Gilbert equation) was considered in [41], but this spin model is simplified and no large-time asymptotics was proved.

More precisely, we decompose the density matrix $N = \frac{1}{2}n_0\sigma_0 + \vec{n} \cdot \vec{\sigma}$ and $N^0 = \frac{1}{2}n_0^0\sigma_0 + \vec{n}^0 \cdot \vec{\sigma}$. Then the spin-up and spin-down densities $n_{\pm} = \frac{1}{2}n_0 \pm \vec{n} \cdot \vec{\mu}$ solve (6)–(8). The information on n_{\pm} is not sufficient to recover the density matrix. Therefore, we also consider the perpendicular component of \vec{n} with respect to $\vec{\mu}$, $\vec{n}_{\perp} = \vec{n} - (\vec{n} \cdot \vec{\mu})\vec{\mu}$, which solves

$$\partial_t \vec{n}_{\perp} - \operatorname{div} \left(\frac{D}{\eta} (\nabla \vec{n}_{\perp} + \vec{n}_{\perp} \nabla V) \right) - 2\gamma (\vec{n}_{\perp} \times \vec{\mu}) = -\frac{\vec{n}_{\perp}}{\tau}, \quad (11)$$

where $\eta = \sqrt{1 - p^2}$, with the boundary and initial conditions $\vec{n}_{\perp} = 0$ on $\partial\Omega$ and $\vec{n}_{\perp} = \vec{n}^0 - (\vec{n}^0 \cdot \vec{\mu})\vec{\mu}$. The density matrix can be reconstructed from $(n_+, n_-, \vec{n}_{\perp})$ by setting $n_0 = n_+ + n_-$ and $\vec{n} = \vec{n}_{\perp} + (\vec{n} \cdot \vec{\mu})\vec{\mu} = \vec{n}_{\perp} + \frac{1}{2}(n_+ - n_-)\vec{\mu}$.

A key element of the proof is the derivation of a uniform positive lower bound for n_{\pm} . This is shown by using the De Giorgi–Moser iteration method inspired by the proof of [18, Lemma 3.6]. More precisely, we choose the test functions $e^t w_{\pm}^{q-1}/n_{\pm}$ in (6) and (7), respectively, where $w_{\pm} = -\min\{0, \log n_{\pm} + m\}$ with $m > 0$, $q \in \mathbb{N}$, and pass to the limit $q \rightarrow \infty$, leading to $\|w_{\pm}(t)\|_{L^{\infty}(\Omega)} \leq K$ and consequently to the desired bound $w_{\pm}(t) \geq e^{-m-K}$ in Ω . Second, we calculate the time derivative of the free energy

$$H(t) = \int_{\Omega} \left(h(n_+|n_{\infty}) + h(n_-|n_{\infty}) + \frac{\lambda^2}{2} |\nabla(V - V_{\infty})|^2 \right) (t) dx, \quad (12)$$

where $h(n_{\pm}|n_{\infty}) = n_{\pm} \log(2n_{\pm}/n_{\infty}) - n_{\pm} + \frac{1}{2}n_{\infty}$, leading to the free energy inequality

$$\begin{aligned} \frac{dH}{dt} + C_1 \int_{\Omega} (n_+ |\nabla(\phi_+ - \phi_D)|^2 + n_- |\nabla(\phi_- - \phi_D)|^2) \\ \leq C_2 \|\nabla \phi_D\|_{L^{\infty}(\Omega)}^2 \int_{\Omega} ((n_+ - \frac{1}{2}n_{\infty})^2 + (n_- - \frac{1}{2}n_{\infty})^2) dx, \end{aligned} \quad (13)$$

where $\phi_{\pm} = \log n_{\pm} + V$ are the electrochemical potentials and $C_1 > 0$ and $C_2 > 0$ are some constants independent of the solution and independent of time. The right-hand side can be estimated, up to a factor, by the free energy H times $\|\nabla \phi_D\|_{L^{\infty}(\Omega)}^2$. Furthermore, using the time-uniform positive lower bound for n_{\pm} , the energy dissipation (the second term on the left-hand side of (13)) is bounded from below by H , up to a factor. Therefore, if $\|\nabla \phi_D\|_{L^{\infty}(\Omega)} \leq \delta$, (13) becomes, for some time-independent constants $C_3 > 0$ and $C_4 > 0$,

$$\frac{dH}{dt} + (C_3 - C_4\delta^2)H \leq 0.$$

Choosing $\delta^2 < C_3/C_4$, the Gronwall inequality implies the exponential decay with respect to the free energy and, as a consequence, in the $L^2(\Omega)$ norm of $n_{\pm} - n_{\infty}$ with rate $\kappa := C_3 - C_4\delta^2 > 0$.

Third, we prove the time decay of \bar{n}_{\perp} . Since we are not aware of an entropy structure for (11), we rely on $L^2(\Omega)$ estimates. This means that we use the test function \bar{n}_{\perp} in the weak formulation of (11) such that the term $(\bar{n}_{\perp} \times \bar{\mu}) \cdot \bar{n}_{\perp}$ vanishes. However, in order to handle the term coming from the doping concentration, we need a smallness condition on the relaxation time $\tau > 0$. Such a condition is not needed in the Van-Roosbroeck model.

The paper is organized as follows. The stationary equations are studied in Section 2. In Section 3, we prove the lower and upper uniform bounds for n_{\pm} , the entropy inequality, and some bounds for the free energy and energy dissipation. Theorem 1 is proved in Section 4. In the appendix, we prove a uniform L^{∞} bound for any function that satisfies an iterative inequality using the De Giorgi–Moser method.

2. The stationary equations

The existence of weak solutions to the stationary drift-diffusion problem

$$\operatorname{div}(\nabla n_{\infty} + n_{\infty} \nabla V_{\infty}) = 0, \quad -\lambda^2 \Delta V_{\infty} = n_{\infty} - g(x) \quad \text{in } \Omega, \quad (14)$$

$$n_{\infty} = n_D, \quad V_{\infty} = V_D \quad \text{on } \partial\Omega \quad (15)$$

with data satisfying the assumptions in Theorem 1 is well known; see [28, Theorem 3.2.1]. The solution satisfies $n_{\infty}, V_{\infty} \in H^1(\Omega) \cap L^{\infty}(\Omega)$ and

$$0 < m_{\infty} \leq n_{\infty} \leq M_{\infty} \quad \text{in } \Omega \quad (16)$$

for some $m_{\infty}, M_{\infty} > 0$. Note that we cannot expect uniqueness of weak solutions in general, since there are devices (thyristors) that allow for multiple physical stationary solutions. However, uniqueness can be expected for data sufficiently close to the (thermal) equilibrium state [2,31]. We call a solution to (14)–(15) a (thermal) equilibrium state if the electrochemical potential $\phi_{\infty} := \log n_{\infty} + V_{\infty}$ vanishes in Ω . This state needs the compatibility condition $\phi_D := \log n_D + V_D = 0$ on $\partial\Omega$.

