

CHARGE TRANSPORT SYSTEMS WITH FERMI–DIRAC STATISTICS FOR MEMRISTORS

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ABSTRACT. An instationary drift–diffusion system for the electron, hole, and oxygen vacancy densities, coupled to the Poisson equation for the electric potential, is analyzed in a bounded domain with mixed Dirichlet–Neumann boundary conditions. The electron and hole densities are governed by Fermi–Dirac statistics, while the oxygen vacancy density is governed by Blakemore statistics. The equations model the charge carrier dynamics in memristive devices used in semiconductor technology. The global existence of weak solutions is proved in up to three space dimensions. The proof is based on the free energy inequality, an iteration argument to improve the integrability of the densities, and estimations of the Fermi–Dirac integral. Under a physically realistic elliptic regularity condition, it is proved that the densities are bounded.

1. INTRODUCTION

Memristors are nonlinear resistors with memory able to exhibit a resistive switching behavior. In neuromorphic computing, they are used to build artificial neurons and synapses [18]. Also perovskite solar cells may show a memristive behavior, emulating synaptic- and neural-like dynamics [26]. In semiconductor technology, often oxide-based memristors are used. They consist of a thin titanium dioxide layer between two metal electrodes [23]. Charge carriers are the electrons, holes (defect electrons), and oxide vacancies which allow for a modulation of the layer conductance.

Generally, the relation between the electron density and its chemical potential (quasi-Fermi potential) is given by Fermi–Dirac statistics. In low-density regimes, this reduces to Maxwell–Boltzmann statistics, leading to particle fluxes with linear diffusion [21], while in high-density regimes, Fermi–Dirac statistics reduce to a power-law density–chemical potential relation, leading to fluxes with degenerate diffusion. A mathematical analysis of the associated low-density drift–diffusion equations was performed in [19], while high-density models were studied in [22]. In this paper, we investigate for the first time a

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general drift-diffusion system with Fermi–Dirac statistics for the electrons and holes as well as physically motivated Blakemore statistics for the oxide vacancies.

1.1. Model equations. The charge transport through the semiconductor device is supposed to be governed by the mass balance equations for the electron density $n(x, t)$, hole density $p(x, t)$, and density $D(x, t)$ of oxide vacancies, and the gradients of the associated chemical potentials (quasi-Fermi potentials) μ_n , μ_p , and μ_D are the driving forces of the flow. This leads to the (scaled) equations

$$\begin{aligned}\partial_t n - \operatorname{div} J_n &= 0, & J_n &= n \nabla \mu_n, \\ \partial_t p + \operatorname{div} J_p &= 0, & J_p &= -p \nabla \mu_p, \\ \partial_t D + \operatorname{div} J_D &= 0, & J_D &= -D \nabla \mu_D,\end{aligned}$$

where J_n , J_p , and J_D are the electron, hole, and oxide vacancy current densities, respectively. Fermi–Dirac statistics is valid for electrons in the conduction band and for holes in the valence band in the parabolic band approximation [21, Sec. 1.6], giving the relations

$$n = \mathcal{F}_{1/2}(\mu_n + V), \quad p = \mathcal{F}_{1/2}(\mu_p - V),$$

where V denotes the electric potential, and the Fermi–Dirac integral is defined by

$$\mathcal{F}_{1/2}(y) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{s}}{1 + e^{s-y}} ds, \quad y \in \mathbb{R}.$$

In the Maxwell–Boltzmann approximation, the Fermi–Dirac integral can be approximated by the exponential, $\mathcal{F}_{1/2}(y) \approx \exp(y)$ for $y \ll -1$, leading to the electron flux $J_n \approx n \nabla(\log n - V) = \nabla n - n \nabla V$. However, the use of Fermi–Dirac statistics is more appropriate in regimes with moderate or high densities. We expect that the oxide vacancies cannot be accumulated excessively such that it is reasonable to use Blakemore statistics [4],

$$D = \mathcal{F}_{-1}(\mu_D - V), \quad \text{where } \mathcal{F}_{-1}(y) = \frac{1}{1 + e^{-y}}, \quad y \in \mathbb{R}.$$

Although being itself an approximation of Fermi–Dirac statistics, Blackmore statistics have the advantage of restricting the oxide vacancy density to the interval $(0, 1)$. Without loss of generality, we have set the upper bound equal to one.

Introducing the inverse functions

$$\begin{aligned}g(z) &= \mathcal{F}_{1/2}^{-1}(z) \quad \text{for } z \in (0, \infty), \\ h(z) &= \mathcal{F}_{-1}^{-1}(z) = \log z - \log(1 - z) \quad \text{for } z \in (0, 1),\end{aligned}$$

the transport equations can be written in a drift–diffusion form as

$$\begin{aligned}(1) \quad & \partial_t n - \operatorname{div} J_n = 0, & J_n &= n \nabla g(n) - n \nabla V, \\ (2) \quad & \partial_t p + \operatorname{div} J_p = 0, & J_p &= -(p \nabla g(p) + p \nabla V), \\ (3) \quad & \partial_t D + \operatorname{div} J_D = 0, & J_D &= -(D \nabla h(D) + D \nabla V) \quad \text{in } \Omega, \quad t > 0,\end{aligned}$$

where $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) is a bounded domain. The electric potential is selfconsistently coupled to the charge densities by the Poisson equation

$$(4) \quad \lambda^2 \Delta V = n - p - D + A(x) \quad \text{in } \Omega,$$

where $\lambda > 0$ is the (scaled) Debye length and $A(x)$ is the given dopant acceptor density. Following [25], we neglect recombination–generation effects. Equations (1)–(4) are supplemented with the initial and mixed Dirichlet–Neumann boundary conditions

$$(5) \quad n(0, \cdot) = n^I, \quad p(0, \cdot) = p^I, \quad D(0, \cdot) = D^I \quad \text{in } \Omega,$$

$$(6) \quad n = \bar{n}, \quad p = \bar{p}, \quad V = \bar{V} \quad \text{on } \Gamma_D, t > 0,$$

$$(7) \quad J_n \cdot \nu = J_p \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N, t > 0,$$

$$(8) \quad J_D \cdot \nu = 0 \quad \text{on } \partial\Omega, t > 0.$$

Here, Γ_D is the union of Ohmic contacts and Γ_N models the insulating boundary parts. Since the oxide vacancies are supposed not to leave the domain, we impose no-flux boundary conditions for D on the whole boundary. These boundary conditions are usually used in the literature [15, 25].

The aim of this paper is to prove (i) the existence of global weak solutions (n, p, D, V) to (1)–(8) and (ii) the regularity $n, p, D \in L^\infty(0, T; L^\infty(\Omega))$ for any $T > 0$.

1.2. Mathematical difficulties. The misfit of the boundary conditions for (n, p) on the one hand and for D on the other hand gives the first main mathematical difficulty. A second difficulty comes from the fact that we consider three species instead of two charge carriers as done in many papers [10, 14, 20]. Indeed, the two-species case allows one to exploit a monotonicity property of the drift term such that the quadratic nonlinearity can be handled [10]. For more than two species, one may use Gagliardo–Nirenberg estimates, but this is possible in two space dimensions only [13]. This issue can be overcome by $W_{\text{loc}}^{1,r}(\Omega)$ estimates with $r > 1$ [19], but leading to very weak solutions and boundedness of solutions in two space dimensions only. The third difficulty are the nonlinearities from the Fermi–Dirac statistics, which complicates the estimates. We prove in Appendix A that

$$(9) \quad g'(z) \sim z^{-1} 1_{\{z \leq \mathcal{F}_{1/2}(0)\}} + z^{-1/3} 1_{\{z > \mathcal{F}_{1/2}(0)\}} \quad \text{for } z > 0,$$

where $A \sim B$ means that there exist constants $C_1, C_2 > 0$ such that $C_1 A \leq B \leq C_2 A$. In particular, the nonlinear diffusion $n \nabla g(n) = n g'(n) \nabla n$ can be approximated by ∇n in the low-density regime and by $(3/5) \nabla n^{5/3}$ in the high-density regime. On the other hand, the Blakemore statistics gives to the diffusion $D \nabla h(D) = -\nabla \log(1 - D)$, which exhibits a singularity at $D = 1$. The technical issues associated to this singularity are overcome by using some ideas from [6], developed for a one-species model.

1.3. State of the art and key ideas. There are only a few works dealing with the drift–diffusion equations for more than two species. General existence results for an n -species model have been proved in [17] for an abstract drift operator satisfying smoothing conditions. In [7, 12, 13, 14], the existence of global weak solutions was shown in at most two space dimensions. The three-dimensional case was investigated in [5] using Robin

boundary conditions for the electric potential. In the work [3], the function $n\nabla g(n) = \nabla(n + \eta n^q)$ with $\eta > 0$ and $q \geq 4$ was chosen to regularize the diffusion term, which allows for an analysis in three space dimensions. The paper [11] studies the drift–diffusion equations with Fermi–Dirac statistics but assuming inhomogeneous Neumann boundary conditions on $\partial\Omega$. A drift–diffusion system with Fermi–Dirac statistics for electrons and holes and with Blakemore statistics for the ionic vacancy carriers, modeling perovskite solar cells, was analyzed recently in [2] in two space dimensions. A free energy inequality for this model in three space dimensions was shown in [1].

Our analysis is based, as in [1, 11], on estimates derived from the free energy inequality. The asymptotic behavior of the Fermi–Dirac integral $\mathcal{F}_{1/2}$ allows for an argument similar to [3] but based on physical bounds. Indeed, the behavior (9) shows that the diffusion is given by

$$n\nabla g(n) \sim n(n^{-1} + n^{-1/3})\nabla n = \nabla\left(n + \frac{3}{5}n^{5/3}\right).$$

The first term corresponds to linear diffusion, while the second term allows for higher integrability estimates. As a by-product, we are able to weaken the condition $q \geq 4$ in [3] to $q \geq 5/3$. (By [22], one may weaken this condition even to $q > 6/5$.)

To specify the free energy inequality, we introduce the anti-derivatives of g and h ,

$$(10) \quad G(s) = \int_{\mathcal{F}_{1/2}(0)}^s g(z)dz, \quad H(s) = \int_{\mathcal{F}_{-1}(0)}^s h(z)dz,$$

the relative energy density

$$\mathcal{G}(s|\bar{s}) = G(s) - G(\bar{s}) - G'(\bar{s})(s - \bar{s}), \quad s, \bar{s} \geq 0,$$

and the free energy

$$E(n, p, D, V) = \int_{\Omega} \left(\mathcal{G}(n|\bar{n}) + \mathcal{G}(p|\bar{p}) + H(D) + D\bar{V} + \frac{\lambda^2}{2} |\nabla(V - \bar{V})|^2 \right) dx.$$

A formal computation, made rigorous in Theorem 1, shows that

$$(11) \quad \frac{dE}{dt}(n, p, D, V) + \frac{1}{2} \int_{\Omega} (n|\nabla(g(n) - V)|^2 + p|\nabla(g(p) + V)|^2 + D|\nabla(h(D) + V)|^2) dx \leq C(\bar{n}, \bar{p}, \bar{D}, T).$$

This yields a priori estimates for n, p in $L^\infty(0, T; L^{5/3}(\Omega))$ and for V in $L^\infty(0, T; H^1(\Omega))$. Moreover, defining \tilde{g} by $\tilde{g}'(n) = \sqrt{n}g'(n)$,

$$|\nabla\tilde{g}(n)| \leq |\nabla\tilde{g}(n) - \sqrt{n}\nabla V| + \sqrt{n}|\nabla V| = \sqrt{n}|\nabla(g(n) - V)| + \sqrt{n}|\nabla V|$$

is uniformly bounded in $L^2(0, T; L^{5/4}(\Omega))$. Unfortunately, this regularity is *not* sufficient to define $n\nabla g(n) = \sqrt{n}\nabla\tilde{g}(n)$ since \sqrt{n} is bounded in $L^\infty(0, T; L^{10/3}(\Omega))$ and $3/10 + 4/5 > 1$. However, we are able to improve the regularity by an iteration argument to $\nabla\tilde{g}(n) \in L^2(0, T; L^r(\Omega))$ with $r < 8/5$ (see Lemma 11), which is sufficient since $3/10 + 5/8 < 1$.

The treatment of the diffusion $D\nabla h(D) = -\nabla \log(1 - D)$ is quite delicate because of the singularity at $D = 1$. The idea is to approximate $L(D) = -\log(1 - D)$ by regular functions

L_k with $k \in \mathbb{N}$. The identification of the limit of the sequence $L_k(D_k)$ of approximating solutions D_k which converge strongly to some function D is then achieved by a monotonicity argument (Minty trick); see Lemma 16. These ideas allow us to prove the existence of global weak solutions.

The second main result is the boundedness of weak solutions. The difficulty comes from the estimate of the quadratic drift terms, which can be overcome in the case of two species by a monotonicity argument. For more than two species, we use the Gagliardo–Nirenberg inequality to estimate this term, similarly as in [12] for two space dimensions. In three dimensions, we need as in [22] the elliptic regularity result $V \in W^{1,r}(\Omega)$ with $r > 3$. This is possible even under mixed boundary conditions if Γ_D and Γ_N do not meet in a “too wild” manner [9, Theorem 4.8]. Then, applying an Alikakos-type iteration argument similar to [19, 22], we obtain q -uniform estimates in $L^\infty(0, T; L^q(\Omega))$ for any $q < \infty$. The boundedness follows after performing the limit $q \rightarrow \infty$.

1.4. Main results. First, we introduce some notation. We set $\Omega_T = \Omega \times (0, T)$ for $T > 0$, denote by $m(B)$ the measure of a set $B \subset \mathbb{R}^d$, and set for $1 \leq q \leq \infty$,

$$W_D^{1,q}(\Omega) = \{u \in W^{1,q}(\Omega) : u = 0 \text{ on } \Gamma_D\}, \quad H_D^1(\Omega) = W_D^{1,2}(\Omega).$$

The function $V^I \in H_D^1(\Omega) + \bar{V}$ is the unique solution to

$$\lambda^2 \Delta V^I = n^I - p^I - D^I + A(x) \text{ in } \Omega, \quad V^I = \bar{V} \text{ on } \Gamma_D, \quad \nabla V^I \cdot \nu = 0 \text{ on } \Gamma_N.$$

Constants $C > 0$ are generic and may change their value from line to line.

We impose the following assumptions.

- (A1) Domain: $\Omega \subset \mathbb{R}^d$ ($1 \leq d \leq 3$) is a bounded domain with Lipschitz boundary, $\partial\Omega = \Gamma_D \cup \Gamma_N$, $\Gamma_D \cap \Gamma_N = \emptyset$, $m(\Gamma_D) > 0$, and Γ_N is relatively open in $\partial\Omega$.
- (A2) Data: $T > 0$, $\lambda > 0$, $A \in L^\infty(\Omega)$.
- (A3) Boundary data: $\bar{n}, \bar{p}, \bar{V} \in W^{1,\infty}(\Omega)$ with $\bar{n}, \bar{p} > 0$ in Ω .
- (A4) Initial data: $n^I, p^I, D^I \in L^2(\Omega)$ satisfy $n^I, p^I, D^I \geq 0$ in Ω , $E(n^I, p^I, D^I, V^I) < \infty$. Furthermore, $\sup_\Omega D^I \leq 1$ and

$$D_\Omega^I := \frac{1}{m(\Omega)} \int_\Omega D^I dx < 1.$$

- (A5) Elliptic Regularity: There exists $r > 3$ such that for some constant $C > 0$ and all $f \in L^{3r/(r+3)}(\Omega)$ the weak solution V to the Poisson problem

$$(12) \quad \Delta V = f \text{ in } \Omega, \quad V = \bar{V} \text{ on } \Gamma_D, \quad \nabla V \cdot \nu = 0 \text{ on } \Gamma_N,$$

satisfies the estimate

$$(13) \quad \|V\|_{W^{1,r}(\Omega)} \leq C \|f\|_{L^{3r/(r+3)}(\Omega)} + C.$$

Let us discuss the assumptions. We can assume higher space dimensions in most of the estimates, but we restrict ourselves to $d \leq 3$ because of the applications. The boundary data in Assumption (A3) is assumed to be independent of time to simplify the computations; time-dependent boundary data are possible, see, e.g., [8, Sec. 2]. Compared to [2], we do not need pointwise positive lower bounds of the densities and we can allow for

vacuum as well as saturation of the oxygen vacancy density. We only prevent $D_\Omega^I = 1$ in Assumption (A4), which would be physically unrealistic.

