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INSTATIONARY DRIFT-DIFFUSION PROBLEMS WITH GAUSS–FERMI STATISTICS AND FIELD-DEPENDENT MOBILITY FOR ORGANIC SEMICONDUCTOR DEVICES*

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Abstract. This paper deals with the analysis of an instationary drift-diffusion model for organic semiconductor devices including Gauss–Fermi statistics and application-specific mobility functions. The charge transport in organic materials is realized by hopping of carriers between adjacent energetic sites and is described by complicated mobility laws with a strong nonlinear dependence on temperature, carrier densities and the electric field strength.

To prove the existence of global weak solutions, we consider a problem with (for small densities) regularized state equations on any arbitrarily chosen finite time interval. We ensure its solvability by time discretization and passage to the time-continuous limit. Positive lower a priori estimates for the densities of its solutions that are independent of the regularization level ensure the existence of solutions to the original problem. Furthermore, we derive for these solutions global positive lower and upper bounds strictly below the density of transport states for the densities. The estimates rely on Moser iteration techniques.

Keywords. Drift-diffusion system; nonlinear parabolic system; organic semiconductor; charge transport; existence of weak solutions; Gauss–Fermi statistics.

AMS subject classifications. 35K20; 35K55; 35B45; 78A35; 82A57; 82A70.

1. Introduction

Organic electronics is a future-oriented green technology using carbon-based semiconductor materials. Today, devices based on these materials surround us in our everyday life, e.g., in smartphone displays or solar cells. On the one hand, the technological adaption to other applications such as advanced lighting applications and thin-film transistors is still at an early stage. On the other hand, the tremendously fast pace in the development of new organic materials with fine-tuned properties yields the potential for smart three-dimensional vertical structures with desired electronic behavior.

Contrary to classical, inorganic semiconductor materials, in the organic case charge transport is realized by temperature-activated hopping of electrons and holes between adjacent molecules. The random alignment of the molecules leads to a disordered system with Gaussian distributed energy levels for the carriers. Therefore, in contrast to inorganic semiconductors (where either Fermi–Dirac or Boltzmann statistics are used), the statistical description of the energetic distribution of the charge carriers here has to be substituted by Gauss–Fermi statistics (see Subsection 2.1).

In the literature (e.g. [16] and the references therein), organic materials are modeled at different scales, ranging from density functional theory for molecules, master equation approaches for carrier dynamics in homogeneous materials, to drift-diffusion equations. However, a master equation approach for the hopping transport with kinetic Monte-Carlo methods as proposed in [15, 23] are in general computationally very costly and are less suited for the description of complicated geometric device structures and the inclusion of other physical effects such as heat flow. On the other hand, coarser models,

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such as the $p(x)$-Laplace thermistor model for the electrothermal interplay in organic light-emitting diodes considered in [19, 20], reduce the computational effort and allow to treat the full geometric device structure but are less accurate.

Within the hierarchy of models, the drift-diffusion modeling is most adequate for the description and simulation of complex, multi-dimensional organic devices. For example, to determine the behavior of advanced organic LEDs or to identify current paths in small scale devices like vertical organic field-effect transistors, a detailed description on the drift-diffusion level incorporating electron and hole currents, recombinations, and heterostructures is needed. The description should be entirely based on the geometrical structure and on the individual properties of each material layer, allowing to simulate the behavior of the device and in perspective, to study optimization strategies for the device layout including efficient doping designs. As a milestone in this direction, stable numerical discretization schemes for non-Boltzmann statistics have been introduced in [5]. Moreover, drift-diffusion modeling is well suited to couple also other physical effects such as heat flow.