The following lemma provides some a priori estimates for (n_{∞}, V_{∞}) and shows that the current density $J_{\infty} := n_{\infty} \nabla \phi_{\infty}$ is arbitrarily small in the $L^{\infty}(\Omega)$ norm if the boundary data is sufficiently close to the equilibrium state $\phi_D = 0$ in the $W^{2,q_0}(\Omega)$ sense.

Lemma 2 (*A priori estimates*). *Under the assumptions of Theorem 1, there exists a constant $C_{\infty} > 0$ independent of (n_{∞}, V_{∞}) such that*

$$\|\nabla \phi_{\infty}\|_{L^{\infty}(\Omega)} \leq C_{\infty} \|\phi_D\|_{W^{2,q_0}(\Omega)}.$$

Proof. Since $n_{\infty} - g(x) \in L^{\infty}(\Omega)$, elliptic regularity yields $V_{\infty} \in W^{2,q_0}(\Omega)$, and the $W^{2,q_0}(\Omega)$ norm of V_{∞} depends on M_{∞} , $\|V_D\|_{W^{2,q_0}(\Omega)}$, and $\|g\|_{L^{\infty}(\Omega)}$. Using the test function $n_{\infty} - n_D$ in the weak formulation of the first equation in (14), we find that

$$\begin{aligned} \int_{\Omega} |\nabla(n_{\infty} - n_D)|^2 dx &= - \int_{\Omega} \nabla n_D \cdot \nabla(n_{\infty} - n_D) dx - \int_{\Omega} n_{\infty} \nabla V_{\infty} \cdot \nabla(n_{\infty} - n_D) dx \\ &\leq (\|\nabla n_D\|_{L^2(\Omega)} + M_{\infty} \|\nabla V_{\infty}\|_{L^2(\Omega)}) \|\nabla(n_{\infty} - n_D)\|_{L^2(\Omega)}. \end{aligned}$$

This implies that

$$\begin{aligned}\|\nabla n_\infty\|_{L^2(\Omega)} &\leq 2\|\nabla n_D\|_{L^2(\Omega)} + M_\infty\|\nabla V_\infty\|_{L^2(\Omega)} \\ &\leq C(1 + \|\nabla n_D\|_{L^2(\Omega)} + \|\nabla V_D\|_{L^2(\Omega)}).\end{aligned}$$

Since $q_0 > 3$, we have $W^{2,q_0}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$. Thus, $b := \nabla V_\infty \in L^\infty(\Omega)$ and elliptic regularity for

$$\Delta n_\infty + b \cdot \nabla n_\infty = \lambda^{-2} n_\infty (n_\infty - g(x)) \in L^\infty(\Omega)$$

shows that $n_\infty \in W^{2,q_0}(\Omega)$ with an a priori bound depending on the norms $\|n_D\|_{W^{2,q_0}(\Omega)}$ and $\|n_\infty\|_{H^1(\Omega)}$. Summarizing,

$$\|n_\infty\|_{W^{2,q_0}(\Omega)} + \|V_\infty\|_{W^{2,q_0}(\Omega)} \leq C.$$

It holds that $W^{2,q_0}(\Omega) \hookrightarrow C^{0,\alpha}(\overline{\Omega})$ for all $0 < \alpha < 1$. Hence, $n_\infty \in C^{0,\alpha}(\overline{\Omega})$. The first equation in (14) can be formulated as

$$\operatorname{div}(n_\infty \nabla(\phi_\infty - \phi_D)) = -\operatorname{div}(n_\infty \nabla \phi_D) \in L^{q_0}(\Omega),$$

which shows that, by elliptic regularity again,

$$\|\phi_\infty - \phi_D\|_{W^{2,q_0}(\Omega)} \leq C(m_\infty, M_\infty)\|\phi_D\|_{W^{2,q_0}(\Omega)}$$

and, in view of the continuous embedding $W^{2,q_0}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$,

$$\|\nabla \phi_\infty\|_{L^\infty(\Omega)} \leq C\|\phi_\infty\|_{W^{2,q_0}(\Omega)} \leq C\|\phi_D\|_{W^{2,q_0}(\Omega)}.$$

This finishes the proof. \square

3. Uniform estimates

In this section, we prove some a priori estimates that are uniform in time. A uniform upper bound for n_\pm was already shown in [25, Theorem 1.1]. For the convenience of the reader, we present the proof.

Lemma 3 (*Uniform upper bound for n_\pm*). *Introduce*

$$M = \max \left\{ \frac{1}{2} \sup_{\partial\Omega} n_D, \sup_{\Omega} \left(\frac{1}{2} n_0^0 + |\vec{n}^0 \cdot \vec{\mu}| \right), \sup_{\Omega} g \right\}.$$

Then

$$n_\pm(t) \leq M \quad \text{in } \Omega, \quad t > 0.$$

Proof. We use the test functions $(n_+ - M)^+$ in (6) and $(n_- - M)^+$ in (7), where $z^+ = \max\{0, z\}$, and add both equations. Observing that $(n_\pm - M)^+ = 0$ on $\partial\Omega$ and $(n_\pm(0) - M)^+ = 0$ in Ω , we find after standard manipulations that

$$\begin{aligned}
& \frac{1}{2} \int_{\Omega} (|(n_+(t) - M)^+|^2 + |(n_-(t) - M)^+|^2) dx \\
& + \int_0^t \int_{\Omega} (D_+ |\nabla(n_+ - M)^+|^2 + D_- |\nabla(n_- - M)^+|^2) dx ds \\
& = -\frac{1}{2\tau} \int_0^t \int_{\Omega} (n_+ - n_-)((n_+ - M)^+ - (n_- - M)^+) dx ds \\
& - D_+ \int_0^t \int_{\Omega} (n_+ - M)^+ \nabla V \cdot \nabla(n_+ - M)^+ dx ds \\
& - D_- \int_0^t \int_{\Omega} (n_- - M)^+ \nabla V \cdot \nabla(n_- - M)^+ dx ds \\
& - D_+ M \int_0^t \int_{\Omega} \nabla V \cdot \nabla(n_+ - M)^+ dx ds - D_- M \int_0^t \int_{\Omega} \nabla V \cdot \nabla(n_- - M)^+ dx ds.
\end{aligned}$$

Since $z \mapsto (z - M)^+$ is monotone, the first integral on the right-hand side is nonnegative. Then, writing $(n_{\pm} - M) \nabla V \cdot \nabla(n_{\pm} - M)^+ = \nabla V \cdot \frac{1}{2} \nabla [(n_{\pm} - M)^+]^2$, integrating by parts, and using the Poisson equation leads to

$$\begin{aligned}
& \frac{1}{2} \int_{\Omega} (|(n_+(t) - M)^+|^2 + |(n_-(t) - M)^+|^2) dx \\
& + \int_0^t \int_{\Omega} (D_+ |\nabla(n_+ - M)^+|^2 + D_- |\nabla(n_- - M)^+|^2) dx ds \\
& \leq -\frac{D_+}{2\lambda^2} \int_0^t \int_{\Omega} |(n_+ - M)^+|^2 (n_+ + n_- - g(x)) dx ds \\
& - \frac{D_-}{2\lambda^2} \int_0^t \int_{\Omega} |(n_- - M)^+|^2 (n_+ + n_- - g(x)) dx ds \\
& - \frac{D_+ M}{\lambda^2} \int_0^t \int_{\Omega} (n_+ - M)^+ (n_+ + n_- - g(x)) dx ds \\
& - \frac{D_- M}{\lambda^2} \int_0^t \int_{\Omega} (n_- - M)^+ (n_+ + n_- - g(x)) dx ds.
\end{aligned}$$