The most restrictive condition is Assumption (A5). Indeed, we can only expect the regularity $V \in W^{1,r}(\Omega)$ with $r > 2$ for the solution V to (12) with mixed boundary conditions [16]. Shamir's counterexample [24] shows that $r < 4$ is generally necessary, even for smooth domains and data. The regularity $r > 3$ can be achieved under reasonable conditions on Γ_D and Γ_N [9, Theorem 4.8]. These conditions are satisfied if Γ_D and Γ_N intersect with an "angle" not larger than π [9, Prop. 3.4]. Assumption (A5) is *not* needed for the existence result but for the proof of the boundedness of solutions.

Our first main result is the existence of global weak solutions.

Theorem 1 (Global existence). *Let Assumptions (A1)–(A4) hold. Then there exists a weak solution (n, p, D, V) to (1)–(8) satisfying $n, p \geq 0$, $0 \leq D < 1$ a.e. in Ω_T ,*

$$n, p \in L^\infty(0, T; L^{5/3}(\Omega)) \cap L^2(0, T; W^{1,\alpha}(\Omega)), \quad D \in L^\infty(\Omega_T) \cap L^2(0, T; H^1(\Omega)),$$

$$n \nabla g(n), p \nabla g(p) \in L^2(0, T; L^{5/4}(\Omega)), \quad D \nabla h(D) \in L^2(0, T; L^2(\Omega)),$$

$$\partial_t n, \partial_t p \in L^{7/5}(0, T; W_D^{1,2\alpha/(4-\alpha)}(\Omega)), \quad \partial_t D \in L^2(0, T; H^1(\Omega)'), \quad V \in L^\infty(0, T; H^1(\Omega)),$$

where $\alpha < 8/5$ if $d = 3$, $\alpha < 2$ if $d = 2$, and $\alpha = 2$ if $d = 1$. The fluxes are understood in the sense

$$J_n = n \nabla(g(n) - V) \in L^2(0, T; L^{5/4}(\Omega)),$$

$$J_p = -p \nabla(g(p) + pV) \in L^2(0, T; L^{5/4}(\Omega)),$$

$$J_D = -D \nabla(h(D) + V) = -\nabla \log(1 - D) + D \nabla V \in L^2(\Omega_T).$$

The solution satisfies the free energy inequality

$$(14) \quad E(n, p, D, V)(t) + \frac{1}{2} \int_0^t \int_\Omega (n |\nabla(g(n) - V)|^2 + p |\nabla(g(p) + V)|^2 + D |\nabla(h(D) + V)|^2) dx ds \leq C(E^I, \Lambda, T),$$

where $E^I := E(n^I, p^I, D^I, V^I)$,

$$\Lambda := 2(\|\nabla(g(\bar{n}) - \bar{V})\|_{L^\infty(\Omega)}^2 + \|\nabla(g(\bar{p}) + \bar{V})\|_{L^\infty(\Omega)}^2),$$

and it holds that $C(E^I, \Lambda, T) = 0$ if $\Lambda = 0$.

The property $\Lambda = 0$ means that the boundary data is in thermal equilibrium. In this situation, the free energy is a Lyapunov functional. For the proof of Theorem 1, we first approximate the problem by truncating the nonlinearities (densities) in the diffusion and drift terms and prove the existence of approximate solutions by using the Leray–Schauder fixed-point theorem. The compactness of the fixed-point operator is a consequence of the approximate free energy inequality. From this inequality, we derive uniform bounds for the approximate solutions, allowing us to take the re-regularizing limit. As mentioned before, the main difficulties are the derivation of improved estimates via an iteration argument and the treatment of the singularity $D = 1$.

Our second main result is the boundedness of weak solutions.

Theorem 2 (Boundedness). *Let Assumptions (A1)–(A5) hold and assume that $n^I, p^I, D^I \in L^\infty(\Omega)$. Then the weak solution constructed in Theorem 1 satisfies*

$$n, p, D \in L^\infty(\Omega_T), \quad V \in L^\infty(0, T; W^{1,r}(\Omega)) \subset L^\infty(\Omega_T),$$

where $r > 3$ is given in Assumption (A5).

The restriction to three space dimensions comes from regularity (13). The boundedness result is not surprising in view of [22, Theorem 2]. Indeed, since $ng'(n) \sim 1 + n^{2/3}$, the diffusion term contains the porous-medium term $\nabla n^{5/3}$, and it is proved in [22] that this nonlinear diffusion leads to an improvement of the integrability of the densities up to $L^\infty(\Omega)$. The idea is first to prove that $n, p \in L^\infty(0, T; L^2(\Omega))$. This is used as the starting point of a recursion showing that $n, p \in L^\infty(0, T; L^q(\Omega))$ for any $q < \infty$, but with bounds that may depend on q . This allows us to use $n^q - \bar{n}^q, p^q - \bar{p}^q$ as test functions in the weak formulations to (1), (2), respectively. By an Alikakos iteration, it turns out that the $L^\infty(0, T; L^q(\Omega))$ bounds are independent of q , and we can pass to the limit $q \rightarrow \infty$ to conclude. To reduce the technicalities and since the first parts of the proof are technically similar to [22, Sec. 3], we detail only the last part of the proof (the Alikakos argument).

Remark 3 (Generalization). Our results hold for an arbitrary number of charged particles, since we use the Poisson equation only through the norm estimates for V and ∇V . In particular, we can consider the transport equations

$$\begin{aligned} \partial_t u_i &= \operatorname{div}(u_i \nabla g(u_i) + z_i u_i \nabla V), \quad i \in I, \\ \partial_t u_i &= \operatorname{div}(u_i \nabla h(u_i) + z_i u_i \nabla V), \quad i \in I_0, \\ \lambda^2 \Delta V &= - \sum_{i \in I \cup I_0} z_i u_i + A(x) \quad \text{in } \Omega, \quad t > 0, \end{aligned}$$

where $z_i \in \mathbb{R}$ are the particle charges, $I, I_0 \subset \mathbb{N}$ are some index sets, and the initial and boundary conditions are as in (5)–(8). \square

The paper is organized as follows. Theorem 1 and 2 are proved in Sections 2 and 3, respectively. Auxiliary inequalities involving Fermi–Dirac integrals are proved in Appendix A. We also need a nonlinear version of the Poincaré–Wirtinger inequality, which is shown in Appendix B.

2. PROOF OF THEOREM 1

We prove the existence of global weak solutions to (1)–(8). To this end, we truncate the coefficients in the parabolic equations with parameter $k \in \mathbb{N}$, solve the corresponding approximate problem, derive uniform estimates from an approximate free energy inequality, and pass to the limit $k \rightarrow \infty$.

2.1. Approximate problem. We introduce for $k \in \mathbb{N}$ and $z \in \mathbb{R}$ the truncations $T_k(z) = \max\{0, \min\{k, z\}\}$ and

$$S_k^1(z) = \begin{cases} 1 & \text{for } z \leq 0, \\ zg'(z) & \text{for } 0 < z \leq k, \\ k^{2/3}z^{1/3}g'(z) & \text{for } z > k, \end{cases} \quad S_k^2(z) = \begin{cases} 1 & \text{for } z \leq 0, \\ zh'(z) & \text{for } 0 < z \leq k/(k+1), \\ 1+k & \text{for } z > k/(k+1). \end{cases}$$

The functions S_k^1 and S_k^2 are continuous, bounded, and strictly positive on \mathbb{R} noting that $zh'(z) = 1/(1-z)$ for $z \in (0, 1)$. The approximate problem reads as follows:

$$\begin{aligned} (15) \quad & \partial_t n_k = \operatorname{div} (S_k^1(n_k) \nabla n_k - T_k(n_k) \nabla V_k), \\ (16) \quad & \partial_t p_k = \operatorname{div} (S_k^1(p_k) \nabla p_k + T_k(p_k) \nabla V_k), \\ (17) \quad & \partial_t D_k = \operatorname{div} (S_k^2(D_k) \nabla D_k + T_{k/(k+1)}(D_k) \nabla V_k), \\ (18) \quad & \lambda^2 \Delta V_k = n_k - p_k - D_k + A(x) \quad \text{in } \Omega, \quad t > 0, \end{aligned}$$

with the initial and boundary conditions (5)–(8), where (n, p, D, V) is replaced by (n_k, p_k, D_k, V_k) . Clearly, if $k \rightarrow \infty$, we recover formulation (1)–(3). The truncation $T_{k/(k+1)}(D_k)$ is chosen since we expect that the limit D of D_k satisfies $D < 1$ a.e.

We show the existence of solutions to (15)–(18) by using a fixed-point argument. For this, let $(n^*, p^*, D^*) \in L^2(\Omega_T)^3$ and $\sigma \in [0, 1]$. We apply [27, Theorem 23.A] to infer that the linearized problem

$$\begin{aligned} (19) \quad & \partial_t n = \operatorname{div} (S_k^1(n^*) \nabla n - \sigma T_k(n^*) \nabla V), \\ (20) \quad & \partial_t p = \operatorname{div} (S_k^1(p^*) \nabla p + \sigma T_k(p^*) \nabla V), \\ (21) \quad & \partial_t D = \operatorname{div} (S_k^2(D^*) \nabla D + \sigma T_{k/(k+1)}(D^*) \nabla V), \\ (22) \quad & \lambda^2 \Delta V = n^* - p^* - D^* + \sigma A(x) \quad \text{in } \Omega, \quad t > 0, \end{aligned}$$

with the initial and boundary conditions

$$\begin{aligned} n(0, \cdot) &= \sigma n^I, \quad p(0, \cdot) = \sigma p^I, \quad D(0, \cdot) = \sigma D^I \quad \text{in } \Omega, \\ n &= \sigma \bar{n}, \quad p = \sigma \bar{p}, \quad V = \sigma \bar{V} \quad \text{on } \Gamma_D, \quad t > 0, \\ \nabla n \cdot \nu &= \nabla p \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N, \quad t > 0, \\ (S_k^2(D^*) \nabla D + \sigma T_{k/(k+1)}(D^*) \nabla V) \cdot \nu &= 0 \quad \text{on } \partial\Omega, \quad t > 0, \end{aligned}$$

has a unique solution $(n, p, D, V) \in L^2(0, T; H^1(\Omega))^4$ such that $n, p, D \in H^1(0, T; H_D^1(\Omega)')$. This defines the fixed-point operator $F : L^2(\Omega)^3 \times [0, 1] \rightarrow L^2(\Omega_T)^3$, $(n^*, p^*, D^*; \sigma) \mapsto (n, p, D)$. Standard arguments show that F is continuous and satisfies $F(n^*, p^*, D^*; 0) = (0, 0, 0)$. To apply the Leray–Schauder fixed-point theorem, we need to find a uniform bound for all fixed points of $F(\cdot, \cdot, \cdot; \sigma)$.

Lemma 4. *Let (n, p, D) be a fixed point of $F(\cdot, \cdot, \cdot; \sigma)$, where $\sigma \in [0, 1]$. Then (n, p, D) is bounded in $L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$ uniformly in σ .*

Proof. Since the proof is similar to that one of [19, Lemma 2.1], we only sketch it. Let $(n^*, p^*, D^*) = (n, p, D)$ be a fixed point of $F(\cdot, \cdot, \cdot; \sigma)$. We use the test function $V - \sigma\bar{V}$ in the weak formulation of (22) and apply the Young and Poincaré inequality to find that

$$\int_0^T \int_{\Omega} |\nabla V|^2 dxdt \leq C + C \int_0^T \int_{\Omega} (n^2 + p^2 + D^2) dxdt,$$

where $C > 0$ is a constant independent of (n, p, D, σ) . Next, we use the test function $n - \sigma\bar{n}$ in the weak formulation of (19) and take into account that $S_k^1(n) \geq c(k) > 0$ and $S_k^2(n) \geq 1$. Then, with the Young inequality,

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} (n(t) - \sigma\bar{n})^2 dx - \frac{1}{2} \int_{\Omega} (n^I - \sigma\bar{n})^2 dx + \int_0^t \int_{\Omega} |\nabla n|^2 dxds \\ & \leq C + C(k) \int_0^t \int_{\Omega} |\nabla V|^2 dxds \leq C + C \int_0^t \int_{\Omega} (n^2 + p^2 + D^2) dxds. \end{aligned}$$

We derive similar estimates when using $p - \sigma\bar{p}$ and D in the weak formulations of (20) and (21), respectively. Adding these estimates yields

$$\begin{aligned} & \int_{\Omega} (n(t)^2 + p(t)^2 + D(t)^2) dx + \int_0^t \int_{\Omega} (|\nabla n|^2 + |\nabla p|^2 + |\nabla D|^2) dxds \\ & \leq C + C \int_0^t \int_{\Omega} (n^2 + p^2 + D^2) dxds. \end{aligned}$$

We deduce from Gronwall's lemma σ -uniform bounds for (n, p, D) in $L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$. \square

The bounds in Lemma 4 imply uniform estimates for $(\partial_t n, \partial_t p, \partial_t D)$ in $L^2(0, T; H_D^1(\Omega)')$. By the Aubin–Lions lemma, the embedding $L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H_D^1(\Omega)') \hookrightarrow L^2(\Omega_T)$ is compact. Thus, $F : L^2(\Omega_T)^3 \times [0, 1] \rightarrow L^2(\Omega_T)^3$ is compact. The assumptions of the Leray–Schauder fixed-point theorem are satisfied, and we conclude the existence of a fixed point of $F(\cdot, \cdot, \cdot; 1)$, i.e. a solution to (15)–(18) and (5)–(8). We summarize:

Lemma 5 (Existence for the approximate problem). *Let Assumptions (A1)–(A4) hold. Then there exists a weak solution to (15)–(18) with initial and boundary conditions (5)–(8).*

The solution (n_k, p_k, D_k) to (15)–(18) is componentwise nonnegative. Indeed, using the test function $n_k^- = \min\{0, n_k\}$ in the weak formulation of (15), we have

$$\frac{1}{2} \int_{\Omega} (n_k^-)(t)^2 dx + \int_0^t \int_{\Omega} S_k^1(n_k) |\nabla n_k^-|^2 dxds = \int_0^t \int_{\{n_k < 0\}} T_k(n_k) \nabla V_k \cdot \nabla n_k dxds = 0,$$

since $T_k(n_k) = 0$ for $n_k < 0$, showing that $n_k^-(t) = 0$ and consequently $n_k(t) \geq 0$ for $t > 0$. We note that the mass of the oxide vacancies is conserved,

$$\int_{\Omega} D_k(t) dx = \int_{\Omega} D^I dx \quad \text{for } t > 0,$$

while this is generally not the case for the electron and hole densities because of the Dirichlet boundary conditions.