In the analytical treatment of drift-diffusion models for organics with Gauss–Fermi statistics we have to overcome two new essential problems in comparison to the usual classical van Roosbroeck system (studied e.g. in [8, 21] and the references therein):

(i) The mobility laws, which arise from fitting to kinetic Monte–Carlo simulations, exhibit strongly nonlinear dependences on the temperature T, carrier density n and the electric field strength F (see Subsection 2.2). They are usually given in product form

$$\mu_n(T, n, F) = \mu_{n0}(T) \times g_1(n, T) \times g_2(F, T).$$

Especially the dependence of the mobility on the field strength has to be managed and requires new arguments in the existence proof.

(ii) The statistical relation in organic semiconductor materials is given by Gauss-Fermi integrals [22], i.e.

$$n = \int_{-\infty}^{\infty} N_{\mathrm{Gauss}}(E) f(E - E_F)\,\mathrm{d}E,$$

where N_{Gauss} denotes a Gaussian density, E_F is the Fermi energy, and f is the Fermi-Dirac occupation probability. In particular, the Gauss–Fermi statistics does not satisfy the standard assumption of monotone and unbounded statistical relations as in Gajewski/Gröger [7, Eq. (2.3)] for the treatment of non-Boltzmann statistics (see also [9, Eq. (3.5)], [6, 10–12]).

In the literature, there are only a few papers dealing with the analysis of drift-diffusion problems in the setting of organics. They mostly concentrate on special aspects arising in photovoltaics (excitons, polarons) and they do not take the Gauss–Fermi statistics into account. However, they consider some field strength-dependent (Poole–Frenkel) mobility laws (see e.g. [2, 24] and the references therein).

For the stationary problem, [4] gives the first existence result taking all the features of an organic drift-diffusion model into account. The present paper now tackles the corresponding instationary problem in two spatial dimensions. We verify existence of weak solutions as well as upper and lower bounds for solutions. The applied techniques work successfully in the two-dimensional case, but cannot be carried over to higher dimensions. This is mainly caused by the fact that the regularity results for the electrostatic potential are not sufficient for the estimation of the drift terms in the Moser estimates to get bounds for the charge carrier densities (comp. last but one lines in

(4.20) and (5.7) and the beginning of Section 4). Moreover, we make use of imbedding, Gagliardo-Nirenberg and trace inequalities that depend on the spatial dimension.

The plan of the paper is as follows: In Section 2, we introduce the model equations and identify the crucial differences to the classical van Roosbroeck system such as the carrier statistics (Subsection 2.1) and nonlinear mobility laws (Subsection 2.2). In Section 3, we rescale the model equations, formulate our assumption for the analytical treatment of the problem, and give the weak formulation of the instationary drift-diffusion system. Moreover we introduce the associated free energy functional, give energy estimates and estimates of the electrostatic potential for weak solutions of the problem (Subsection 3.4). Section 4 is devoted to the existence of weak solutions (Theorem 4.1). In Subsection 4.1, we consider a problem with (for small densities) regularized state equations. Its solvability is ensured by time discretization and passage to the limit. Positive lower a priori estimates for the densities of its solutions that are independent of the regularization level (Lemma 4.3) ensure the solvability of the original problem. Finally, in Section 5 we derive global positive lower bounds (Theorem 5.1) and global upper bounds strictly less than the number of transport states (Theorem 5.2) for the carrier densities by Moser iteration.

2. Drift-diffusion modeling of organic semiconductor devices

In organic semiconductor devices, which are based on organic molecules or polymers, the transport of electrons (and holes) happens via hopping processes of charge carriers between discrete energy levels of adjacent molecular sites, see Figure 2.1 for the case of electrons. For charge carriers, there exist two energy states on organic molecules: the Highest Occupied Molecular Orbital (HOMO, energy E_H) as well as the Lowest Unoccupied Molecular Orbital (LUMO, energy E_L). The LUMO-states describe delocalized electrons in the π-bindings, whereas the HOMO-states describe the electrons in the localized electron pair-bindings between the atoms of the molecule. By crossing the HOMO-LUMO gap (e.g. by optical excitation) electrons in the molecule can change from the HOMO-state into the LUMO-state. Thereby there arises a positively charged cavity in the charge cloud of the molecule which is called a hole. Since charge carriers can move by hopping transport between energy levels of neighboring molecules, organic semiconductor materials behave like amorphous semiconductors. This process is depicted schematically in Figure 2.1 for electrons, a corresponding Gaussian centered at a lower energy value $E_H < E_L$ and with a variance σ_p describes the situation for the holes.