As $M \geq \|g\|_{L^\infty(\Omega)}$ and we integrate only over $\{n_{\pm} > M\}$, we have $n_+ + n_- - g(x) \geq 0$ on this set. Therefore, all integrals on the right-hand side are nonnegative, and we conclude that

$$\frac{1}{2} \int_{\Omega} (|(n_+(t) - M)^+|^2 + |(n_-(t) - M)^+|^2) dx$$

$$+ \int_0^t \int_{\Omega} (D_+ |\nabla(n_+ - M)^+|^2 + D_- |\nabla(n_- - M)^+|^2) dx ds \leq 0.$$

This shows that $(n_{\pm}(t) - M)^+ = 0$ and hence $n_{\pm}(t) \leq M$ in Ω , $t > 0$. \square

Lemma 4 (Uniform positive lower bound for n_{\pm}). *There exists $m > 0$ such that for all $t > 0$,*

$$n_{\pm}(t) \geq m > 0 \quad \text{in } \Omega.$$

Proof. We show first that n_{\pm} is strictly positive with a lower bound that depends on time. For this, we use the test functions $(n_{\pm} - m^*(t))^- = \min\{0, n_{\pm} - m^*(t)\}$, where $m^*(t) = m_0 e^{-\mu t}$, $\mu = 2\lambda^{-2} D_- M$, and

$$m_0 = \min \left\{ \inf_{\partial\Omega} \frac{n_D}{2}, \inf_{\Omega} \left(\frac{1}{2} n_0^0 + \vec{n}^0 \cdot \vec{\mu} \right) \right\} > 0,$$

in (6), (7), respectively, and add both equations. Proceeding similarly as in the proof of Lemma 3, we obtain

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} ((n_+ - m^*)^-(t)^2 + (n_- - m^*)^-(t)^2) dx \\ & + D_+ \int_0^t \int_{\Omega} |\nabla(n_+ - m^*)^-|^2 dx ds + D_- \int_0^t \int_{\Omega} |\nabla(n_- - m^*)^-|^2 dx ds \\ & = -\frac{1}{2\tau} \int_0^t \int_{\Omega} (n_+ - n_-) ((n_+ - m^*)^- - (n_- - m^*)^-) dx ds \\ & - \frac{D_+}{2} \int_0^t \int_{\Omega} \nabla[(n_+ - m^*)^-]^2 \cdot \nabla V dx ds - \frac{D_-}{2} \int_0^t \int_{\Omega} \nabla[(n_- - m^*)^-]^2 \cdot \nabla V dx ds \\ & - D_+ \int_0^t m^*(s) \int_{\Omega} \nabla(n_+ - m^*)^- \cdot \nabla V dx ds \\ & - D_- \int_0^t m^*(s) \int_{\Omega} \nabla(n_- - m^*)^- \cdot \nabla V dx ds \\ & + \mu \int_0^t m^*(s) \int_{\Omega} ((n_+ - m^*)^- + (n_- - m^*)^-) dx ds. \end{aligned}$$

The first term on the right-hand side is nonpositive since $z \mapsto (z - m^*)^-$ is monotone. For the remaining terms, we use the Poisson equation and the estimate $n_0 = n_+ + n_- \leq 2M$:

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} ((n_+ - m^*)^-(t)^2 + (n_- - m^*)^-(t)^2) dx \\ & \leq -\frac{D_+}{2\lambda^2} \int_0^t \int_{\Omega} |(n_+ - m^*)^-|^2 (n_0 - g(x)) dx ds \end{aligned}$$

$$\begin{aligned}
& -\frac{D_-}{2\lambda^2} \int_0^t \int_{\Omega} |(n_- - m^*)^-|^2 (n_0 - g(x)) dx ds \\
& -\frac{D_+}{\lambda^2} \int_0^t m^*(s) \int_{\Omega} (n_+ - m^*)^- (n_0 - g(x)) dx ds \\
& -\frac{D_-}{\lambda^2} \int_0^t m^*(s) \int_{\Omega} (n_- - m^*)^- (n_0 - g(x)) dx ds \\
& + \mu \int_0^t m^*(s) \int_{\Omega} ((n_+ - m^*)^- + (n_- - m^*)^-) dx ds \\
& \leq \frac{D_-}{2\lambda^2} \|g\|_{L^\infty(\Omega)} \int_0^t \int_{\Omega} (|(n_+ - m^*)^-|^2 + |(n_- - m^*)^-|^2) dx ds \\
& -\frac{D_+}{\lambda^2} \int_0^t m^*(s) \int_{\Omega} (n_+ - m^*)^- \left(2M - \frac{\lambda^2}{D_+} \mu\right) dx ds \\
& -\frac{D_-}{\lambda^2} \int_0^t m^*(s) \int_{\Omega} (n_- - m^*)^- \left(2M - \frac{\lambda^2}{D_-} \mu\right) dx ds \\
& \leq \frac{D_-}{2\lambda^2} \|g\|_{L^\infty(\Omega)} \int_0^t \int_{\Omega} (|(n_+ - m^*)^-|^2 + |(n_- - m^*)^-|^2) dx ds.
\end{aligned}$$

In the last inequality, we used $2M - \lambda^2 D_{\pm}^{-1} \mu \leq 0$. By Gronwall's lemma, this shows that $n_{\pm} \geq m^*(t) > 0$ in Ω .

In the second step, we prove that n_{\pm} is strictly positive uniformly in time. The idea is to use the Di Giorgi–Moser iteration method similarly as in the proof of Lemma 3.6 in [18]. We set $w_{\pm} = -(\log n_{\pm} + m)^- \in L^2(0, T; H^1(\Omega))$ and take the test function $e^t w_{\pm}^{q-1}/n_{\pm}$ in (6), (7), respectively, where $0 < -\log(m_*/2) < m < 1$ and $q \in \mathbb{N}, q \geq 2$. Because of the previous step, which ensures that $n_{\pm} > 0$, this test function is well defined. Moreover, $\log(n_D/2) + m \geq \log(m_*/2) + m \geq 0$ and $\log(n_0^0/2 \pm \vec{n}^0 \cdot \vec{\mu}) + m \geq \log(m_*/2) + m \geq 0$ such that $w_{\pm} = 0$ on $\partial\Omega$ and $w_{\pm}(0) = 0$ in Ω . Formally, we compute $\partial_t(e^t w_{\pm}^q) - e^t w_{\pm}^q = -q e^t w_{\pm}^{q-1} n_{\pm}^{-1} \partial_t n_{\pm}$. Therefore, integrating this identity formally over Ω and $(0, t)$ and using (6)–(7),