2.2. Approximate energy inequality. We derive the discrete analog of the free energy inequality (11). Similarly as in [19, Sec. 2.3], we define for $0 < \delta < \mathcal{F}_{1/2}(0)$ the approximations

$$(23) \quad \begin{aligned} G_{k,\delta}(s) &= \int_{\mathcal{F}_{1/2}(0)}^s \int_{\mathcal{F}_{1/2}(0)}^y \frac{S_k^1(z)}{T_k(z) + \delta} dz dy, & \tilde{g}_{k,\delta}(s) &= \int_0^s \frac{S_k^1(y)}{\sqrt{T_k(y) + \delta}} dy, \\ H_{k,\delta}(s) &= \int_{\mathcal{F}_{-1}(0)}^s \int_{\mathcal{F}_{-1}(0)}^y \frac{S_k^2(z)}{T_{k/(k+1)}(z) + \delta} dz dy, & \tilde{h}_{k,\delta}(s) &= \int_0^s \frac{S_k^2(y)}{\sqrt{T_{k/(k+1)}(y) + \delta}} dy. \end{aligned}$$

Recalling that $S_k^1(z) \rightarrow z g'(z)$, $S_k^2(z) \rightarrow z h'(z)$, and $T_k(z) \rightarrow z$ pointwise as $k \rightarrow \infty$, the functions $G_{k,\delta}$ and $H_{k,\delta}$ approximate the anti-derivatives of g and h , respectively (see (10)), while $\tilde{g}_{k,\delta}$ and $\tilde{h}_{k,\delta}$ approximate

$$\begin{aligned} \tilde{g}(s) &:= \int_{\mathcal{F}_{1/2}(0)}^s \sqrt{z} g'(z) dz, \\ \tilde{h}(s) &:= \int_{\mathcal{F}_{-1}(0)}^s \sqrt{z} h'(z) dz = 2 \tanh^{-1}(\sqrt{s}) - 2 \tanh^{-1}(1/\sqrt{2}), \end{aligned}$$

respectively, since $\mathcal{F}_{-1}(0) = 1/2$. These definitions yield the following chain rules:

$$(24) \quad \begin{aligned} S_k^1(n_k) \nabla n_k &= \sqrt{T_k(n_k) + \delta} \nabla \tilde{g}_{k,\delta}(n_k), \\ S_k^2(D_k) \nabla D_k &= \sqrt{T_{k/(k+1)}(D_k) + \delta} \nabla \tilde{h}_{k,\delta}(D_k), \end{aligned}$$

and similarly for p_k instead of n_k . They are the truncated analogs of the chain rules $n_k g'(n_k) \nabla n_k = \sqrt{n_k} \nabla \tilde{g}(n_k)$ and $D_k h'(D_k) \nabla D_k = \sqrt{D_k} \nabla \tilde{h}(D_k)$. Choosing $\delta = 0$ in (24), we see that the approximate fluxes can be formulated as

$$(25) \quad \begin{aligned} S_k^1(n_k) \nabla n_k - T_k(n_k) \nabla V_k &= \sqrt{T_k(n_k)} (\nabla \tilde{g}_k(n_k) - \sqrt{T_k(n_k)} \nabla V_k), \\ S_k^1(p_k) \nabla p_k + T_k(p_k) \nabla V_k &= \sqrt{T_k(p_k)} (\nabla \tilde{g}_k(p_k) + \sqrt{T_k(p_k)} \nabla V_k), \\ S_k^2(D_k) \nabla D_k + T_k(D_k) \nabla V_k &= \sqrt{T_k(D_k)} (\nabla \tilde{h}_k(D_k) + \sqrt{T_k(D_k)} \nabla V_k). \end{aligned}$$

Next, we define for $s, \bar{s} \geq 0$ the approximate relative energies

$$(26) \quad \mathcal{G}_{k,\delta}(s|\bar{s}) = G_{k,\delta}(s) - G_{k,\delta}(\bar{s}) - G'_{k,\delta}(\bar{s})(s - \bar{s}), \quad \mathcal{H}_{k,\delta}(s) = H_{k,\delta}(s) + s\bar{V}$$

and the approximate free energy

$$(27) \quad E_{k,\delta}(n_k, p_k, D_k, V_k) = \int_{\Omega} \left(\mathcal{G}_{k,\delta}(n_k|\bar{n}) + \mathcal{G}_{k,\delta}(p_k|\bar{p}) + \mathcal{H}_{k,\delta}(D_k) + \frac{\lambda^2}{2} |\nabla(V - \bar{V})|^2 \right) dx.$$

We set

$$(28) \quad E_{k,\delta}^I := E_{k,\delta}(n^I, p^I, D^I, V^I),$$

$$(29) \quad \Lambda_{k,\delta} := 2 \|\nabla(G'_{k,\delta}(\bar{n}) - \bar{V})\|_{L^\infty(\Omega)}^2 + 2 \|\nabla(G'_{k,\delta}(\bar{p}) + \bar{V})\|_{L^\infty(\Omega)}^2.$$

For the derivation of the approximate free energy inequality, we need the following lemma.

Lemma 6. *There exists a constant $C > 0$ such that for any $k, \delta > 0$ satisfying $0 < \delta < \mathcal{F}_{1/2}(0) < k$,*

$$T_k(s)^{5/3} \leq C(1 + G_{k,\delta}(s)) \quad \text{for } s > 0.$$

Proof. Let $0 < s \leq \mathcal{F}_{1/2}(0)$. Since $s < k$, we have $T_k(s)^{5/3} = s^{5/3} \leq \mathcal{F}_{1/2}(0)^{5/3} \leq C$. Next, let $\mathcal{F}_{1/2}(0) < s \leq k$. Then $S_k^1(s) = sg(s)$ and, by Lemma 20,

$$\begin{aligned} G_{k,\delta}(s) &= \int_{\mathcal{F}_{1/2}(0)}^s \int_{\mathcal{F}_{1/2}(0)}^y \frac{zg'(z)}{z + \delta} dz dy \geq C \int_{\mathcal{F}_{1/2}(0)}^s \int_{\mathcal{F}_{1/2}(0)}^y \frac{z(z^{-1} + z^{-1/3})}{z + \delta} dz dy \\ &\geq \frac{C}{2} \int_{\mathcal{F}_{1/2}(0)}^s \int_{\mathcal{F}_{1/2}(0)}^y z^{-1/3} dz dy, \end{aligned}$$

since $\delta < \mathcal{F}_{1/2}(0) \leq z$. An integration of the right-hand side leads to

$$G_{k,\delta}(s) \geq \frac{3C}{4} \left(\frac{3}{5} s^{5/3} - \mathcal{F}_{1/2}(0)^{2/3} s + \frac{2}{5} \mathcal{F}_{1/2}(0)^{5/3} \right) \geq CT_k(s)^{5/3} - C.$$

Finally, if $s > k$, we have $T_k(s)^{5/3} = k^{5/3} \leq CG_{k,\delta}(k) \leq CG_{k,\delta}(s)$. This finishes the proof. \square

Lemma 7 (Approximate free energy inequality for $E_{k,\delta}$). *Let Assumptions (A1)–(A4) hold and let (n_k, p_k, D_k, V_k) be the weak solution constructed in Lemma 5. Then, for all $0 < t < T$,*

$$\begin{aligned} (30) \quad E_{k,\delta}(n_k, p_k, D_k, V_k)(t) &+ \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta} \nabla V_k|^2 dx ds \\ &+ \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(p_k) + \sqrt{T_k(p_k) + \delta} \nabla V_k|^2 dx ds \\ &+ \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{h}_{k,\delta}(D_k) + (T_{k/(k+1)}(D_k) + \delta)^{1/2} \nabla V_k|^2 dx ds \\ &\leq C(E_{k,\delta}^I, \Lambda_{k,\delta}, T). \end{aligned}$$

The constant $C(E_{k,\delta}^I, \Lambda_{k,\delta}, T) \geq 0$ vanishes if $\Lambda_{k,\delta} = 0$ and $\delta = 0$.

Proof. We use the test function $G'_{k,\delta}(n_k) - G'_{k,\delta}(\bar{n}) - V_k + \bar{V}$ (see definition (23)) in the weak formulation of (15):

$$\begin{aligned} &\langle \partial_t n_k, G'_{k,\delta}(n_k) - G'_{k,\delta}(\bar{n}) - V_k + \bar{V} \rangle \\ &= - \int_{\Omega} (S_k^1(n_k) \nabla n_k - T_k(n_k) \nabla V_k) \cdot \nabla ((G'_{k,\delta}(n_k) - V_k) - (G'_{k,\delta}(\bar{n}) - \bar{V})) dx. \end{aligned}$$

We use the identities

$$\langle \partial_t n_k, G'_{k,\delta}(n_k) - G'_{k,\delta}(\bar{n}) \rangle = \frac{d}{dt} \int_{\Omega} (G_{k,\delta}(n_k) - G_{k,\delta}(\bar{n}) - G'_{k,\delta}(\bar{n})(n_k - \bar{n})) dx,$$

$$S_k^1(n_k)\nabla n_k - T_k(n_k)\nabla V_k = \sqrt{T_k(n_k) + \delta}(\nabla\tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta}\nabla V_k) + \delta\nabla V_k,$$

$$\nabla(G'_{k,\delta}(n_k) - V_k) = \frac{\nabla\tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta}\nabla V_k}{\sqrt{T_k(n_k) + \delta}},$$

which follow from the chain rules (24), to obtain

$$(31) \quad \begin{aligned} & \frac{d}{dt} \int_{\Omega} (G_{k,\delta}(n_k) - G_{k,\delta}(\bar{n}) - G'_{k,\delta}(\bar{n})(n_k - \bar{n})) dx - \langle \partial_t n_k, V_k - \bar{V} \rangle \\ &= - \int_{\Omega} |\nabla\tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta}\nabla V_k|^2 dx \\ & \quad - \int_{\Omega} \frac{\delta}{\sqrt{T_k(n_k) + \delta}} \nabla V_k \cdot (\nabla\tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta}\nabla V_k) dx \\ & \quad + \int_{\Omega} \sqrt{T_k(n_k) + \delta} (\nabla\tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta}\nabla V_k) \cdot \nabla(G'_{k,\delta}(\bar{n}) - \bar{V}) dx \\ & \quad + \delta \int_{\Omega} \nabla V_k \cdot \nabla(G'_{k,\delta}(\bar{n}) - \bar{V}) dx \\ & \leq -\frac{1}{2} \int_{\Omega} |\nabla\tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta}\nabla V_k|^2 dx + \frac{\delta}{2} \int_{\Omega} |\nabla(G'_{k,\delta}(\bar{n}) - \bar{V})|^2 dx \\ & \quad + \frac{3\delta}{2} \int_{\Omega} |\nabla V_k|^2 dx + \|\nabla(G'_{k,\delta}(\bar{n}) - \bar{V})\|_{L^\infty(\Omega)}^2 \int_{\Omega} (T_k(n_k) + \delta) dx, \end{aligned}$$

where we used the inequality $\delta/(\sqrt{T_k(n_k) + \delta}) \leq \sqrt{\delta}$ and Young's inequality in the last step. Similarly, the test function $G'_{k,\delta}(p_k) - G'_{k,\delta}(\bar{p}) + V_k - \bar{V}$ in the weak formulation of (16) leads to

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega} (G_{k,\delta}(p_k) - G_{k,\delta}(\bar{p}) - G'_{k,\delta}(\bar{p})(p_k - \bar{p})) dx + \langle \partial_t p_k, V_k - \bar{V} \rangle \\ & \leq -\frac{1}{2} \int_{\Omega} |\nabla\tilde{g}_{k,\delta}(p_k) + \sqrt{T_k(p_k) + \delta}\nabla V_k|^2 dx + \frac{\delta}{2} \int_{\Omega} |\nabla(G'_{k,\delta}(\bar{p}) + \bar{V})|^2 dx \\ & \quad + \frac{3\delta}{2} \int_{\Omega} |\nabla V_k|^2 dx + \|\nabla(G'_{k,\delta}(\bar{p}) + \bar{V})\|_{L^\infty(\Omega)}^2 \int_{\Omega} (T_k(p_k) + \delta) dx. \end{aligned}$$

Similarly, with the test function $H'_{k,\delta}(D_k) + V_k$ in the weak formulation of (17),

$$(32) \quad \begin{aligned} & \frac{d}{dt} \int_{\Omega} \mathcal{H}_{k,\delta}(D_k) dx + \langle \partial_t D_k, V_k - \bar{V} \rangle = \langle \partial_t D_k, H'_{k,\delta}(D_k) + V_k \rangle \\ & \leq -\frac{1}{2} \int_{\Omega} |\nabla\tilde{h}_{k,\delta}(D_k) + (T_{k/(k+1)}(D_k) + \delta)^{1/2}\nabla V_k|^2 dx + \frac{\delta}{2} \int_{\Omega} |\nabla V_k|^2 dx. \end{aligned}$$

We add (31)–(32) and take into account definition (26) of the relative energies and definition (29) of $\Lambda_{k,\delta}$:

$$(33) \quad \frac{d}{dt} \int_{\Omega} (\mathcal{G}_{k,\delta}(n_k|\bar{n}) + \mathcal{G}_{k,\delta}(p_k|\bar{p}) + \mathcal{H}_{k,\delta}(D_k)) dx - \langle \partial_t(n_k - p_k - D_k), V_k - \bar{V} \rangle$$

$$\begin{aligned}
& + \frac{1}{2} \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta} \nabla V_k|^2 dx \\
& + \frac{1}{2} \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(p_k) + \sqrt{T_k(p_k) + \delta} \nabla V_k|^2 dx \\
& + \frac{1}{2} \int_{\Omega} |\nabla \tilde{h}_{k,\delta}(D_k) + (T_{k/(k+1)}(D_k) + \delta)^{1/2} \nabla V_k|^2 dx \\
& \leq \Lambda_{k,\delta} \int_{\Omega} (T_k(n_k) + T_k(p_k) + 2\delta) dx + \frac{7\delta}{2} \int_{\Omega} |\nabla V_k|^2 dx + \frac{\delta}{2} |\Omega| \Lambda_{k,\delta}.
\end{aligned}$$

In view of Poisson's equation (18), the last term in the first line of (33) can be written as

$$-\langle \partial_t(n_k - p_k - D_k), V_k - \bar{V} \rangle = -\lambda^2 \langle \partial_t \Delta V_k, V_k - \bar{V} \rangle = \frac{\lambda^2}{2} \frac{d}{dt} \int_{\Omega} |\nabla(V_k - \bar{V})|^2 dx.$$

Integrating (33) over $(0, t)$ and taking into account

$$\int_{\Omega} |\nabla V_k|^2 dx \leq 2 \int_{\Omega} |\nabla(V_k - \bar{V})|^2 dx + 2 \int_{\Omega} |\nabla \bar{V}|^2 dx$$

as well as definitions (27) for $E_{k,\delta}$ and (28) for $E_{k,\delta}^I$, we arrive at

$$\begin{aligned}
& E_{k,\delta}(n_k, p_k, D_k, V_k)(t) + \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta} \nabla V_k|^2 dx ds \\
& + \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(p_k) + \sqrt{T_k(p_k) + \delta} \nabla V_k|^2 dx ds \\
& + \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{h}_{k,\delta}(D_k) + (T_{k/(k+1)}(D_k) + \delta)^{1/2} \nabla V_k|^2 dx ds \\
& \leq E_{k,\delta}^I + \Lambda_{k,\delta} \int_0^t \int_{\Omega} (T_k(n_k) + T_k(p_k) + 2\delta) dx ds \\
& + 7\delta \int_0^t \int_{\Omega} |\nabla(V_k - \bar{V})|^2 dx ds + 7\delta \int_0^t \int_{\Omega} |\nabla \bar{V}|^2 dx ds + \frac{\delta}{2} |\Omega| \Lambda_{k,\delta} t.
\end{aligned}$$

We conclude from Young's inequality and Lemma 6 that

$$T_k(n_k) \leq C + T_k(n_k)^{5/3} \leq C + CG_{k,\delta}(n_k),$$

and consequently, the second term on the right-hand side can be replaced by

$$C_1 \Lambda_{k,\delta} \int_0^t E_{k,\delta}(n_k, p_k, D_k, V_k) ds + C(\Omega)(\delta + 1) \Lambda_{k,\delta} t.$$

Thus, applying Gronwall's lemma,

$$\begin{aligned}
& E_{k,\delta}(n_k, p_k, D_k, V_k)(t) + \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta} \nabla V_k|^2 dx ds \\
& + \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_{k,\delta}(p_k) + \sqrt{T_k(p_k) + \delta} \nabla V_k|^2 dx ds
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{h}_{k,\delta}(D_k) + (T_{k/(k+1)}(D_k) + \delta)^{1/2} \nabla V_k|^2 dx ds \\
& \leq (E_{k,\delta}^I + C(\Omega)(\delta + 1)\Lambda_{k,\delta}t) \exp(C_1\Lambda_{k,\delta}t).
\end{aligned}$$

This proves the lemma. \square

2.3. **Limit $\delta \rightarrow 0$.** We set

$$\begin{aligned}
\tilde{g}_k(s) &= \tilde{g}_{k,0}(s), \quad G_k(s) = G_{k,0}(s), \quad \tilde{h}_k(s) = \tilde{h}_{k,0}(s), \quad H_k(s) = H_{k,0}(s), \\
\mathcal{G}_k(s|\bar{s}) &= \mathcal{G}_{k,0}(s|\bar{s}), \quad \mathcal{H}_k(s|\bar{s}) = \mathcal{H}_{k,0}(s|\bar{s})
\end{aligned}$$

and introduce

$$\begin{aligned}
E_k(n_k, p_k, D_k, V_k) &= \int_{\Omega} \left(\mathcal{G}_k(n_k|\bar{n}) + \mathcal{G}_k(p_k|\bar{p}) + \mathcal{H}_k(V_k) + \frac{\lambda^2}{2} |\nabla(V_k - \bar{V})|^2 \right) dx, \\
E_k^I &= E_k(n^I, p^I, D^I, V^I), \quad \Lambda_k = \Lambda_{k,0}.
\end{aligned}$$

Lemma 8 (Approximate free energy inequality for E_k). *Under the assumptions of Lemma 7, it holds for all $0 < t < T$ that*

$$\begin{aligned}
(34) \quad E_k(n_k, p_k, D_k, V_k)(t) &+ \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_k(n_k) - \sqrt{T_k(n_k)} \nabla V_k|^2 dx ds \\
&+ \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{g}_k(p_k) + \sqrt{T_k(p_k)} \nabla V_k|^2 dx ds \\
&+ \frac{1}{2} \int_0^t \int_{\Omega} |\nabla \tilde{h}_k(D_k) + T_{k/(k+1)}(D_k)^{1/2} \nabla V_k|^2 dx ds \leq C(E_k^I, \Lambda_k, T),
\end{aligned}$$

and the constant $C(E_k^I, \Lambda_k, T) \geq 0$ vanishes if $\Lambda_k = 0$.

Proof. The proof essentially follows from the monotone and dominated convergence theorems as in the proof of Lemma 2.3 of [19]. The only difference is the treatment of the functions $\tilde{g}_{k,\delta}$, $G_{k,\delta}$, $\tilde{h}_{k,\delta}$, and $H_{k,\delta}$. In fact, by the monotone convergence theorem, $\tilde{g}_{k,\delta}(n_k) \rightarrow \tilde{g}_k(n_k)$, $G_{k,\delta}(n_k) \rightarrow G_k(n_k)$, $\tilde{h}_{k,\delta}(D_k) \rightarrow \tilde{h}_k(D_k)$, and $H_{k,\delta}(D_k) \rightarrow H_k(D_k)$ a.e. in Ω_T as $\delta \rightarrow 0$. We derive upper bounds for the limit functions. Let $s > k$. Then, using Lemma 20,

$$\begin{aligned}
\tilde{g}_k(s) &= \int_0^s \tilde{g}'_k(z) dz = \int_0^k \sqrt{z} g'(z) dz + \int_k^s k^{1/6} z^{1/3} g'(z) dz \\
&\leq C \int_0^k (z^{1/6} + z^{-1/2}) dz + C k^{1/6} \int_k^s (1 + z^{-2/3}) dz \leq C(k)(s + 1),
\end{aligned}$$

and this inequality also holds for any $s \geq 0$. We obtain for $s > k/(k+1)$:

$$\tilde{h}_k(s) = \int_0^{k/(k+1)} \frac{dz}{\sqrt{z}(1-z)} + \int_{k/(k+1)}^s (k+1) \sqrt{\frac{k+1}{k}} dz \leq C(k)(s + 1),$$

and this bound holds in fact for all $s \geq 0$. Similar arguments lead to

$$G_{k,\delta}(s) \leq C(k)(s^2 + 1), \quad H_{k,\delta}(s) \leq C(k)(s^2 + 1) \quad \text{for } s \geq 0.$$

The approximate free energy inequality (30) implies that n_k, p_k, D_k are bounded in $L^2(\Omega_T)$ uniformly in δ . Hence, we can apply the dominated convergence theorem to find that

$$\begin{aligned} \tilde{g}_{k,\delta}(n_k) &\rightarrow \tilde{g}_k(n_k), \quad \tilde{h}_{k,\delta}(D_k) \rightarrow \tilde{h}_k(D_k) \quad \text{strongly in } L^2(\Omega_T), \\ G_{k,\delta}(n_k) &\rightarrow G_k(n_k), \quad H_{k,\delta}(D_k) \rightarrow H_k(D_k) \quad \text{strongly in } L^1(\Omega_T). \end{aligned}$$

The sequence $(\nabla \tilde{g}_{k,\delta}(n_k) - \sqrt{T_k(n_k) + \delta} \nabla V_k)_\delta$ is uniformly bounded in $L^2(\Omega_T)$. Therefore, there exists a subsequence that converges weakly in $L^2(\Omega_T)$ as $\delta \rightarrow 0$. The previous arguments allow us to identify the weak limit, showing the claim. The other terms in (30) can be treated in a similar way. The limit $\delta \rightarrow 0$ in (30) then proves (34). \square

2.4. Uniform estimates. We first show some inequalities relating g, G_k, T_k , and \tilde{g} .

Lemma 9. *There exists $C > 0$ such that for all $k > 1$ and $s > 0$,*

$$\begin{aligned} g'(s) &\leq G_k''(s), \quad s^{5/3} \leq C(G_k(s) + 1), \quad T_k(s)^{7/6} \leq C\tilde{g}_k(s), \\ \tilde{g}_k(s)^{10/7} &\leq C(G_k(s) + 1), \quad T_k(s)^{5/3} \leq C(G_k(s) + 1), \\ \tilde{h}_k(s) &\geq s^{-1/2}, \quad \tilde{h}'_k(s) \geq 1. \end{aligned}$$

Proof. The first inequality follows from $G_k''(s) = g'(s)$ for $0 < s \leq k$ and $G_k''(s) = (s/k)^{1/3}g'(s) \geq g'(s)$ for $s > k$. Since $g'(s) \sim s^{-1} + s^{-1/3}$ by Lemma 20,

$$G_k(s) \geq C \int_{\mathcal{F}_{1/2}(0)}^s \int_{\mathcal{F}_{1/2}(0)}^y (z^{-1} + z^{-1/3}) dz dy \geq C(s^{5/3} - 1),$$

which proves the second inequality. For the third one, let $0 < s \leq k$. Then, again by Lemma 20,

$$\tilde{g}'_k(z) = \sqrt{z}g'(z) \geq C(z^{-1/2} + z^{1/6}) \geq Cz^{1/6}.$$

We integrate this inequality over $z \in (0, s)$ to find that $\tilde{g}_k(s) = \tilde{g}_k(s) - \tilde{g}_k(0) \geq Cs^{7/6} = CT_k(s)^{7/6}$. If $s > k$, we compute

$$\tilde{g}_k(s) \geq \int_0^k \frac{yg'(y)}{\sqrt{T_k(y)}} dy = \int_0^k \sqrt{y}g'(y) dy \geq C \int_0^k y^{1/6} dy = Ck^{7/6} = CT_k(s)^{7/6}.$$

We turn to the fourth inequality. By Lemma 20, we have for $0 < s \leq k$,

$$\tilde{g}_k(s) = \int_0^s \sqrt{y}g'(y) dy \leq C \int_0^s (y^{-1/2} + y^{1/6}) dy \leq C(s^{7/6} + 1).$$

Furthermore, if $s > k$,

$$\begin{aligned} \tilde{g}_k(s) &= \int_0^k \sqrt{y}g'(y) dy + \int_k^s k^{1/6}y^{1/3}g'(y) dy \\ &\leq C(k^{1/2} + k^{7/6}) + Ck^{1/6}(s^{1/3} + s) \leq C(s^{7/6} + 1), \end{aligned}$$

and the conclusion follows after raising the inequality to the power $10/7$ and using the second inequality. The fifth inequality follows from the third and fourth ones since $T_k(s)^{5/3} \leq C\tilde{g}_k(s)^{10/7} \leq C(G_k(s) + 1)$.

To estimate \tilde{h}' , we observe that $h'(s) = 1/(s(1-s))$ and hence $\tilde{h}'_k(s) = 1/(\sqrt{s}(1-s)) \geq s^{-1/2}$ for $s < k/(k+1)$ and $\tilde{h}'_k(s) = (1+k)/k \geq s^{-1} \geq s^{-1/2}$ for $k/(k+1) \leq s < 1$. Moreover, in both cases, $\tilde{h}'(s) \geq 1$. This proves the inequalities for \tilde{h}'_k . \square

The previous lemma and the approximate energy inequality (34) lead to the following a priori estimates.

Lemma 10 (Uniform estimates I). *There exists a constant $C > 0$ such that for all $k \in \mathbb{N}$,*

$$\begin{aligned} \|T_k(n_k)\|_{L^\infty(0,T;L^{5/3}(\Omega))} + \|T_k(p_k)\|_{L^\infty(0,T;L^{5/3}(\Omega))} &\leq C, \\ \|n_k\|_{L^\infty(0,T;L^{5/3}(\Omega))} + \|p_k\|_{L^\infty(0,T;L^{5/3}(\Omega))} &\leq C, \\ \|\tilde{g}_k(n_k)\|_{L^\infty(0,T;L^{10/7}(\Omega))} + \|\tilde{g}_k(p_k)\|_{L^\infty(0,T;L^{10/7}(\Omega))} &\leq C, \\ \|\sqrt{T_k(n_k)}\nabla V_k\|_{L^\infty(0,T;L^{5/4}(\Omega))} + \|\sqrt{T_k(p_k)}\nabla V_k\|_{L^\infty(0,T;L^{5/4}(\Omega))} &\leq C, \\ \|\nabla\tilde{g}_k(n_k)\|_{L^2(0,T;L^{5/4}(\Omega))} + \|\nabla\tilde{g}_k(p_k)\|_{L^2(0,T;L^{5/4}(\Omega))} &\leq C, \\ \|\nabla n_k\|_{L^2(0,T;L^{5/4}(\Omega))} + \|\nabla p_k\|_{L^2(0,T;L^{5/4}(\Omega))} &\leq C, \\ \|\nabla\tilde{h}_k(D_k)\|_{L^2(\Omega_T)} + \|(T_{k/(k+1)}(D_k))^{1/2}\nabla V_k\|_{L^\infty(0,T;L^2(\Omega))} &\leq C, \\ \|\nabla D_k\|_{L^2(\Omega_T)} + \|\nabla\sqrt{D_k}\|_{L^2(\Omega_T)} &\leq C. \end{aligned}$$

Proof. The approximate energy inequality (34) shows that $(G_k(n_k))$ and $(G_k(p_k))$ are bounded in $L^\infty(0, T; L^1(\Omega))$. By Lemma 9, this yields a uniform bound for $T_k(n_k)$, $T_k(p_k)$ and n_k , p_k in $L^\infty(0, T; L^{5/3}(\Omega))$ and for $\tilde{g}_k(n_k)$, $\tilde{g}_k(p_k)$ in $L^\infty(0, T; L^{10/7}(\Omega))$. The energy estimate (34) implies a uniform bound for ∇V_k in $L^\infty(0, T; L^2(\Omega))$. Consequently, using Hölder's inequality,

$$\|\sqrt{T_k(n_k)}\nabla V_k\|_{L^\infty(0,T;L^{5/4}(\Omega))} \leq \|\sqrt{T_k(n_k)}\|_{L^\infty(0,T;L^{10/3}(\Omega))} \|\nabla V_k\|_{L^\infty(0,T;L^2(\Omega))} \leq C,$$

and similarly for $\sqrt{T_k(p_k)}\nabla V_k$. Then we deduce from the $L^2(\Omega_T)$ bound for $\nabla\tilde{g}_k(n_k) - \sqrt{T_k(n_k)}\nabla V_k$ that $\nabla\tilde{g}_k(n_k)$ is uniformly bounded in $L^2(0, T; L^{5/4}(\Omega))$. It follows from Lemma 20 that $\tilde{g}'_k(s) = \sqrt{s}g'(s) \geq C(s^{1/6} + s^{-1/2}) \geq C$ for $0 < s \leq k$ and $\tilde{g}'_k(s) = k^{1/6}s^{1/3}g'(s) \geq k^{1/6}(1 + s^{-2/3}) \geq 1$ for $s > k$. Thus, \tilde{g}'_k is bounded from below by a positive constant. Then the bounds for $\nabla\tilde{g}_k(n_k)$ and $\nabla\tilde{g}_k(p_k)$ imply the same bounds for ∇n_k and ∇p_k .

We turn to the estimates for D_k . Since $T_{k/(k+1)}(D_k) < 1$, we infer from the energy inequality (34) that $(T_{k/(k+1)}(D_k))^{1/2}\nabla V_k$ is bounded in $L^\infty(0, T; L^2(\Omega))$ and consequently, $\nabla\tilde{h}_k(D_k)$ is uniformly bounded in $L^2(\Omega_T)$. We deduce from $\tilde{h}'_k(s) \geq s^{-1/2}$ and $\tilde{h}'_k(s) \geq 1$ for $s > 0$ (see Lemma 9) that $\nabla\sqrt{D_k}$ and ∇D_k are uniformly bounded in $L^2(\Omega_T)$. \square

We can improve the regularity stated in Lemma 10 by using the inequality $T_k(s)^{7/6} \leq C\tilde{g}_k(s)$ and an iteration argument.

Lemma 11 (Uniform estimates II). *Let $q, r \leq \infty$ if $d = 1$, $q, r < \infty$ if $d = 2$, and $q < 8$, $r < 24/7$ if $d = 3$. There exists a constant $C > 0$ such that for all $k \in \mathbb{N}$,*

$$\begin{aligned} & \|\sqrt{T_k(n_k)}\|_{L^{14/3}(0,T;L^q(\Omega))} + \|\sqrt{T_k(n_k)}\|_{L^{14/3}(0,T;L^q(\Omega))} \leq C, \\ & \|\sqrt{T_k(n_k)}\nabla V_k\|_{L^{14/3}(0,T;L^r(\Omega))} + \|\sqrt{T_k(n_k)}\nabla V_k\|_{L^{14/3}(0,T;L^r(\Omega))} \leq C, \\ & \|\tilde{g}_k(n_k)\|_{L^2(0,T;L^r(\Omega))} + \|\tilde{g}_k(p_k)\|_{L^2(0,T;L^r(\Omega))} \leq C, \\ & \|\nabla\tilde{g}_k(n_k)\|_{L^2(0,T;L^{2q/(2+q)}(\Omega))} + \|\nabla\tilde{g}_k(p_k)\|_{L^2(0,T;L^{2q/(2+q)}(\Omega))} \leq C, \\ & \|\nabla n_k\|_{L^2(0,T;L^{2q/(2+q)}(\Omega))} + \|\nabla p_k\|_{L^2(0,T;L^{2q/(2+q)}(\Omega))} \leq C \end{aligned}$$

Observe that $2q/(2+q) < 8/5$ if $d = 3$.