$$\begin{aligned}
& \int_{\Omega} e^t (w_+^q(t) + w_-^q(t)) dx - \int_0^t \int_{\Omega} e^s (w_+^q + w_-^q) dx ds \\
& = -q \int_0^t e^s \left(\left\langle \partial_t n_+, \frac{w_+^{q-1}}{n_+} \right\rangle + \left\langle \partial_t n_-, \frac{w_-^{q-1}}{n_-} \right\rangle \right) ds \\
& = \frac{q}{2\tau} \int_0^t e^s \int_{\Omega} (n_+ - n_-) \left(\frac{w_+^{q-1}}{n_+} - \frac{w_-^{q-1}}{n_-} \right) dx ds \\
& \quad - D_+ q \int_0^t e^s \int_{\Omega} (\nabla n_+ + n_+ \nabla V) \cdot ((q-1)w_+^{q-2} + w_+^{q-1}) \frac{\nabla n_+}{n_+^2} dx ds
\end{aligned}$$

$$-D_-q \int_0^t e^s \int_{\Omega} (\nabla n_- + n_- \nabla V) \cdot ((q-1)w_-^{q-2} + w_-^{q-1}) \frac{\nabla n_-}{n_-^2} dx ds,$$

where $\langle \cdot, \cdot \rangle$ is the duality product of $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. The computation can be made rigorous by a density argument; see [23, (5.18)] for a similar statement. Since $z \mapsto (-\log z + m)^{-q-1}/z$ is nonincreasing for $z > 0$, the first term on the right-hand side is nonpositive, giving

$$\begin{aligned} & \int_{\Omega} e^t (w_+^q(t) + w_-^q(t)) dx - \int_0^t \int_{\Omega} e^s (w_+^q + w_-^q) dx ds \\ & \leq -D_+q \int_0^t e^s \int_{\Omega} ((q-1)w_+^{q-2} + w_+^{q-1}) (|\nabla w_+|^2 - \nabla V \cdot \nabla w_+) dx ds \\ & \quad - D_-q \int_0^t e^s \int_{\Omega} ((q-1)w_-^{q-2} + w_-^{q-1}) (|\nabla w_-|^2 - \nabla V \cdot \nabla w_-) dx ds. \end{aligned}$$

Taking into account the Poisson equation and the inequalities $D_+ \leq D_-$, $w_{\pm} \geq 0$, and $n_0 \leq 2M$, this becomes

$$\begin{aligned} & \int_{\Omega} e^t (w_+^q(t) + w_-^q(t)) dx - \int_0^t \int_{\Omega} e^s (w_+^q + w_-^q) dx ds \\ & \quad + \frac{4D_+(q-1)}{q} \int_0^t e^s \int_{\Omega} (|\nabla w_+^{q/2}|^2 + |\nabla w_-^{q/2}|^2) dx ds \\ & \quad + \frac{4D_+q}{(q+1)^2} \int_0^t e^s \int_{\Omega} (|\nabla w_+^{(q+1)/2}|^2 + |\nabla w_-^{(q+1)/2}|^2) dx ds \\ & \leq \frac{D_+q}{\lambda^2} \int_0^t e^s \int_{\Omega} \left(w_+^{q-1} + \frac{1}{q} w_+^q \right) (n_0 - g(x)) dx ds \\ & \quad + \frac{D_-q}{\lambda^2} \int_0^t e^s \int_{\Omega} \left(w_-^{q-1} + \frac{1}{q} w_-^q \right) (n_0 - g(x)) dx ds \\ & \leq \frac{2D_+M}{\lambda^2} \int_0^t e^s \int_{\Omega} (qw_+^{q-1} + w_+^q) dx ds + \frac{2D_-M}{\lambda^2} \int_0^t e^s \int_{\Omega} (qw_-^{q-1} + w_-^q) dx ds \\ & \leq \frac{2D_-Mq}{\lambda^2} \int_0^t e^s \int_{\Omega} (w_+^q + w_-^q) dx ds + \frac{4D_-M}{\lambda^2} \int_0^t e^s \int_{\Omega} dx ds. \end{aligned} \tag{17}$$

In the last inequality, we used Young's inequality: $qw_{\pm}^{q-1} \leq (q-1)w_{\pm}^q + 1$. We infer that

$$\int_{\Omega} e^t (w_+^q(t) + w_-^q(t)) dx + K_0 \int_0^t \int_{\Omega} e^s (|\nabla w_+^{q/2}|^2 + |\nabla w_-^{q/2}|^2) dx ds$$

$$\leq K_1 q \int_0^t \int_{\Omega} e^s (w_+^q + w_-^q) dx ds + K_2 e^t$$

for some constants $K_0, K_1, K_2 > 0$ which are independent of q and time.

Lemma 11 in the appendix shows that w_{\pm} is bounded in L^{∞} with a constant which depends on the $L^{\infty}(0, T; L^1(\Omega))$ norm of w_{\pm} . Therefore, it remains to estimate w_{\pm} in this norm. To this end, we take $q = 2$ in (17):

$$\begin{aligned} & \int_{\Omega} e^t (w_+^2(t) + w_-^2(t)) dx - \int_0^t e^s \int_{\Omega} (w_+^2 + w_-^2) dx ds \\ & + \frac{8}{9} D_+ \int_0^t e^s \int_{\Omega} (|\nabla w_+^{3/2}|^2 + |\nabla w_-^{3/2}|^2) dx ds \\ & \leq \frac{4D_- M}{\lambda^2} \int_0^t e^s \int_{\Omega} (w_+^2 + w_-^2) dx ds + \frac{4D_- M}{\lambda^2} \int_0^t e^s \int_{\Omega} dx ds. \end{aligned}$$

By the Poincaré inequality, for some constants $C_i > 0$, we obtain

$$\int_{\Omega} e^t (w_+^2(t) + w_-^2(t)) dx \leq \int_0^t e^s \int_{\Omega} (-C_1(w_+^3 + w_-^3) + C_2(w_+^2 + w_-^2)) dx ds + C_3 e^t.$$

Since $f(x) = -C_1 x^3 + C_2 x^2 = (-C_1 x + C_2)x^2$ has a maximum $\tilde{C}_4 > 0$ for $x \geq 0$, we can estimate the right-hand side by $e^t(\tilde{C}_4 \text{meas}(\Omega) + C_3)$. Division by e^t leads to

$$\int_{\Omega} (w_+^2(t) + w_-^2(t)) dx \leq C_4 := \tilde{C}_4 \text{meas}(\Omega) + C_3,$$

which does not depend on time. In particular, this shows that w_{\pm} is bounded in $L^{\infty}(0, T; L^1(\Omega))$ uniformly in time. Thus, by Lemma 11, $\|w_{\pm}(t)\|_{L^{\infty}(\Omega)} \leq K$ for some constant $K > 0$ and $n_{\pm}(t) \geq \exp(-K - m)$ in Ω , $t > 0$. This finishes the proof. \square

Remark 5. The factor e^t is necessary to derive time-uniform bounds. Indeed, without this factor, the last term on the right-hand side of (17) becomes $4D_- M \lambda^{-2} \int_0^t \int_{\Omega} ds dx$ which is unbounded as $t \rightarrow \infty$. \square

We introduce the relative free energy

$$H(t) = \int_{\Omega} \left(h(n_+ | n_{\infty}) + h(n_- | n_{\infty}) + \frac{\lambda^2}{2} |\nabla(V - V_{\infty})|^2 \right) (t) dx,$$

where $h(n_{\pm} | n_{\infty}) = n_{\pm} \log(2n_{\pm}/n_{\infty}) - n_{\pm} + \frac{1}{2}n_{\infty}$, and the electrochemical potentials $\phi_{\pm} = \log n_{\pm} + V$.