Proof. We assume that $(\sqrt{T_k(n_k)})$ is bounded in $L^{14/3}(0, T; L^{q_m}(\Omega))$ and $(\tilde{g}_k(n_k))$ is bounded in $L^2(0, T; L^{r_m}(\Omega))$ for some numbers $q_m, r_m \geq 1$ with $m \in \mathbb{N}$. By Lemma 10, we have $q_1 = 10/3$ and $r_1 = 10/7$. We estimate

$$(35) \quad \|\sqrt{T_k(n_k)}\nabla V_k\|_{L^{14/3}(0,T;L^a(\Omega))} \leq \|\sqrt{T_k(n_k)}\|_{L^{14/3}(0,T;L^{q_m}(\Omega))} \|\nabla V_k\|_{L^\infty(0,T;L^2(\Omega))} \leq C,$$

where $1/a = 1/q_m + 1/2$. This shows that

$$(36) \quad \begin{aligned} \|\nabla\tilde{g}_k(n_k)\|_{L^2(0,T;L^a(\Omega))} & \leq \|\nabla\tilde{g}_k(n_k) - \sqrt{T_k(n_k)}\nabla V_k\|_{L^2(0,T;L^a(\Omega))} \\ & \quad + \|\sqrt{T_k(n_k)}\nabla V_k\|_{L^2(0,T;L^a(\Omega))} \leq C. \end{aligned}$$

Then the continuous embedding $W^{1,a}(\Omega) \hookrightarrow L^{r_{m+1}}(\Omega)$ with $1/r_{m+1} = 1/a - 1/d = 1/q_m + 1/2 - 1/d$ implies that $\tilde{g}_k(n_k)$ is uniformly bounded in $L^2(0, T; L^{r_{m+1}}(\Omega))$. We deduce from $\sqrt{T_k(s)} \leq C\tilde{g}_k(s)^{3/7}$ (see Lemma 9) that $\sqrt{T_k(n_k)}$ is uniformly bounded in $L^{14/3}(0, T; L^{q_{m+1}}(\Omega))$, where $q_{m+1} = 7r_{m+1}/3$. This leads to the recursion

$$\frac{1}{q_{m+1}} = \frac{3}{7} \frac{1}{r_{m+1}} = \frac{3}{7} \left(\frac{1}{q_m} + \frac{1}{2} - \frac{1}{d} \right).$$

The sequence $(1/q_m)$ is nonincreasing (if $d \leq 4$) and bounded from below. Thus, it possesses the limit q^* that satisfies

$$\frac{1}{q^*} = \frac{3}{7} \left(\frac{1}{q^*} + \frac{1}{2} - \frac{1}{d} \right) \quad \text{and hence} \quad q^* = \frac{8d}{3(d-2)}.$$

We can perform this recursion only a finite number of times as otherwise the powers of the embedding constant may diverge. Thus, $q < q^* = 8$ if $d = 3$ and, since $q_{m+1} = 7q_m/3 \rightarrow \infty$ as $m \rightarrow \infty$, $q < \infty$ if $d = 2$. Furthermore, $1/r = 1/q + 1/2 - 1/d$, which gives $r < 24/7$ if $d = 3$ and $r < \infty$ if $d = 2$.

The uniform bound for $\sqrt{T_k(n_k)}\nabla V_k$ follows from (35) because of $1/a = 1/q + 1/2 = (2+q)/(2q)$. Estimate (36) then implies the bound for $\nabla\tilde{g}_k(n_k)$. We have shown in the proof of Lemma 10 that \tilde{g}'_k is bounded from below by a positive constant such that $C|\nabla n_k| \leq |\tilde{g}'_k(n_k)\nabla n_k| = |\nabla\tilde{g}_k(n_k)|$, proving the last uniform bound. Finally, the estimates for p_k are proved analogously. \square

The following bounds are needed for the Aubin–Lions lemma.

Lemma 12 (Uniform estimates III). *Under the assumptions of Lemma 11, there exists a constant $C > 0$ such that for all $k \in \mathbb{N}$,*

$$\begin{aligned} \|n_k\|_{L^2(0,T;W^{1,2q/(2+q)}(\Omega))} + \|p_k\|_{L^2(0,T;W^{1,2q/(2+q)}(\Omega))} &\leq C, \\ \|\partial_t n_k\|_{L^{7/5}(0,T;W_D^{1,2q/(q+4)}(\Omega)')} + \|\partial_t p_k\|_{L^{7/5}(0,T;W_D^{1,2q/(q+4)}(\Omega)')} &\leq C, \\ \|D_k\|_{L^2(0,T;H^1(\Omega))} + \|\partial_t D_k\|_{L^2(0,T;H^1(\Omega)')} &\leq C. \end{aligned}$$

Proof. The bound for n_k follows from the gradient bounds in Lemma 11 and the bound for n_k in $L^\infty(0, T; L^{5/3}(\Omega))$, which is a consequence of the energy inequality (34) and the inequality $s^{5/3} \leq C(G_k(s) + 1)$ from Lemma 9. By the chain rule (24) (for $\delta = 0$), the evolution equation for n_k reads as

$$\partial_t n_k = \operatorname{div} \left[\sqrt{T_k(n_k)} (\nabla \tilde{g}_k(n_k) - \sqrt{T_k(n_k)} \nabla V_k) \right].$$

The term $\sqrt{T_k(n_k)}$ is uniformly bounded in $L^{14/3}(0, T; L^q(\Omega))$, while $\nabla \tilde{g}_k(n_k) - \sqrt{T_k(n_k)} \nabla V_k$ is uniformly bounded in $L^2(0, T; L^{2q/(2+q)}(\Omega))$. Hence, $(\partial_t n_k)$ is bounded in $L^{7/5}(0, T; L^{2q/(4+q)}(\Omega))$ (we choose $q \geq 4$ to guarantee that $2q/(4+q) \geq 1$). The estimates for p_k are shown in a similar way.

We turn to the bounds for D_k . We know from the energy inequality (34) that $(H_k(D_k))$ is bounded in $L^\infty(0, T; L^1(\Omega))$ and from Lemma 10 that (∇D_k) is bounded in $L^2(\Omega_T)$. Proceeding as in the proof of Lemma 9, we infer that $S_k^2/T_{k/(k+1)}$ is bounded from below by a positive constant. This implies that $H_k(D_k) \geq CD_k^2$, which yields a bound for (D_k) in $L^\infty(0, T; L^2(\Omega))$. This shows that (D_k) is bounded in $L^2(0, T; H^1(\Omega))$. Finally, since $(T_{k/(k+1)}(D_k))$ is bounded in $L^\infty(\Omega_T)$, the sequence

$$(\nabla \tilde{h}_k(D_k) + T_{k/(k+1)}(D_k)^{1/2} \nabla V_k)$$

is bounded in $L^2(\Omega_T)$. Therefore,

$$\partial_t D_k = \operatorname{div} \left[T_{k/(k+1)}(D_k)^{1/2} (\nabla \tilde{h}_k(D_k) + T_{k/(k+1)}(D_k)^{1/2} \nabla V_k) \right]$$

is uniformly bounded in $L^2(0, T; H^1(\Omega)')$, finishing the proof. \square

2.5. Limit $k \rightarrow \infty$ in the equations for n_k and p_k . Lemma 12 and the compact embedding $W^{1,2q/(2+q)}(\Omega) \hookrightarrow L^r(\Omega)$ for $r < 24/7$ (if $d \leq 3$) allow us to apply the Aubin–Lions lemma to infer the existence of a subsequence that is not relabeled such that, as $k \rightarrow \infty$,

$$\begin{aligned} (n_k, p_k) &\rightarrow (n, p) \quad \text{strongly in } L^2(0, T; L^r(\Omega))^2, \\ D_k &\rightarrow D \quad \text{strongly in } L^2(\Omega_T), \\ (\nabla n_k, \nabla p_k) &\rightharpoonup (\nabla n, \nabla p) \quad \text{weakly in } L^2(0, T; L^{2q/(2+q)}(\Omega)), \\ (\partial_t n_k, \partial_t p_k) &\rightharpoonup (\partial_t n, \partial_t p) \quad \text{weakly in } L^{7/5}(0, T; W_D^{1,2q/(q+4)}(\Omega)')^2, \\ \partial_t D_k &\rightharpoonup \partial_t D \quad \text{weakly in } L^2(0, T; H^1(\Omega)'). \end{aligned}$$

The $L^\infty(0, T; L^{5/3}(\Omega))$ bound for n_k from Lemma 10 implies that

$$\|T_k(n_k) - n_k\|_{L^1(\Omega_T)} = \int_0^T \int_{\{n_k > k\}} |k - n_k| dx dt \leq \int_0^T \int_\Omega \frac{n_k^{5/3}}{k^{2/3}} dx dt \leq \frac{C}{k^{2/3}} \rightarrow 0.$$

This shows that $\sqrt{T_k(n_k)} - \sqrt{n_k} \rightarrow 0$ strongly in $L^2(\Omega_T)$ and in particular $\sqrt{T_k(n_k)} \rightarrow \sqrt{n}$ strongly in $L^2(\Omega_T)$. In fact, in view of the $L^\infty(0, T; L^{5/3}(\Omega))$ bound for n_k , we even have strong convergence for $\sqrt{T_k(n_k)}$ in $L^s(\Omega_T)$ for any $s < 10/3$. The $L^2(\Omega_T)$ bound for ∇V_k shows that $\nabla V_k \rightharpoonup \nabla V$ weakly in $L^2(\Omega_T)$. Hence,

$$\sqrt{T_k(n_k)} \nabla V_k \rightharpoonup \sqrt{n} \nabla V \quad \text{weakly in } L^1(\Omega_T).$$

Thanks to Lemma 11, this convergence also holds in $L^{14/3}(0, T; L^r(\Omega))$ with $r < 8/5$. Then, since $s < 10/3$ and $q < 8$ can be chosen in such a way that $1/s + (2 + q)/(2q) < 1$,

$$(37) \quad T_k(n_k) \nabla V_k = \sqrt{T_k(n_k)} \cdot \sqrt{T_k(n_k)} \nabla V_k \rightharpoonup n \nabla V \quad \text{weakly in } L^1(\Omega_T).$$

Similarly, we have $T_k(p_k) \nabla V_k \rightharpoonup T_k(p_k) \nabla V_k$ weakly in $L^1(\Omega_T)$.

Next, we prove the weak convergence of $(\sqrt{T_k(n_k)} \nabla \tilde{g}_k(n_k))$.

Lemma 13. *It holds that, up to a subsequence,*

$$\begin{aligned} \sqrt{T_k(n_k)} (\nabla \tilde{g}_k(n_k) - \sqrt{T_k(n_k)} \nabla V_k) &\rightharpoonup n \nabla g(n) - n \nabla V \quad \text{weakly in } L^1(\Omega_T), \\ \sqrt{T_k(p_k)} (\nabla \tilde{g}_k(p_k) + \sqrt{T_k(p_k)} \nabla V_k) &\rightharpoonup p \nabla g(p) + p \nabla V \quad \text{weakly in } L^1(\Omega_T). \end{aligned}$$

Proof. First, we show that $\sqrt{T_k(n_k)} \tilde{g}'_k(n_k)$ converges strongly. To this end, we estimate

$$(38) \quad \begin{aligned} &\left\| \sqrt{T_k(n_k)} \tilde{g}'_k(n_k) - n g'(n) \right\|_{L^2(0, T; L^5(\Omega))} \\ &\leq \left\| \sqrt{T_k(n_k)} \tilde{g}'_k(n_k) - n_k g'(n_k) \right\|_{L^2(0, T; L^5(\Omega))} + \|n_k g'(n_k) - n g'(n)\|_{L^2(0, T; L^5(\Omega))}. \end{aligned}$$

The first integrand vanishes on $\{n_k \leq k\}$. Therefore, on the set $\{n_k > k\}$, using Lemma 20,

$$\begin{aligned} &\left| \sqrt{T_k(n_k)} \tilde{g}'_k(n_k) - n_k g'(n_k) \right|^5 = |(n_k^{2/3} - k^{2/3}) n_k^{1/3} g'(n_k)|^5 \\ &\leq |n_k g'(n_k)|^5 \leq C |n_k (n_k^{-1} + n_k^{-1/3})|^5 \leq C (1 + n_k^{10/3}) \leq C \left(\frac{n_k}{k} + \frac{n_k^{10/3+\varepsilon}}{k^\varepsilon} \right) \end{aligned}$$

for $\varepsilon > 0$ such that $10/3 + \varepsilon \leq r < 24/7$, which shows that

$$\left\| \sqrt{T_k(n_k)} \tilde{g}'_k(n_k) - n_k g'(n_k) \right\|_{L^2(0, T; L^5(\Omega))}^2 \leq \frac{C}{k^{2\varepsilon}} \int_0^T (\|n_k\|_{L^1(\Omega)} + \|n_k\|_{L^r(\Omega)}^r)^{2/5} dt \rightarrow 0,$$

since (n_k) is bounded in $L^2(0, T; L^r(\Omega))$. We show in Lemma 21 that $|(zg'(z))'| = |g'(z) + zg''(z)|$ is bounded for $z > 0$. Hence,

$$|n_k g'(n_k) - n g'(n)|^r = \left| \int_{n_k}^n \frac{d}{dz} (zg'(z)) dz \right|^r \leq C |n_k - n|^r.$$

Then the strong convergence $n_k \rightarrow n$ in $L^2(0, T; L^r(\Omega))$ implies that

$$\|n_k g'(n_k) - n g'(n)\|_{L^2(0, T; L^r(\Omega))} \rightarrow 0.$$

We conclude from (38) that

$$\sqrt{T_k(n_k)} \tilde{g}'_k(n_k) \rightarrow n g'(n) \quad \text{strongly in } L^2(0, T; L^r(\Omega)).$$

Consequently, the weak convergence $\nabla n_k \rightharpoonup \nabla n$ in $L^2(0, T; L^{2q/(2+q)}(\Omega))$ gives

$$\sqrt{T_k(n_k)} \nabla \tilde{g}_k(n_k) = \sqrt{T_k(n_k)} \tilde{g}'_k(n_k) \nabla n_k \rightharpoonup n g'(n) \nabla n = n \nabla g(n)$$

weakly in $L^1(\Omega_T)$. Combining this result with (37) shows that

$$\sqrt{T_k(n_k)} (\nabla \tilde{g}_k(n_k) - \sqrt{T_k(n_k)} \nabla V_k) \rightharpoonup n \nabla g(n) - n \nabla V \quad \text{weakly in } L^1(\Omega_T),$$

which ends the proof. \square

We need the convergence of $(\nabla \tilde{g}(n_k))$ and $(\nabla \tilde{g}(p_k))$ to pass to the limit in the energy inequality.

Lemma 14. *It holds that*

$$\begin{aligned} (\nabla \sqrt{n_k}, \nabla \sqrt{p_k}) &\rightharpoonup (\nabla \sqrt{n}, \nabla \sqrt{p}) \quad \text{weakly in } L^2(0, T; L^{2q/(2+q)}(\Omega))^2, \\ (\nabla \tilde{g}_k(n_k), \nabla \tilde{g}_k(p_k)) &\rightharpoonup (\sqrt{n} \nabla g(n), \sqrt{p} \nabla g(p)) \quad \text{weakly in } L^1(\Omega_T)^2. \end{aligned}$$

Proof. It follows from Lemma 20 that $\tilde{g}'_k(s) = \sqrt{s} g'(s) \geq C(s^{-1/2} + s^{1/6}) \geq C s^{-1/2}$ for $s < k$ and $\tilde{g}'_k(s) = k^{-1/6} s^{1/3} g'(s) \geq C C (s/k)^{1/6} (s^{-5/6} + s^{-1/2}) \geq C s^{-1/2}$ for $s > k$. Then the uniform bound for $\nabla \tilde{g}_k(n_k)$ in Lemma 11 implies directly the bound for $\nabla \sqrt{n_k}$ in $L^2(0, T; L^{2q/(2+q)}(\Omega))$, showing the first statement. The limit for $\nabla \sqrt{p_k}$ is shown analogously. Repeating the proof of Lemma 13 with $\sqrt{n_k}$ instead of $\sqrt{T_k(n_k)}$, we obtain the convergence

$$\sqrt{n_k} \tilde{g}'_k(n_k) \rightarrow n g'(n) \quad \text{strongly in } L^2(0, T; L^r(\Omega)).$$

We combine this result with the weak convergence of $(\nabla \sqrt{n_k})$ to conclude that

$$\nabla \tilde{g}_k(n_k) = 2 \sqrt{n_k} \tilde{g}'_k(n_k) \nabla \sqrt{n_k} \rightharpoonup 2 n g'(n) \nabla \sqrt{n} = \sqrt{n} \nabla g(n) \quad \text{weakly in } L^1(\Omega_T),$$

using that $(2+q)/(2q) + 1/r < 1$ if we choose $q < 8$ and $r < 24/7$ sufficiently large. \square

2.6. Limit $k \rightarrow \infty$ in the equation for D_k . We prove the convergence of the terms in the equation for D_k . First, we consider $T_{k/(k+1)}(D_k)^{1/2} \nabla \tilde{h}_k(D_k) = T_{k/(k+1)}(D_k)^{1/2} \tilde{h}'_k(D_k) \nabla D_k$. We introduce the functions

$$\begin{aligned} L(s) &= -\log(1-s) \quad \text{for } 0 \leq s < 1, \\ L_k(s) &= \begin{cases} -\log(1-s) & \text{for } 0 \leq s \leq k/(k+1), \\ (k+1)s - k + \log(k+1) & \text{for } s > k/(k+1). \end{cases} \end{aligned}$$

They satisfy the property $L'_k(D_k) = T_{k/(k+1)}(D_k)^{1/2} \tilde{h}'_k(D_k)$ for all $0 \leq s < 1$. Moreover, L_k is nondecreasing, $L_k \leq L_{k+1}$ on $[0, 1)$, and L_k converges to L locally uniformly on $[0, 1)$. The aim is to derive uniform bounds for $L_k(D_k)$ and to identify its weak limit.

Lemma 15. *There exists a constant $C > 0$ such that*

$$\|L_k(D_k)\|_{L^2(0,T;H^1(\Omega))} \leq C.$$

Proof. The gradient bound follows immediately from $L'_k(s) < \tilde{h}'_k(s)$ for $0 < s < 1$ and $|\nabla L_k(D_k)| = L'_k(D_k)|\nabla n_k| \leq \tilde{h}'_k(n_k)|\nabla n_k| = |\nabla \tilde{h}_k(n_k)|$, showing that $(\nabla L_k(D_k))$ is bounded in $L^2(\Omega_T)$. By mass conservation and Assumption (A4), we have

$$\frac{1}{\mathfrak{m}(\Omega)} \int_{\Omega} D_k dx = \frac{1}{\mathfrak{m}(\Omega)} \int_{\Omega} D^I dx = D_{\Omega}^I < 1.$$

Thus, the conditions of Lemma 22 in Appendix B are satisfied, and we infer from the gradient bound that $L_k(D_k)$ is bounded in $L^2(\Omega_T)$. Lemma 22 now finishes the proof. \square

The uniform bound in Lemma 15 implies the existence of a subsequence such that

$$L_k(D_k) \rightharpoonup L^* \quad \text{weakly in } L^2(\Omega_T) \text{ as } k \rightarrow \infty.$$

The next aim is to identify $L^* = L(D)$, where we recall that D is the strong $L^2(\Omega_T)$ limit of (D_k) .

First, we claim that $L(D) \in L^2(\Omega_T)$ and $D < 1$ a.e. in Ω_T . Indeed, we have $D_{\ell} \rightarrow D$ a.e. in Ω_T as $\ell \rightarrow \infty$, up to a subsequence. Hence, since L_k is continuous and $L_k \leq L_{k+1}$, for any $k \in \mathbb{N}$,

$$\begin{aligned} \int_0^T \int_{\Omega} L_k(D)^2 dx dt &= \int_0^T \int_{\Omega} \lim_{\ell \rightarrow \infty} L_k(D_{\ell})^2 dx dt = \int_0^T \int_{\Omega} \liminf_{\ell \rightarrow \infty} L_k(D_{\ell})^2 dx dt \\ &\leq \int_0^T \int_{\Omega} \liminf_{\ell \rightarrow \infty} L_{\ell}(D_{\ell})^2 dx dt \leq \liminf_{\ell \rightarrow \infty} \int_0^T \int_{\Omega} L_{\ell}(D_{\ell})^2 dx dt, \end{aligned}$$

where the last step follows from Fatou's lemma. The last integral is uniformly bounded. Therefore, $(L_k(D))$ is bounded in $L^2(\Omega_T)$, and again by Fatou's lemma,

$$\int_0^T \int_{\Omega} L(D)^2 dx dt \leq \liminf_{k \rightarrow \infty} \int_0^T \int_{\Omega} L_k(D)^2 dx dt \leq C.$$

The $L^2(\Omega_T)$ -bound for $L(D) = -\log(1 - D)$ implies that $D < 1$ a.e.

To identify L^* with $L(D)$, we set

$$D_{\eta} := (1 - \eta)D + \eta, \quad D_{k,\eta} := (1 - \eta)D_k + \eta \quad \text{for } 0 < \eta < 1.$$

Because of the strong convergence of D_k , we clearly have $D_{k,\eta} \rightarrow D_{\eta}$ strongly in $L^2(\Omega_T)$ for any fixed $0 < \eta < 1$. The proof of Lemma 15 shows that $(L_k(D_{k,\eta}))$ is bounded in $L^2(0, T; H^1(\Omega))$, and the previous arguments imply that $L(D_{\eta}) \in L^2(\Omega_T)$. With these preparations, we can prove that $L^* = L(D)$.

Lemma 16. *It holds that $L^* = L(D)$ and*

$$L_k(D_k) \rightharpoonup L(D) \quad \text{weakly in } L^2(0, T; H^1(\Omega)).$$

Proof. The proof is based on the monotonicity of L_k (Minty trick). We pass to the limit $k \rightarrow \infty$ in

$$0 \leq \int_0^T \int_{\Omega} (L_k(D_\eta) - L_k(D_k))(D_\eta - D_k) dx dt,$$

leading to

$$0 \leq \frac{1}{\eta} \int_0^T \int_{\Omega} (L(D_\eta) - L^*)(D_\eta - D) dx dt = \int_0^T \int_{\Omega} (L(D_\eta) - L^*)(1 - D) dx dt.$$

By dominated convergence, the limit $\eta \rightarrow 0$ gives

$$(39) \quad 0 \leq \int_0^T \int_{\Omega} (L(D) - L^*)(1 - D) dx dt.$$

Next, we show the inverse inequality. The monotonicity $L_k \leq L_{k+1}$, the weak convergence of $(L_k(D_k))$, and Fatou's lemma yield the following inequalities:

$$\begin{aligned} \int_0^T \int_{\Omega} (1 - D) L_k(D) dx dt &= \int_0^T \int_{\Omega} (1 - D) \lim_{\ell \rightarrow \infty} L_k(D_\ell) dx dt \\ &\leq \int_0^T \int_{\Omega} (1 - D) \liminf_{\ell \rightarrow \infty} L_\ell(D_\ell) dx dt \leq \liminf_{\ell \rightarrow \infty} \int_0^T \int_{\Omega} (1 - D) L_\ell(D_\ell) dx dt \\ &\leq \int_0^T \int_{\Omega} (1 - D) L^* dx dt. \end{aligned}$$

It follows from dominated convergence that

$$\int_0^T \int_{\Omega} (1 - D) L(D) dx dt \leq \int_0^T \int_{\Omega} (1 - D) L^* dx dt,$$

or equivalently,

$$\int_0^T \int_{\Omega} (L(D) - L^*)(1 - D) dx dt \leq 0.$$

Together with (39) and the fact that $D < 1$ a.e., we conclude that $L^* = L(D)$ a.e. Hence, by Lemma 15, $L_k(D_k) \rightharpoonup L(D)$ weakly in $L^2(0, T; H^1(\Omega))$. \square

The previous lemma implies that

$$(40) \quad \begin{aligned} T_{k/(k+1)}(D_k)^{1/2} \nabla \tilde{h}_k(D_k) &= T_{k/(k+1)}(D_k)^{1/2} \tilde{h}'_k(D_k) \nabla D_k = L'_k(D_k) \nabla D_k \\ &= \nabla L_k(D_k) \rightharpoonup \nabla L(D) = -\nabla \log(1 - D) = D \nabla h(D) \quad \text{weakly in } L^2(\Omega_T). \end{aligned}$$

The next step is the convergence of $(T_{k/(k+1)}(D_k) \nabla V_k)$ and the identification of the limit.

Set $T_1(s) = \max\{0, \min\{1, s\}\}$. We deduce from

$$\begin{aligned} |T_{k/(k+1)}(D_k) - T_1(D)| &= |T_{k/(k+1)}(D_k) - T_{k/(k+1)}(D)| + |T_{k/(k+1)}(D) - T_1(D)| \\ &\leq |D_k - D| + \frac{1}{k+1} \end{aligned}$$

and the strong convergence of (D_k) that

$$\int_0^T \int_{\Omega} |T_{k/(k+1)}(D_k) - T_1(D)|^2 dx dt \leq 2 \int_0^T \int_{\Omega} |D_k - D|^2 dx dt + \frac{C}{(k+1)^2} \rightarrow 0.$$

The property $D < 1$ a.e. implies that $T_1(D) = D$ and thus $T_{k/(k+1)}(D_k) \rightarrow D$ strongly in $L^2(\Omega_T)$. We deduce from the convergence of $\nabla V_k \rightharpoonup \nabla V$ weakly in $L^2(\Omega_T)$ that $T_{k/(k+1)}(D_k) \nabla V_k \rightharpoonup D \nabla V$ weakly in $L^1(\Omega_T)$. We know from Lemma 10 that $T_{k/(k+1)}(D_k) \nabla V_k = T_{k/(k+1)}(D_k)^{1/2} \cdot T_{k/(k+1)}(D_k)^{1/2} \nabla V_K$ is uniformly bounded in $L^\infty(0, T; L^2(\Omega))$. This yields the convergence

$$T_{k/(k+1)}(D_k) \nabla V_k \rightharpoonup D \nabla V \quad \text{weakly in } L^2(\Omega_T).$$

It follows from (40) that

$$T_{k/(k+1)}(D_k)^{1/2} (\nabla \tilde{h}_k(D_k) + T_{k/(k+1)}(D_k)^{1/2} \nabla V_K) \rightharpoonup D \nabla h(D) + D \nabla V$$

weakly in $L^2(\Omega_T)$.

Performing the limit $k \rightarrow \infty$ in the weak formulation (15)–(18), using formulation (25) of the fluxes, leads to the weak formulation of (1)–(4). The limit (n, p, V) satisfies the Dirichlet boundary conditions (6) since $n_k = \bar{n}$, $p_k = \bar{p}$, and $V_k = \bar{V}$ on Γ_D . Finally, the limit $n_k \rightharpoonup n$ weakly in $W^{1,7/5}(0, T; W_D^{1,2q/(q+4)}(\Omega)')$ $\hookrightarrow C^0([0, T]; W_D^{1,2q/(q+4)}(\Omega)')$ and the property $n_k(\cdot, 0) = n^I$ in the sense of $W_D^{1,2q/(q+4)}(\Omega)'$ show that n satisfies the initial condition in (5) in a weak sense. Similarly, p and D also satisfy the initial conditions.

2.7. Energy inequality. We identify the weak limit of $\nabla \tilde{h}_k(D_k)$, which is needed in the limit of the energy inequality (34), leading to (14).

Lemma 17. *Recall that $\tilde{h}(s) = 2 \tanh^{-1} \sqrt{s} - 2 \tanh^{-1} \sqrt{1/2}$. It holds that*

$$\nabla \tilde{h}_k(D_k) \rightharpoonup \nabla \tilde{h}(D) \quad \text{weakly in } L^2(\Omega_T).$$

Proof. The function \tilde{h}_k is written explicitly as

$$\tilde{h}_k(s) = \begin{cases} 2 \tanh^{-1} \sqrt{s} - 2 \tanh^{-1} \sqrt{1/2} & \text{for } 0 \leq s \leq \frac{k}{k+1}, \\ \sqrt{\frac{k+1}{k}} ((k+1)s - k) + 2 \tanh^{-1} \sqrt{\frac{k}{k+1}} & \text{for } s > \frac{k}{k+1}. \end{cases}$$

By Lemma 10, the sequence $(\nabla \tilde{h}_k(D_k))$ is bounded in $L^2(\Omega_T)$. Proceeding as in the proof of Lemma 15, we can show that $(\tilde{h}_k(D_k))$ is bounded in $L^2(0, T; H^1(\Omega))$. We deduce from

$$|\nabla \tilde{h}_k(D_{k,\eta})| \leq \begin{cases} |\nabla \tilde{h}_k(D_k)| & \text{for } D_{k,\eta} \leq k/(k+1), \\ \sqrt{2} |\nabla L_k(D_{k,\eta})| & \text{for } D_{k,\eta} > k/(k+1) \end{cases}$$

a uniform bound for $\nabla \tilde{h}_k(D_{k,\eta})$ in $L^2(\Omega_T)$. The bound for $(\tilde{h}_k(D_k))$ implies a bound for $(\tilde{h}_k(D_{k,\eta}))$ in $L^2(\Omega_T)$, and we have $\tilde{h}(D_\eta) \in L^2(\Omega_T)$. Finally, the proof of Lemma 16 shows that

$$\tilde{h}_k(D_k) \rightharpoonup 2 \tanh^{-1} \sqrt{D} - 2 \tanh^{-1} \sqrt{1/2} \quad \text{weakly in } L^2(\Omega_T),$$

$$\nabla \tilde{h}_k(D_k) \rightharpoonup 2\nabla \tanh^{-1} \sqrt{D} \quad \text{weakly in } L^2(\Omega_T),$$

ending the proof. \square

3. PROOF OF THEOREM 2

Since the proof is similar to that one of [22, Theorem 2], we present only the key ideas, proceeding formally. First, we notice that Assumption (A5) with $r = 3 + \varepsilon > 3$ yields

$$(41) \quad \|V\|_{L^\infty(0,T;W^{1,r}(\Omega))} \leq C\|n - p - D + A\|_{L^\infty(0,T;L^{3r/(r+3)}(\Omega))} + C \leq C,$$

by Lemma 10, since $3r/(r+3) \leq 5/3$ if $\varepsilon > 0$ is sufficiently small. To simplify, we assume that $\bar{n} = 0$. The proof can be extended in a straightforward way to general boundary data \bar{n} , but at the price of more elaborate technical estimations (see, e.g., [22, Section 3]). We wish to use n^q for $q \in \mathbb{N}$ as a test function in the weak formulation of (1). To justify this step, we need to show that $n \in L^\infty(0, T; L^q(\Omega))$. This property is proved in [22, Sec. 3] in a similar context and therefore, we do not present the quite technical proof here. With this test function, we obtain

$$\frac{1}{q+1} \frac{d}{dt} \int_{\Omega} n^{q+1} dx + q \int_{\Omega} n g'(n) n^{q-1} |\nabla n|^2 dx = q \int_{\Omega} n^q \nabla V \cdot \nabla n dx.$$

We deduce from Lemma 20 that $n g'(n) \geq c(1 + n^{2/3})$ and hence, using Hölder's inequality for the drift term, integrating over $(0, t)$, and possibly lowering the constant $c > 0$,

$$(42) \quad \begin{aligned} & \frac{1}{q+1} \int_{\Omega} (n(t)^{q+1} - n(0)^{q+1}) dx + \frac{c}{q+1} \int_0^t \int_{\Omega} (|\nabla n^{(q+1)/2}|^2 + |\nabla n^{(3q+5)/6}|^2) dx ds \\ & \leq \frac{6q}{3q+5} \int_{\Omega} n^{(3q+1)/6} \nabla V \cdot \nabla n^{(3q+5)/6} dx \\ & \leq C \int_0^t \|n^{(3q+1)/6}\|_{L^{(6+2\varepsilon)/(1+\varepsilon)}(\Omega)} \|\nabla V\|_{L^{3+\varepsilon}(\Omega)} \|\nabla n^{(3q+5)/6}\|_{L^2(\Omega)} ds \\ & \leq C \int_0^t \|n^{(3q+1)/6}\|_{L^{(6+2\varepsilon)/(1+\varepsilon)}(\Omega)} \|\nabla n^{(3q+5)/6}\|_{L^2(\Omega)} ds, \end{aligned}$$

where in the last step we have taken into account (41). We apply the Gagliardo–Nirenberg inequality with $\theta = (15 + 3\varepsilon)/(15 + 5\varepsilon) < 1$ (at this point we need the regularity in $W^{1,r}(\Omega)$ with $r = 3 + \varepsilon > 3$; $\varepsilon = 0$ would not be sufficient) and Young's inequality:

$$\begin{aligned} \|n^{(3q+1)/6}\|_{L^{(6+2\varepsilon)/(1+\varepsilon)}(\Omega)} &= \|n^{(3q+5)/6}\|_{L^{(3q+1)(6+2\varepsilon)/((3q+5)(1+\varepsilon))}(\Omega)}^{(3q+1)/(3q+5)} \\ &\leq C + C \|n^{(3q+5)/6}\|_{L^{(3q+1)(6+2\varepsilon)/((3q+5)(1+\varepsilon))}(\Omega)} \\ &\leq C + C \|\nabla n^{(3q+5)/6}\|_{L^2(\Omega)}^\theta \|n^{(3q+5)/6}\|_{L^1(\Omega)}^{1-\theta}. \end{aligned}$$