Lemma 6 (Relative free energy estimate). *It holds that*

$$\frac{dH}{dt} \leq -\frac{D_+}{2} \int_{\Omega} (n_+ |\nabla(\phi_+ - \phi_{\infty})|^2 + n_- |\nabla(\phi_- - \phi_{\infty})|^2) dx$$

$$\begin{aligned}
 & + \frac{D_-}{2} \int_{\Omega} ((n_+ - \tfrac{1}{2}n_{\infty})^2 + (n_- - \tfrac{1}{2}n_{\infty})^2) |\nabla \phi_{\infty}|^2 dx \\
 & - \frac{1}{8\tau} \int_{\Omega} (\sqrt{n_+} - \sqrt{n_-})^2 dx.
 \end{aligned}$$

Proof. Using the Poisson equation and the definitions $\phi_{\pm} = \log n_{\pm} + V$ and $\phi_{\infty} = \log n_{\infty} + V_{\infty}$, it follows that

$$\begin{aligned}
 \frac{dH}{dt} &= \left\langle \partial_t n_+, \log \frac{2n_+}{n_{\infty}} \right\rangle + \left\langle \partial_t n_-, \log \frac{2n_-}{n_{\infty}} \right\rangle - \lambda^2 \langle \partial_t \Delta(V - V_{\infty}), V - V_{\infty} \rangle \\
 &= \left\langle \partial_t n_+, \log \frac{n_+}{n_{\infty}} + \log 2 \right\rangle + \left\langle \partial_t n_-, \log \frac{n_-}{n_{\infty}} + \log 2 \right\rangle + \langle \partial_t (n_+ + n_-), V - V_{\infty} \rangle \\
 &= \langle \partial_t n_+, \phi_+ - \phi_{\infty} + \log 2 \rangle + \langle \partial_t n_-, \phi_- - \phi_{\infty} + \log 2 \rangle
 \end{aligned} \tag{18}$$

This can be made rigorous similarly as in [23, formula (5.18)], together with the techniques in [14, Theorem 3, p. 287].

Next, we subtract $\frac{1}{2}D_{\pm} \times (14)$ from (6) and (7), respectively:

$$\begin{aligned}
 \partial_t n_+ - D_+ \operatorname{div} (n_+ \nabla (\phi_+ - \phi_{\infty}) + (n_+ - \tfrac{1}{2}n_{\infty}) \nabla \phi_{\infty}) &= -\frac{1}{2\tau} (n_+ - n_-), \\
 \partial_t n_- - D_- \operatorname{div} (n_- \nabla (\phi_- - \phi_{\infty}) + (n_- - \tfrac{1}{2}n_{\infty}) \nabla \phi_{\infty}) &= -\frac{1}{2\tau} (n_- - n_+).
 \end{aligned}$$

Inserting these equations into (18), we find that

$$\begin{aligned}
 \frac{dH}{dt} &= -D_+ \int_{\Omega} n_+ |\nabla (\phi_+ - \phi_{\infty})|^2 dx - D_- \int_{\Omega} n_- |\nabla (\phi_- - \phi_{\infty})|^2 dx \\
 &\quad - D_+ \int_{\Omega} (n_+ - \tfrac{1}{2}n_{\infty}) \nabla \phi_{\infty} \cdot \nabla (\phi_+ - \phi_{\infty}) dx \\
 &\quad - D_- \int_{\Omega} (n_- - \tfrac{1}{2}n_{\infty}) \nabla \phi_{\infty} \cdot \nabla (\phi_- - \phi_{\infty}) dx \\
 &\quad - \frac{1}{2\tau} \int_{\Omega} (n_+ - n_-) (\log n_+ - \log n_-) dx.
 \end{aligned}$$

We use the elementary inequality

$$(y - z)(\log y - \log z) \geq \frac{1}{4} (\sqrt{y} - \sqrt{z})^2 \quad \text{for } y, z > 0 \tag{19}$$

to estimate the last term. Then the Young inequality and the lower bound $n_{\pm} \geq m$ lead to

$$\begin{aligned}
 \frac{dH}{dt} &\leq -\frac{D_+}{2} \int_{\Omega} n_+ |\nabla (\phi_+ - \phi_{\infty})|^2 dx - \frac{D_-}{2} \int_{\Omega} n_- |\nabla (\phi_- - \phi_{\infty})|^2 dx \\
 &\quad + \frac{D_+}{2m} \int_{\Omega} (n_+ - \tfrac{1}{2}n_{\infty})^2 |\nabla \phi_{\infty}|^2 dx + \frac{D_-}{2m} \int_{\Omega} (n_- - \tfrac{1}{2}n_{\infty})^2 |\nabla \phi_{\infty}|^2 dx \\
 &\quad - \frac{1}{8\tau} \int_{\Omega} (\sqrt{n_+} - \sqrt{n_-})^2 dx,
 \end{aligned}$$

finishing the proof. \square

Lemma 7 (Lower bound for the chemical potentials). *It holds that*

$$\begin{aligned} & \|\nabla(\phi_+ - \phi_\infty)\|_{L^2(\Omega)}^2 + \|\nabla(\phi_- - \phi_\infty)\|_{L^2(\Omega)}^2 \\ & \geq C(\|n_+ - \tfrac{1}{2}n_\infty\|_{L^2(\Omega)}^2 + \|n_- - \tfrac{1}{2}n_\infty\|_{L^2(\Omega)}^2 + \|\nabla(V - V_\infty)\|_{L^2(\Omega)}^2), \end{aligned}$$

where $C > 0$ depends only on M , M_∞ , λ , and Ω .

Recall that M is the upper bound for n_\pm (see Lemma 3) and M_∞ is the upper bound for n_∞ (see (16)).