We insert this expression into (42), multiply by $q+1$, and use the Young inequality $(q+1)a^{1+\theta}b^{1-\theta} \leq a^2 + C_\theta(q+1)^{2/(1-\theta)}b^2$, with $C_\theta > 0$ depending solely on θ :

$$\|n(t)\|_{L^{q+1}(\Omega)}^{q+1} + c \int_0^t \|\nabla n^{(3q+5)/6}\|_{L^2(\Omega)}^2 ds$$

$$\begin{aligned}
&\leq \|n^I\|_{L^\infty(\Omega)}^{q+1} + C(q+1) \int_0^t (1 + \|\nabla n^{(3q+5)/6}\|_{L^2(\Omega)}^{1+\theta} \|n^{(3q+5)/6}\|_{L^1(\Omega)}^{1-\theta}) ds \\
&\leq \|n^I\|_{L^\infty(\Omega)}^{q+1} + CT(q+1) + \frac{C}{2} \int_0^t \|\nabla n^{(3q+5)/6}\|_{L^2(\Omega)}^2 ds \\
&\quad + C(q+1)^{2/(1-\theta)} \int_0^t \|n^{(3q+5)/6}\|_{L^1(\Omega)}^2 ds.
\end{aligned}$$

The third term on the right-hand side can be absorbed by the left-hand side. Then, taking the supremum over $(0, T)$ and observing that $\|n^{(3q+5)/6}\|_{L^1(\Omega)}^2 = \|n\|_{L^{(3q+5)/6}(\Omega)}^{(3q+5)/3}$:

$$(43) \quad \|n\|_{L^\infty(0,T;L^{q+1}(\Omega))}^{q+1} \leq \|n^I\|_{L^\infty(\Omega)}^{q+1} + C(q+1) + C(q+1)^{2/(1-\theta)} \|n\|_{L^\infty(0,T;L^{(3q+5)/6}(\Omega))}^{(3q+5)/3}.$$

We set $q_k := q+1$ and $q_{k-1} := (3q+5)/6$, which defines the recursion $q_{k-1} = (3q_k+2)/6$ or $q_k = 2q_{k-1} - 2/3$ with the explicit solution

$$q_k = 2^k \frac{3q_0 - 2}{3} + \frac{2}{3}, \quad k \in \mathbb{N},$$

where the initialization $q_0 > 2/3$ is arbitrary. Setting

$$b_k = \|n\|_{L^\infty(0,T;L^{q_k}(\Omega))}^{q_k} + \|n^I\|_{L^\infty(\Omega)}^{q_k} + 1,$$

an elementary computation shows that (43) can be written as

$$b_k \leq C^k q_k^{2/(1-\theta)} b_{k-1}^2, \quad k \in \mathbb{N}.$$

This inequality can be solved as in [22, Sec. 3]:

$$\|n\|_{L^\infty(0,T;L^{q_k}(\Omega))} \leq (C3^{2/(1-\theta)})^{(2^{k+1}-k-2)/q_k} (\|n\|_{L^\infty(0,T;L^{q_0}(\Omega))}^{q_0} + \|n^I\|_{L^\infty(\Omega)}^{q_0} + 1)^{2^k/q_k}.$$

It is shown in [22, Sec. 3] that the exponents on the right-hand side are bounded uniformly in k . Choosing $q_0 \leq 5/3$, it follows from Lemma 10 that $N := \|n\|_{L^\infty(0,T;L^{q_0}(\Omega))}$ is bounded. Then the limit $k \rightarrow \infty$ shows that $\|n\|_{L^\infty(0,T;L^\infty(\Omega))} \leq C(n^I, N)$.

APPENDIX A. FERMI-DIRAC INTEGRALS

The Fermi-Dirac integral of order $j > -1$ is defined by

$$\mathcal{F}_j(z) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{s^j}{1+e^{s-z}} ds, \quad z \in \mathbb{R},$$

where $\Gamma(j+1) = \int_0^\infty s^j e^{-s} ds$ is the Gamma function. This function has the property $\mathcal{F}'_j = \mathcal{F}_{j-1}$ for $j > 0$. In the following, we write $A \sim B$ if there exist constants $C_1, C_2 > 0$ such that $A \leq C_1 B \leq C_2 A$.

Lemma 18. *It holds for any $j > -1$ and $z \in \mathbb{R}$ that*

$$\mathcal{F}_j(z) \sim e^z 1_{\{z \leq 0\}} + (z^{j+1} + 1) 1_{\{z > 0\}}.$$

Proof. Let first $z \leq 0$. Then $e^{s-z} < 1 + e^{s-z} \leq 2e^{s-z}$ and

$$\mathcal{F}_j(z) \geq \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{s^j}{2e^{s-z}} ds = \frac{e^z}{2}, \quad \mathcal{F}_j(z) \leq \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{s^j}{e^{s-z}} ds = e^z.$$

This shows that $\mathcal{F}_j(z) \sim e^z$ for $z \leq 0$. For $z > 0$, we write $\mathcal{F}_j(z) = I_1 + I_2$, where

$$I_1 = \frac{1}{\Gamma(j+1)} \int_0^z \frac{s^j}{1+e^{s-z}} ds, \quad I_2 = \frac{1}{\Gamma(j+1)} \int_z^\infty \frac{s^j}{1+e^{s-z}} ds.$$

We infer from $s \leq z$ and hence $e^{s-z} \leq 1$ that

$$\begin{aligned} I_1 &\geq \frac{1}{2\Gamma(j+1)} \int_0^z s^j ds = \frac{z^{j+1}}{2(j+1)\Gamma(j+1)} = \frac{z^{j+1}}{2\Gamma(j+2)}, \\ I_1 &\leq \frac{1}{\Gamma(j+1)} \int_0^z s^j ds = \frac{z^{j+1}}{\Gamma(j+2)}, \end{aligned}$$

To estimate I_2 , we assume first that $j \geq 0$ and substitute $y = s - z \geq 0$:

$$\begin{aligned} I_2 &= \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{(y+z)^j}{1+e^y} dy \geq \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{y^j}{2e^y} dy = \frac{1}{2}, \\ I_2 &\leq \frac{1}{\Gamma(j+1)} \left(\int_0^z + \int_z^\infty \right) \frac{(y+z)^j}{1+e^y} dy \\ &\leq \frac{1}{\Gamma(j+1)} \int_0^z \frac{(2z)^j}{1+e^y} dy + \frac{1}{\Gamma(j+1)} \int_z^\infty \frac{(2y)^j}{1+e^y} dy \\ &\leq \frac{(2z)^j}{\Gamma(j+1)} \int_0^z e^{-y} dy + \frac{2^j}{\Gamma(j+1)} \int_z^\infty \frac{y^j}{e^y} dy \leq \frac{(2z)^j}{\Gamma(j+1)} + 2^j. \end{aligned}$$

We conclude that

$$\mathcal{F}_j(z) \leq \frac{z^{j+1}}{\Gamma(j+2)} + \frac{(2z)^j}{\Gamma(j+1)} + 2^j, \quad \mathcal{F}_j(z) \geq \frac{z^{j+1}}{2\Gamma(j+2)} + \frac{1}{2},$$

proving that $\mathcal{F}_j(z) \sim z^{j+1} + 1$ for $z > 0$ and $j \geq 0$.

Finally, let $-1 < j < 0$. Then, arguing as before, $I_1 \leq z^{j+1}/\Gamma(j+2)$,

$$I_2 = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{(y+z)^j}{1+e^y} dy \leq \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{y^j}{e^y} dy = 1,$$

and hence $\mathcal{F}_j(z) \leq z^{j+1}/\Gamma(j+2) + 1$. The estimate from below requires a more careful computation. As the function \mathcal{F}_j is continuous and strictly increasing, its minimum on $[0, 1]$ equals $\mathcal{F}_j(0)$. Thus, for $z \in [0, 1]$,

$$\mathcal{F}_j(z) \geq \mathcal{F}_j(0) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{s^j}{1+e^s} ds > \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{s^j}{2e^s} ds = \frac{1}{2}.$$

Let $z > 1$. We always have $I_2 \geq 0$. The inequality $s^j \geq 1 \geq z^{-1}$ for $1 \leq s \leq z$ implies that $s^j \geq \frac{1}{2}(s^j + z^{-1})$ and hence,

$$\begin{aligned} I_1 &= \frac{1}{\Gamma(j+1)} \left(\int_0^1 + \int_1^z \right) \frac{s^j}{1+e^{s-z}} ds \\ &\geq \frac{1}{2\Gamma(j+1)} \int_0^1 s^j ds + \frac{1}{2\Gamma(j+1)} \int_1^z \frac{1}{2}(s^j + z^{-1}) ds \\ &= \frac{1}{4\Gamma(j+1)} \int_0^z s^j ds + \frac{1}{4\Gamma(j+1)} \int_0^1 s^j ds + \frac{1}{4\Gamma(j+1)} \int_1^z z^{-1} ds \\ &= \frac{z^{j+1}}{4\Gamma(j+2)} + \frac{1}{4\Gamma(j+1)} \left(\frac{1}{j+1} + 1 - \frac{1}{z} \right) \geq \frac{z^{j+1}}{4\Gamma(j+2)} + \frac{1}{4\Gamma(j+2)}. \end{aligned}$$

Combining the estimates for $z \in [0, 1]$ and $z > 1$ yields $\mathcal{F}_j(z) \geq C(z^{j+1} + 1)$ for all $z \geq 0$. This is the desired lower bound, which concludes the proof. \square

Corollary 19. *Let $j > 0$. Then for $z \in \mathbb{R}$,*

$$\mathcal{F}'_j(z) = \mathcal{F}_{j-1}(z) \sim \mathcal{F}_j(z)1_{\{z \leq 0\}} + \mathcal{F}_j(z)^{j/(j+1)}1_{\{z > 0\}}.$$

Proof. If $z \leq 0$ then, by Lemma 18, $\mathcal{F}_{j-1}(z) \sim e^z \sim \mathcal{F}_j(z)$. Furthermore, by the same lemma, if $z > 0$, we have $\mathcal{F}_{j-1}(z) \sim z^j = (z^{j+1})^{j/(j+1)} \sim \mathcal{F}_j(z)^{j/(j+1)}$. \square

Lemma 20. *Recall that $g = \mathcal{F}_{1/2}^{-1}$. It holds for $z > 0$ that*

$$g'(z) \sim z^{-1} + z^{-1/3}.$$

Proof. Let $z > 0$ and $y = \mathcal{F}_{1/2}^{-1}(z)$. Then, by Corollary 19,

$$\begin{aligned} g'(z) &= \frac{1}{\mathcal{F}'_{1/2}(y)} = \frac{1}{\mathcal{F}_{-1/2}(y)} \sim \frac{1}{\mathcal{F}_{1/2}(y)1_{\{y \leq 0\}} + \mathcal{F}_{1/2}(y)^{1/3}1_{\{y > 0\}}} \\ &= \frac{1}{z1_{\{y \leq 0\}} + z^{1/3}1_{\{y > 0\}}} = z^{-1}1_{\{y \leq 0\}} + z^{-1/3}1_{\{y > 0\}}, \end{aligned}$$

which shows that $g'(z) \leq C(z^{-1} + z^{-1/3})$ for $z > 0$. For the lower bound, we distinguish the cases $0 < z \leq \mathcal{F}_{1/2}(0)$ (or $y \leq 0$) and $z > \mathcal{F}_{1/2}(0)$ (or $y > 0$). The case $z \leq \mathcal{F}_{1/2}(0)$ implies that $z < 1$ (since $1/2 < \mathcal{F}_{1/2}(0) < 1$). Then the inequality $z^{-1} > z^{-1/3}$ yields $z^{-1}1_{\{y \leq 0\}} > (z^{-1} + z^{-1/3})/2$ and $g'(z) \geq C(z^{-1} + z^{-1/3})$.

Let $z > \mathcal{F}_{1/2}(0)$. If $z \geq 1$, we have $z^{-1/3}1_{\{y > 0\}} \geq z^{-1}1_{\{y > 0\}}$ and $g'(z) \geq C(z^{-1} + z^{-1/3})$. If $\mathcal{F}_{1/2}(0) < z < 1$, we observe that $\mathcal{F}_{1/2}(0) < z$ yields $\mathcal{F}_{1/2}(0)z^{-1} < 1 < z^{-1/3}$, showing that

$$z^{-1/3}1_{\{y > 0\}} > \frac{\mathcal{F}_{1/2}(0)}{2}(z^{-1} + z^{-1/3})1_{\{y > 0\}}$$

and again $g'(z) \geq C(z^{-1} + z^{-1/3})$. Summarizing these estimates, we conclude the proof. \square

Our final result is used in the proof of Lemma 13.

Lemma 21. *There exists a constant $C > 0$ such that for $z > 0$,*

$$\frac{d}{dz}(zg'(z)) \leq C(1_{\{z < \mathcal{F}_{1/2}(0)\}} + z^{-1/3}1_{\{z \geq \mathcal{F}_{1/2}(0)\}}).$$

Proof. Let $z < \mathcal{F}_{1/2}(0)$ and set $y = \mathcal{F}_{1/2}^{-1}(z) < 0$. Then

$$(44) \quad \frac{d}{dz}(zg'(z)) = g'(z) + zg''(z) = \frac{\mathcal{F}'_{1/2}(y)^2 - \mathcal{F}_{1/2}(y)\mathcal{F}''_{1/2}(y)}{\mathcal{F}'_{1/2}(y)^3}.$$

Let $N(y) := \mathcal{F}'_{1/2}(y)^2 - \mathcal{F}_{1/2}(y)\mathcal{F}''_{1/2}(y)$. We compute the derivatives

$$\mathcal{F}'_{1/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{s}e^{s-z}}{(1+e^{s-z})^2} ds, \quad \mathcal{F}''_{1/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{s}e^{s-z}(e^{s-z}-1)}{(1+e^{s-z})^3} ds,$$

yielding

$$\begin{aligned} N(y) &= \frac{4}{\pi} \int_0^\infty \int_0^\infty \frac{\sqrt{ste}^{s-y} e^{t-y} ds dt}{(1+e^{s-y})^2(1+e^{t-y})^2} - \frac{4}{\pi} \int_0^\infty \int_0^\infty \frac{\sqrt{ste}^{s-y}(e^{s-y}-1) ds dt}{(1+e^{s-y})^3(1+e^{t-y})} \\ &= \frac{4}{\pi} \int_0^\infty \int_0^\infty \sqrt{ste}^{s-y} \frac{2e^{t-y} - e^{s-y} + 1}{(1+e^{s-y})^3(1+e^{t-y})^2} ds dt \\ &= \frac{4}{\pi} \int_0^\infty \int_0^\infty \sqrt{ste}^{s-y} \left(\frac{2}{(1+e^{s-y})^3(1+e^{t-y})} - \frac{1}{(1+e^{s-y})^2(1+e^{t-y})^2} \right) ds dt \\ &= \frac{2}{\sqrt{\pi}} \mathcal{F}_{1/2}(y) \int_0^\infty \frac{2\sqrt{s}e^{s-y}}{(1+e^{s-y})^3} ds - \frac{2}{\sqrt{\pi}} \mathcal{F}'_{1/2}(y) \int_0^\infty \frac{\sqrt{t}}{(1+e^{t-y})^2} dt \\ &\leq \frac{2}{\sqrt{\pi}} \mathcal{F}_{1/2}(y) \int_0^\infty \frac{2\sqrt{s}e^{s-y}}{(1+e^{s-y})^3} ds. \end{aligned}$$

We estimate the remaining integral:

$$\frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{s}e^{s-y}}{(1+e^{s-y})^3} ds \leq \frac{2}{\sqrt{\pi}} e^y \int_0^\infty \frac{\sqrt{s}e^{s-y}}{(1+e^{s-y})^2} ds = e^y \mathcal{F}'_{1/2}(y).$$

Therefore, using Lemma 18 for $y = \mathcal{F}_{1/2}^{-1}(z) < 0$,

$$N(y) \leq 2e^y \mathcal{F}_{1/2}(y) \mathcal{F}'_{1/2}(y) \leq C_1 e^{3y}, \quad \mathcal{F}'_{1/2}(y)^3 = \mathcal{F}_{-1/2}(y)^3 \geq C_2 e^{3y}.$$

We conclude from (44) for $z < \mathcal{F}_{1/2}(0)$ that

$$\frac{d}{dz}(zg'(z)) = \frac{N(y)}{\mathcal{F}'_{1/2}(y)^3} \leq \frac{C_1}{C_2}.$$

Next, let $z \geq \mathcal{F}_{1/2}(0)$ (or $y \geq 0$). We know from the proof of Lemma 20 that in this case $g'(z) \leq Cz^{-1/3}$. According to (44), it remains to show that

$$zg''(z) = -\frac{\mathcal{F}_{1/2}(y)\mathcal{F}''_{1/2}(y)}{\mathcal{F}'_{1/2}(y)^3} \leq Cz^{-1/3} \quad \text{for } z \geq \mathcal{F}_{1/2}(0).$$

To this end, we fix some $y_0 > \mathcal{F}_{1/2}(0)$ and choose $0 < \varepsilon < y_0$. For $y > y_0$, we split the integral $-\mathcal{F}_{1/2}''$ into two parts, $-\mathcal{F}_{1/2}''(y) = I_3 + I_4$, where

$$I_3 = -\frac{2}{\sqrt{\pi}} \int_0^\varepsilon \frac{\sqrt{s}e^{s-y}(e^{s-y} - 1)}{(1 + e^{s-y})^3} ds, \quad I_4 = -\frac{2}{\sqrt{\pi}} \int_\varepsilon^\infty \frac{\sqrt{s}e^{s-y}(e^{s-y} - 1)}{(1 + e^{s-y})^3} ds.$$

The estimate of I_3 is straightforward:

$$I_3 \leq \frac{2}{\sqrt{\pi}} e^{\varepsilon-y} \int_0^\varepsilon \sqrt{s} ds = \frac{4}{3\sqrt{\pi}} e^{\varepsilon-y} \varepsilon^{3/2}.$$

We integrate by parts in I_4 twice and split the resulting integral into two parts:

$$\begin{aligned} I_4 &= \frac{2}{\sqrt{\pi}} \left(\left. \frac{\sqrt{s}e^{s-y}}{(1 + e^{s-y})^2} \right|_\varepsilon^\infty + \int_\varepsilon^\infty \frac{s^{-1/2}e^{s-y}}{2(1 + e^{s-y})^2} ds \right) \\ &= \frac{2}{\sqrt{\pi}} \left\{ -\frac{\sqrt{\varepsilon}e^{\varepsilon-y}}{(1 + e^{\varepsilon-y})^2} + \left(\left. \frac{s^{-1/2}}{2(1 + e^{s-y})} \right|_\varepsilon^\infty + \int_\varepsilon^\infty \frac{s^{-3/2}}{4(1 + e^{s-y})} ds \right) \right\} \\ &= -\frac{2}{\sqrt{\pi}} \left(\frac{\sqrt{\varepsilon}e^{\varepsilon-y}}{(1 + e^{\varepsilon-y})^2} + \frac{\varepsilon^{-1/2}}{2(1 + e^{\varepsilon-y})} \right) + \frac{2}{\sqrt{\pi}} (I_5 + I_6), \end{aligned}$$

where

$$\begin{aligned} I_5 &= \int_\varepsilon^y \frac{s^{-3/2}}{4(1 + e^{s-y})} ds \leq \frac{1}{4(1 + e^{\varepsilon-y})} \int_\varepsilon^y s^{-3/2} ds = \frac{\varepsilon^{-1/2} - y^{-1/2}}{2(1 + e^{\varepsilon-y})}, \\ I_6 &= \int_y^\infty \frac{s^{-3/2}}{4(1 + e^{s-y})} ds \leq \frac{1}{2} \int_y^\infty s^{-3/2} ds = y^{-1/2}. \end{aligned}$$

Summarizing these estimates, we observe that the contributions that are singular for $\varepsilon \rightarrow 0$ cancel, and we end up with

$$\begin{aligned} -\mathcal{F}_{1/2}''(y) &\leq \frac{2}{\sqrt{\pi}} \left\{ \frac{2}{3} e^{\varepsilon-y} \varepsilon^{3/2} - \left(\frac{\sqrt{\varepsilon}e^{\varepsilon-y}}{(1 + e^{\varepsilon-y})^2} + \frac{\varepsilon^{-1/2}}{2(1 + e^{\varepsilon-y})} \right) + \frac{\varepsilon^{-1/2} - y^{-1/2}}{2(1 + e^{\varepsilon-y})} + y^{-1/2} \right\} \\ &= \frac{2}{\sqrt{\pi}} \left(\frac{2}{3} e^{\varepsilon-y} \varepsilon^{3/2} - \frac{\sqrt{\varepsilon}e^{\varepsilon-y}}{(1 + e^{\varepsilon-y})^2} + \frac{1 + 2e^{\varepsilon-y}}{2(1 + e^{\varepsilon-y})} y^{-1/2} \right). \end{aligned}$$

Since $\varepsilon > 0$ is arbitrary, we can pass to the limit $\varepsilon \rightarrow 0$ to find that for all $y \geq 0$,

$$-\mathcal{F}_{1/2}''(y) \leq \frac{2}{\sqrt{\pi}} \frac{1 + 2e^{-y}}{2(1 + e^{-y})} y^{-1/2} \leq C y^{-1/2}.$$

We use the previous inequality to estimate the nominator and Corollary 19 to estimate the denominator in (44):

$$zg''(z) = -\frac{\mathcal{F}_{1/2}(y)\mathcal{F}_{1/2}''(y)}{\mathcal{F}_{1/2}'(y)^3} \leq C \frac{\mathcal{F}_{1/2}(y)y^{-1/2}}{\mathcal{F}_{1/2}'(y)} \leq \frac{C}{y^{1/2}} \quad \text{for } y > y_0.$$

For $0 \leq y \leq y_0$, the expression $zg''(z)$ is bounded since $\mathcal{F}_{1/2}$ and its derivatives are bounded in $[0, y_0]$. In case $y > y_0$, we wish to have an upper bound in terms of z . For this, we

notice that, by Lemma 18, $z = \mathcal{F}_{1/2}(y) \leq C_1(y^{3/2} + 1)$. It follows from $y > y_0$ that $z \leq C_1(1 + y_0^{-3/2})y^{3/2} =: C_2y^{3/2}$ and

$$zg''(z) \leq Cy^{-1/2} \leq CC_2^{1/3}z^{-1/3}.$$

This concludes the proof. \square

APPENDIX B. A NONLINEAR POINCARÉ–WIRTINGER-TYPE LEMMA

We show a nonlinear version of the Poincaré–Wirtinger inequality.

Lemma 22. *Let $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) be a bounded domain, let $f : [0, b) \rightarrow [0, \infty)$ with $b \in \mathbb{R} \cup \{+\infty\}$, be a strictly increasing function, let $u \in L^1(\Omega)$ satisfy $f(u) \in H^1(\Omega)$ and $u_\Omega := m(\Omega)^{-1} \int_\Omega u dx < b$. Then for any $\hat{u} \in (u_\Omega, b)$ one has*

$$\|f(u)\|_{L^2(\Omega)}^2 \leq 2m(\Omega)f(\hat{u})^2 + 4C_P \left(1 + \frac{\hat{u}}{\hat{u} - u_\Omega}\right) \|\nabla f(u)\|_{L^2(\Omega)}^2,$$

where $C_P > 0$ is the square of the constant of the Poincaré–Wirtinger inequality.

Notice that the function f may be singular at b . Therefore, we need the condition $u_\Omega < b$ to ensure that the right-hand side is finite. We apply this lemma in the proof of Lemma 15 with $f(u) = -\log(1 - u)$, $u \in (0, 1)$.

Proof. The proof is based on the arguments of [6, Lemma 4.1]. We set $A := (f(u) - f(\hat{u}))^+$ and $A_\Omega = m(\Omega)^{-1} \int_\Omega A dx$. Since $f(u)^2 \leq 2f(\hat{u})^2 + 2[(f(u) - f(\hat{u}))^+]^2 = 2f(\hat{u})^2 + 2A^2$, we have

$$(45) \quad \int_\Omega f(u)^2 dx \leq 4 \int_\Omega (A - A_\Omega)^2 dx + 4 \int_\Omega A_\Omega^2 dx + 2m(\Omega)f(\hat{u})^2.$$

We set $C_1 := 2m(\Omega)f(\hat{u})^2$ for the last term. The first term is estimated according to the Poincaré–Wirtinger inequality as

$$(46) \quad \int_\Omega (A - A_\Omega)^2 dx \leq C_P \|\nabla A\|_{L^2(\Omega)}^2 \leq C_P \|\nabla f(u)\|_{L^2(\Omega)}^2.$$

Furthermore,

$$\int_\Omega (A - A_\Omega)^2 dx = \int_{\{A=0\}} A_\Omega^2 dx + \int_{\{A>0\}} (A - A_\Omega)^2 dx \geq m(\{A=0\})A_\Omega^2.$$

The previous two inequalities yield

$$(47) \quad A_\Omega^2 \leq \frac{C_P}{m(\{A=0\})} \|\nabla f(u)\|_{L^2(\Omega)}^2.$$

We need to derive a lower bound for $m(\{A=0\})$. To this end, we observe that $A > 0$ if and only if $u > \hat{u}$ since f is assumed to be strictly increasing. Then

$$(m(\Omega) - m(\{A=0\}))\hat{u} = m(\{A>0\})\hat{u} = \int_{\{u>\hat{u}\}} \hat{u} dx \leq \int_\Omega u dx = m(\Omega)u_\Omega.$$

It follows that

$$m(\{A = 0\}) \geq m(\Omega) \frac{\hat{u} - u_\Omega}{\hat{u}} > 0,$$

and we infer from (47) that

$$A_\Omega^2 \leq \frac{\hat{u}}{\hat{u} - u_\Omega} \frac{C_P}{m(\Omega)} \|\nabla f(u)\|_{L^2(\Omega)}^2.$$

Combining this inequality with (45) and (46), we obtain the result. \square

REFERENCES

- [1] D. Abdel, C. Chainais-Hillairet, P. Farrell, and M. Herda. Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells. *IMA J. Numer. Anal.* 44 (2023), 1090–1129.
- [2] D. Abdel, A. Glitzky, and M. Liero. Analysis of a drift–diffusion model for perovskite solar cells. *Discrete Cont. Dyn. Sys.*, online first, 2024. DOI: 10.3934/dcdsb.2024081.
- [3] A. Bhattacharya, M. Gahn, and M. Neuss-Radu. Homogenization of a nonlinear drift–diffusion system for multiple charged species in a porous medium. *Nonlin. Anal. Real World Appl.* 68 (2022), no. 103651, 28 pages.
- [4] J. Blakemore. Approximations for Fermi–Dirac integrals. *Solid State Electron.* 25 (1982), 1067–1076.
- [5] D. Bothe, A. Fischer, M. Pierre, and G. Rolland. Global existence for diffusion–electromigration systems in space dimension three and higher. *Nonlin. Anal.* 99 (2014), 152–166.
- [6] C. Cancès, C. Chanais-Hillairet, J. Fuhrmann, and B. Gaudeul. A numerical-analysis-focused comparison of several finite volume schemes for a unipolar degenerate drift–diffusion model. *IMA J. Numer. Anal.* 41 (2021), 271–314.
- [7] Y. Choi and R. Lui. Multi-dimensional electrochemistry model. *Arch. Ration. Mech. Anal.* 130 (1995), 315–342.
- [8] P. Degond, S. Génieys, and A. Jüngel. A system of parabolic equations in nonequilibrium thermodynamics including thermal and electrical effects. *J. Math. Pures Appl.* 76 (1997), 991–1015.
- [9] K. Disser and J. Rehberg. Optimal Sobolev regularity for linear second-order divergence elliptic operators occurring in real-world problems. *SIAM J. Math. Anal.* 47 (2015), 1719–1746.
- [10] H. Gajewski, K. Gröger. Semiconductor equations for variable mobilities based on Boltzmann statistics or Fermi–Dirac statistics. *Math. Nachr.* 140 (1989), 7–36.
- [11] H. Gajewski and K. Gröger. Reaction–diffusion processes of electrically charged species. *Math. Nachr.* 177 (1996), 109–130.
- [12] A. Glitzky and R. Hünlich. Global estimates and asymptotics for electro-reaction-diffusion systems in heterostructures. *Appl. Anal.* 66 (1997), 206–226.
- [13] A. Glitzky and R. Hünlich. Global existence result for pair diffusion models. *SIAM J. Math. Anal.* 36 (2005), 1200–1225.
- [14] A. Glitzky and M. Liero. Instationary drift–diffusion problems with Gauss–Fermi statistics and field-dependent mobility for organic semiconductor devices. *Commun. Math. Sci.* 17 (2019), 33–59.
- [15] J. Greenlee, J. Shank, M. Tellekamp, and A. Doolittle. Spatiotemporal drift–diffusion simulations of analog circuit memristors. *J. Appl. Phys.* 114 (2013), no. 034504, 9 pages.
- [16] K. Gröger. Boundedness and continuity of solutions to linear elliptic boundary value problems in two dimensions. *Math. Ann.* 298 (1994), 719–728.
- [17] A. Heibig, A. Petrov, and C. Reichert. Solvability for a drift–diffusion system with Robin boundary conditions. *J. Differ. Eqs.* 267 (2019), 2331–2356.
- [18] D. Ielmini and S. Ambrogio. Emerging neuromorphic devices. *Nanotechnology* 31 (2020), no. 092001, 24 pages.

- [19] C. Jourdana, A. Jüngel, and N. Zamponi. Three-species drift–diffusion models for memristors. *Math. Models Meth. Appl. Sci.* 33 (2023), 2113–2156.
- [20] A. Jüngel. Asymptotic analysis of a semiconductor model based on Fermi–Dirac statistics. *Math. Meth. Appl. Sci.* 19 (1996), 401–424.
- [21] A. Jüngel. *Transport Equations for Semiconductors*. Lect. Notes Phys. 773, Springer, Berlin, 2009.
- [22] A. Jüngel and M. Vetter. Degenerate drift–diffusion systems for memristors. Submitted for publication, 2023. arXiv:2311.16591.
- [23] V. Mladenov. *Advanced Memristor Modeling*. MDPI, Basel, 2019.
- [24] E. Shamir. Regularization of mixed second-order elliptic problems. *Israel J. Math.* 6 (1968), 150–168.
- [25] D. Strukov, J. Borghetti, and S. Williams. Coupled ionic and electronic transport model of thin-film semiconductor memristive behavior. *Small* 5 (2009), 1058–1063.
- [26] N. Tessler and Y. Vaynzof. Insights from device modeling of perovskite solar cells. *ACS Energy Lett.* 5 (2020), 1260–1270.
- [27] E. Zeidler. *Nonlinear Functional Analysis and Its Applications II/A: Linear Monotone Operators*. Springer, New York, 1990.

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