Proof. It holds that $\phi_\pm - \phi_\infty + \log 2 = 0$ on $\partial\Omega$. Thus, the Young and Poincaré inequalities yield for any $\varepsilon > 0$,

$$\begin{aligned} \int_{\Omega} (n_\pm - \tfrac{1}{2}n_\infty)(\phi_\pm - \phi_\infty + \log 2) dx & \leq \varepsilon \|n_\pm - \tfrac{1}{2}n_\infty\|_{L^2(\Omega)}^2 + C(\varepsilon) \|\phi_\pm - \phi_\infty + \log 2\|_{L^2(\Omega)}^2 \\ & \leq \varepsilon \|n_\pm - \tfrac{1}{2}n_\infty\|_{L^2(\Omega)}^2 + C(\varepsilon, \Omega) \|\nabla(\phi_\pm - \phi_\infty)\|_{L^2(\Omega)}^2. \end{aligned} \quad (20)$$

Inserting the definitions of ϕ_\pm and ϕ_∞ , taking into account the Poisson equation $-\lambda^2 \Delta(V - V_\infty) = n_0 - n_\infty$ and inequality (19), and finally using the bounds $m \leq n_\pm \leq M$ and $m_\infty \leq n_\infty \leq M_\infty$, we obtain

$$\begin{aligned} & \int_{\Omega} (n_+ - \tfrac{1}{2}n_\infty)(\phi_+ - \phi_\infty + \log 2) dx + \int_{\Omega} (n_- - \tfrac{1}{2}n_\infty)(\phi_- - \phi_\infty + \log 2) dx \\ & = \int_{\Omega} (n_+ - \tfrac{1}{2}n_\infty)(\log n_+ - \log(\tfrac{1}{2}n_\infty)) dx + \int_{\Omega} (n_- - \tfrac{1}{2}n_\infty)(\log n_- - \log(\tfrac{1}{2}n_\infty)) dx \\ & \quad + \int_{\Omega} (n_0 - n_\infty)(V - V_\infty) dx \\ & \geq \frac{1}{4} \int_{\Omega} \left(\sqrt{n_+} - \sqrt{\tfrac{1}{2}n_\infty} \right)^2 dx + \frac{1}{4} \int_{\Omega} \left(\sqrt{n_-} - \sqrt{\tfrac{1}{2}n_\infty} \right)^2 dx + \lambda^2 \int_{\Omega} |\nabla(V - V_\infty)|^2 dx \\ & = \frac{1}{4} \int_{\Omega} \frac{(n_+ - n_\infty/2)^2}{(\sqrt{n_+} + \sqrt{n_\infty/2})^2} dx + \frac{1}{4} \int_{\Omega} \frac{(n_- - n_\infty/2)^2}{(\sqrt{n_-} + \sqrt{n_\infty/2})^2} dx + \lambda^2 \int_{\Omega} |\nabla(V - V_\infty)|^2 dx \\ & \geq C_2 \int_{\Omega} (n_+ - \tfrac{1}{2}n_\infty)^2 dx + C_2 \int_{\Omega} (n_- - \tfrac{1}{2}n_\infty)^2 dx + \lambda^2 \int_{\Omega} |\nabla(V - V_\infty)|^2 dx, \end{aligned}$$

where $C_2 = \frac{1}{4}(\sqrt{M} + \sqrt{M_\infty/2})^{-2}$. Combining this estimate with (20) and taking $\varepsilon < C_1$, we conclude the proof. \square

Lemma 8 (Bounds for the relative free energy). *There exist constants C_ϕ , $C_H > 0$ independent of the solution and time such that*

$$\begin{aligned} H & \leq C_\phi (\|\nabla(\phi_+ - \phi_\infty)\|_{L^2(\Omega)}^2 + \|\nabla(\phi_- - \phi_\infty)\|_{L^2(\Omega)}^2), \\ H & \geq C_H (\|n_+ - \tfrac{1}{2}n_\infty\|_{L^2(\Omega)}^2 + \|n_- - \tfrac{1}{2}n_\infty\|_{L^2(\Omega)}^2). \end{aligned}$$

Proof. Set $f(y) = y \log(y/z) - y + z$ for some fixed $z > 0$. A Taylor expansion shows that

$$y \log \frac{y}{z} - y + z = f(y) = f(z) + f'(z)(y - z) + \frac{1}{2} f''(\xi)(y - z)^2 = \frac{(y - z)^2}{2\xi},$$

where ξ is between y and z . Consequently, since $n_{\pm} \geq m$ and $n_{\infty} \geq m_{\infty}$,

$$n_{\pm} \log \frac{2n_{\pm}}{n_{\infty}} - n_{\pm} + \frac{1}{2} n_{\infty} \leq \frac{1}{2C_1} (n_{\pm} - \frac{1}{2} n_{\infty})^2,$$

where $C_1 = \min\{m, m_{\infty}/2\}$, and, using Lemma 7, we find that

$$\begin{aligned} H &\leq \max \left\{ \frac{1}{2C_1}, \frac{\lambda^2}{2} \right\} (\|n_+ - \frac{1}{2} n_{\infty}\|_{L^2(\Omega)}^2 + \|n_- - \frac{1}{2} n_{\infty}\|_{L^2(\Omega)}^2 + \|\nabla(V - V_{\infty})\|_{L^2(\Omega)}^2) \\ &\leq \max \left\{ \frac{1}{2C_1}, \frac{\lambda^2}{2} \right\} C (\|\nabla(\phi_+ - \phi_{\infty})\|_{L^2(\Omega)}^2 + \|\nabla(\phi_- - \phi_{\infty})\|_{L^2(\Omega)}^2). \end{aligned}$$

For the second estimate, we use

$$n_{\pm} \log \frac{2n_{\pm}}{n_{\infty}} - n_{\pm} + \frac{1}{2} n_{\infty} \geq \frac{(n_{\pm} - \frac{1}{2} n_{\infty})^2}{2C_2}, \quad \text{where } 2C_2 = \max\{M, M_{\infty}/2\},$$

to conclude that

$$H \geq \frac{1}{2C_2} \int_{\Omega} ((n_+ - \frac{1}{2} n_{\infty})^2 + (n_- - \frac{1}{2} n_{\infty})^2) dx.$$

This finishes the proof. \square

4. Proof of Theorem 1

The starting point is the free-energy inequality in Lemma 6. We need to estimate the integral containing $\nabla \phi_{\infty}$. In view of Lemmas 2 and 8,

$$\begin{aligned} \int_{\Omega} (n_{\pm} - \frac{1}{2} n_{\infty})^2 |\nabla \phi_{\infty}|^2 dx &\leq \|\nabla \phi_{\infty}\|_{L^{\infty}(\Omega)}^2 \|n_{\pm} - \frac{1}{2} n_{\infty}\|_{L^2(\Omega)}^2 \\ &\leq C_{\infty}^2 \|\phi_D\|_{W^{2,q_0}(\Omega)}^2 \|n_{\pm} - \frac{1}{2} n_{\infty}\|_{L^2(\Omega)}^2 \leq C_{\infty}^2 C_H^{-1} \|\phi_D\|_{W^{2,q_0}(\Omega)}^2 H. \end{aligned} \quad (21)$$

By the lower bound of n_{\pm} and Lemma 7, the free-energy inequality in Lemma 6 becomes

$$\frac{dH}{dt} + \left(\frac{D_+ m}{2C_{\phi}} - \frac{D_- C_{\infty}^2}{C_H} \|\phi_D\|_{W^{2,q_0}(\Omega)}^2 \right) H + \frac{1}{8\tau} \|\sqrt{n_+} - \sqrt{n_-}\|_{L^2(\Omega)}^2 \leq 0.$$

Let $\delta > 0$ satisfy $2\kappa := D_+ m/(2C_{\phi}) - D_- (C_{\infty}^2/C_H) \delta^2 > 0$ and choose n_D and V_D such that $\|\phi_D\|_{W^{2,q_0}(\Omega)} \leq \delta$. Then Gronwall's lemma implies that $H(t) \leq H(0) \exp(-2\kappa t)$ for $t > 0$. By Lemma 8,

$$\|n_+(t) - \frac{1}{2} n_{\infty}\|_{L^2(\Omega)} + \|n_-(t) - \frac{1}{2} n_{\infty}\|_{L^2(\Omega)} \leq C_H^{-1/2} H(0)^{1/2} e^{-\kappa t}, \quad t > 0.$$

The $H^1(\Omega)$ elliptic estimate for the Poisson problem $-\lambda^2 \Delta(V - V_{\infty}) = (n_+ - \frac{1}{2} n_{\infty}) + (n_- - \frac{1}{2} n_{\infty})$ in Ω , $V - V_{\infty} = 0$ on $\partial\Omega$ gives

$$\|V(t) - V_\infty\|_{H^1(\Omega)} \leq C\|n_+(t) - \frac{1}{2}n_\infty\|_{L^2(\Omega)} + C\|n_-(t) - \frac{1}{2}n_\infty\|_{L^2(\Omega)} \leq Ce^{-\kappa t},$$

which proves the first estimate. For the second result, recall that we can decompose $N(t)$ as $N(t) = \frac{1}{2}(n_+ + n_-)\sigma_0 + (\vec{n}_\perp + \frac{1}{2}(n_+ - n_-)\vec{\mu}) \cdot \vec{\sigma}$. We use \vec{n}_\perp as a test function in (11):

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\Omega} |\vec{n}_\perp|^2 dx + \frac{D}{\eta} \int_{\Omega} |\nabla \vec{n}_\perp|^2 dx + \frac{1}{\tau} \int_{\Omega} |\vec{n}_\perp|^2 dx \\ &= -\frac{D}{2\eta} \int_{\Omega} \nabla |\vec{n}_\perp|^2 \cdot \nabla V dx = -\frac{D}{2\eta\lambda^2} \int_{\Omega} |\vec{n}_\perp|^2 (n_0 - g(x)) dx \\ &\leq \frac{D}{2\eta\lambda^2} \|g\|_{L^\infty(\Omega)} \int_{\Omega} |\vec{n}_\perp|^2 dx. \end{aligned}$$

Thus, if $\tau \leq 2\eta\lambda^2/(D\|g\|_{L^\infty(\Omega)})$, the Poincaré inequality shows that

$$\frac{d}{dt} \int_{\Omega} |\vec{n}_\perp|^2 dx + 2C(D, \eta, \Omega) \int_{\Omega} |\vec{n}_\perp|^2 dx \leq 0.$$

By Gronwall's lemma,

$$\|\vec{n}_\perp(t)\|_{L^2(\Omega)} \leq \|\vec{n}_\perp(0)\|_{L^2(\Omega)} e^{-C(D, \eta, \Omega)t}, \quad t > 0.$$

Therefore, we find that

$$\begin{aligned} \|N(t) - \frac{1}{2}n_\infty\sigma_0\|_{L^2(\Omega; \mathbb{C}^{2 \times 2})} &\leq \|(\frac{1}{2}(n_+ - \frac{1}{2}n_\infty) + \frac{1}{2}(n_- - \frac{1}{2}n_\infty))\sigma_0\|_{L^2(\Omega; \mathbb{C}^{2 \times 2})} \\ &\quad + \|\vec{n}_\perp + \frac{1}{2}(n_+ - n_-)\vec{\mu}\|_{L^2(\Omega; \mathbb{C}^{2 \times 2})} \\ &\leq C_H^{-1/2} H(0)^{1/2} e^{-\kappa t} + \|\vec{n}_\perp(0)\|_{L^2(\Omega)} e^{-C(D, \eta, \Omega)t} \leq C_0^* e^{-\kappa^* t}, \end{aligned}$$

where $C_0^* = \max(2C_H^{-1/2} H(0)^{1/2}, \|\vec{n}_\perp(0)\|_{L^2(\Omega)})$ and $\kappa^* = \min(\kappa, C(D, \eta, \Omega)t)$. This concludes the proof of Theorem 1.

Remark 9 (*Special initial spin-vector density*). Let $\vec{\mu} = (0, 0, 1)^\top$ and $\vec{n}^0 = (0, 0, n_3^0)$. Then the components n_1 and n_2 of the spin-vector density satisfy the equation

$$\partial_t n_i = \operatorname{div} \left(\frac{D}{\eta^2} (\nabla n_i + n_i \nabla V) \right), \quad i = 1, 2,$$

with boundary conditions $n_i = 0$ on $\partial\Omega$ and initial conditions $n_i(0) = 0$ in Ω . The unique solution is given by $n_i(t) = 0$ for all $t > 0$ and $i = 1, 2$. Since $\vec{n} = \vec{n}_\perp + (\vec{n} \cdot \vec{\mu})\vec{\mu} = \vec{n}_\perp + n_3\vec{\mu}$, the perpendicular component vanishes, $\vec{n}_\perp(t) = 0$. We conclude that the dynamics of the system is completely determined by n_\pm , and the proof of Theorem 1 gives the exponential decay without any condition on τ . In particular, the density matrix $N(t) = \frac{1}{2}(n_+ + n_-)\sigma_0 + \frac{1}{2}(n_+ - n_-)\sigma_3$ converges exponentially fast towards $\frac{1}{2}n_\infty\sigma_0$ as $t \rightarrow \infty$. \square

Remark 10 (*Smallness condition on the relaxation time*). We discuss the physical relevance of the smallness condition of the scaled relaxation time $\tau \leq 2\eta\lambda^2/(D\|g\|_{L^\infty(\Omega)})$. In scaled variables, we may assume that $D = 1$ and $\|g\|_{L^\infty(\Omega)} = 1$. The scaled Debye length is given by $\lambda^2 = \varepsilon_s U_T / (qL^2 g^*) = 2.7 \cdot 10^{-1}$, where the physical parameters are explained in Table 1. We have assumed that the semiconductor material is lowly

Table 1
Physical parameters.

Parameter	Physical meaning	Numerical value
q	elementary charge	$1.6 \cdot 10^{-19}$ As
ε_s	permittivity constant	10^{-12} As/(Vcm)
μ_0	(low field) mobility constant	$1.5 \cdot 10^3$ cm ² /(Vs)
U_T	thermal voltage at $T = 50$ K	$4.3 \cdot 10^{-3}$ V
g^*	maximal doping concentration	10^{15} /cm ³
τ_0	spin-flip relaxation time	10^{-12} s
L	length of the device	10^{-5} cm

doped. The scaled relaxation time is $\tau = \tau_0/t^*$, where the typical time is defined by $t^* = L^2/(\mu_0 U_T) = 1.5 \cdot 10^{-11}$ s. The spin-flip relaxation time is assumed to be $\tau_0 = 1$ ps. This value is realistic in GaAs quantum wells at temperature $T = 50$ K; see [7, Figure 1]. It follows that $\tau = 6 \cdot 10^{-2}$. Thus, the inequality $\tau \leq 2\eta\lambda^2/(D\|g\|_{L^\infty(\Omega)})$ is satisfied if $\eta \geq 0.11$ or $p \leq 0.99$. This covers almost the full range of $p \in [0, 1)$. \square

Appendix A. A boundedness result

The following lemma is an extension of a result due to Kowalczyk [27], based on an iteration technique [3]. It slightly generalizes [25, Lemma A.1]. Although the result should be known to experts, we present a proof for completeness.

Lemma 11 (*Boundedness from iteration*). *Let $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) be a bounded domain and let $w_i^{q/2} \in L^2(0, T; H^1(\Omega)) \cap C^0([0, T]; L^2(\Omega))$ for all $q \in \mathbb{N}$ with $q \geq 2$ with $w_i \geq 0$, $w_i = 0$ on $\partial\Omega$, and $w_i(0) = 0$ in Ω for $i = 1, \dots, n$. Assume that there are constants $K_0, K_1, K_2 > 0$ and $\alpha, \beta \geq 0$ such that for all $q \geq 2$, $t > 0$,*

$$\begin{aligned} & \int_{\Omega} e^t \sum_{i=1}^n w_i(t)^q dx + K_0 \int_0^t \int_{\Omega} e^s \sum_{i=1}^n |\nabla w_i^{q/2}|^2 dx ds \\ & \leq K_1 q^\alpha \int_0^t \int_{\Omega} e^s \sum_{i=1}^n w_i^q dx ds + K_2 q^\beta e^t. \end{aligned} \quad (22)$$

Then

$$w_i(t) \leq K = K_3 \left(\sum_{i=1}^n \|w_i\|_{L^\infty(0, \infty; L^1(\Omega))} + 1 \right) \quad \text{in } \Omega, \quad t > 0,$$

where K_3 depends only on $\alpha, \beta, d, \Omega, K_0, K_1$, and K_2 .

Proof. We apply the Gagliardo–Nirenberg inequality [42, p. 1034] with $\theta = d/(d+2) < 1$ and the Poincaré inequality to deal with the integral over w_i^q on the right-hand side of (22):

$$\begin{aligned} \int_{\Omega} w_i^q dx &= \|w_i^{q/2}\|_{L^2(\Omega)}^2 \leq C_1 \|\nabla w_i^{q/2}\|_{L^2(\Omega)}^{2\theta} \|w_i^{q/2}\|_{L^1(\Omega)}^{2(1-\theta)} \\ &\leq \varepsilon \|\nabla w_i^{q/2}\|_{L^2(\Omega)}^2 + C_1^{1+d/2} \varepsilon^{-d/2} \|w_i^{q/2}\|_{L^1(\Omega)}^2 \end{aligned}$$

for any $\varepsilon > 0$. Choosing $\varepsilon = K_0/(2q^\alpha K_1)$, which is equivalent to $K_1 q^\alpha \varepsilon = K_0/2$, (22) becomes

$$\begin{aligned} & \int_{\Omega} e^t \sum_{i=1}^n w_i(t)^q dx + \frac{K_0}{2} \int_0^t \int_{\Omega} e^s \sum_{i=1}^n |\nabla w_i^{q/2}|^2 dx ds \\ & \leq C_2 q^{\alpha(1+d/2)} \int_0^t e^s \sum_{i=1}^n \|w_i\|_{L^{q/2}(\Omega)}^q ds + K_2 q^{\beta} e^t, \end{aligned}$$

where C_2 depends on d , K_0 , and K_1 . We obtain

$$\sum_{i=1}^n \|w_i(t)\|_{L^q(\Omega)}^q \leq C_2 q^{\alpha(1+d/2)} \int_0^t e^{-(t-s)} \sum_{i=1}^n \|w_i(s)\|_{L^{q/2}(\Omega)}^q ds + K_2 q^{\beta}$$

and, taking the supremum over time,

$$\begin{aligned} \sup_{0 < s < t} \sum_{i=1}^n \|w_i(s)\|_{L^q(\Omega)}^q & \leq C_2 q^{\alpha(1+d/2)} (1 - e^{-t}) \sup_{0 < s < t} \sum_{i=1}^n \|w_i(s)\|_{L^{q/2}(\Omega)}^q + K_2 q^{\beta} \\ & \leq C_2 q^{\alpha(1+d/2)} \sup_{0 < s < t} \sum_{i=1}^n \|w_i(s)\|_{L^{q/2}(\Omega)}^q + K_2 q^{\beta}. \end{aligned}$$

We choose $q = 2^k$ for $k \geq 0$ and set $b_k = \sum_{i=1}^n \|w_i\|_{L^{\infty}(0,T;L^{2^k}(\Omega))}^{2^k} + 1$. Then

$$\begin{aligned} b_k & \leq C_2 2^{\alpha(1+d/2)k} \sum_{i=1}^n \|w_i\|_{L^{\infty}(0,T;L^{2^{k-1}}(\Omega))}^{2^k} + (K_2 + 1) 2^{\beta k} \\ & \leq \max \{C_2 2^{\alpha(1+d/2)}, (K_2 + 1)^{1/k} 2^{\beta}\}^k \left(\sum_{i=1}^n \|w_i\|_{L^{\infty}(0,T;L^{2^{k-1}}(\Omega))}^{2^k} + 1 \right) \\ & \leq \max \{C_2 2^{\alpha(1+d/2)}, (K_2 + 1) 2^{\beta}\}^k \left(\sum_{i=1}^n \|w_i\|_{L^{\infty}(0,T;L^{2^{k-1}}(\Omega))}^{2^{k-1}} + 1 \right)^2 \\ & = \gamma^k b_{k-1}^2, \end{aligned}$$

where

$$\gamma = \max \{C_2 2^{\alpha(1+d/2)}, (K_2 + 1) 2^{\beta}\}.$$

To solve this recursion, we set $c_k = \gamma^{k+2} b_k$. Then

$$c_k \leq \gamma^{2(k+1)} b_{k-1}^2 = (\gamma^{k+1} b_{k-1})^2 = c_{k-1}^2,$$

which gives $c_k \leq c_0^{2^k} \leq \gamma^{2^{k+1}} b_0^{2^k}$. Consequently, $b_k = \gamma^{-k-2} c_k \leq \gamma^{2^{k+1}-k-2} b_0^{2^k}$ and, after taking the 2^k th root,

$$\|w_i\|_{L^{\infty}(0,T;L^{2^k}(\Omega))} \leq b_k^{2^{-k}} \leq \gamma^{2^{-2-k}(k+2)} \left(\sum_{i=1}^n \|w_i\|_{L^{\infty}(0,T;L^1(\Omega))} + 1 \right).$$

The limit $k \rightarrow \infty$ concludes the proof. \square

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