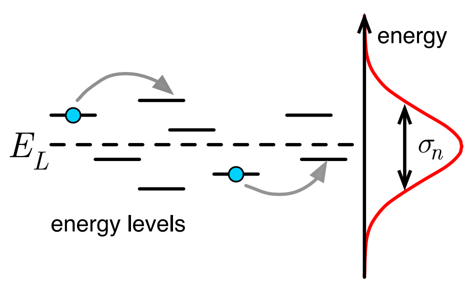

FIG. 2.1. *Hopping-transport of electrons between Gaussian distributed energy levels (centered at E_L with variance σ_n) of neighboring molecules.*

Charge transport in organic semiconductor devices, neglecting thermal effects, is described by generalized drift-diffusion models of van Roosbroeck type. The model contains continuity equations for the densities n and p of electrons and holes, respectively, and a Poisson equation for the electrostatic potential ψ considered on the product of a time interval and a spatial domain Ω:

$$\begin{aligned} -\nabla\cdot(\varepsilon_0\varepsilon_r\nabla\psi) &= q(C-n+p), \\ q\frac{\partial n}{\partial t} - \nabla\cdot j_n &= -qR, \qquad j_n = -qn\mu_n\nabla\varphi_n, \\ q\frac{\partial p}{\partial t} + \nabla\cdot j_p &= -qR, \qquad j_p = -qp\mu_p\nabla\varphi_p. \end{aligned} \tag{2.1}$$

Here q is the elementary charge, ε_r the relative permittivity, and R the recombination rate. Further, φ_n and φ_p denote the quasi-Fermi potentials, j_n and j_p are the electron- and hole current densities that are characterized by the electric mobilities μ_n, μ_p. In principle, (2.1) looks like the van Roosbroeck system for classical inorganic semiconductors. However, there are essential differences with respect to statistical relations and mobility functions that depend in the organic case on the gradient of the electrostatic potential. These cause additional difficulties in the mathematical analysis for the model. The essential features are shortly explained in the next subsections, for a more detailed discussion see also [4].

2.1. Statistical relation between densities and chemical potentials via Gaussian Disorder Model (GDM). In organic semiconductors, the energy positions are Gaussian distributed, such that both, the electrons and holes, can be described by a Gaussian density of state, see Figure 2.1

$$N_{\mathrm{Gauss}}(E) = \frac{N_0}{\sqrt{2\pi}\,\sigma}\exp\Big[-\Big(\frac{E-E_0}{\sqrt{2}\sigma}\Big)^2\Big],$$

where N_0 gives the total density of transport states. E_0 denotes the corresponding average HOMO- and LUMO-levels, respectively, and σ their variance. Note that σ is also called the disorder parameter which characterizes the disorder of the organic material. The density of electrons (and similarly also for holes) is given by the Gauss–Fermi integral

$$n = \frac{N_{n0}}{\sqrt{2\pi}\,\sigma_n}\int_{-\infty}^{\infty}\exp\Big(-\frac{(E-E_L+q\psi)^2}{2\sigma_n^2}\Big)\frac{1}{\exp\big(\frac{E-E_F}{k_{\mathrm{B}}T}\big)+1}\,\mathrm{d}E \tag{2.2}$$

where E_L stands for the LUMO-energy, E_F denotes the Fermi energy, k_{B} is Boltzmann's constant, and the Fermi function $f(E,T) = \big(\exp\big(\frac{E-E_F}{k_{\mathrm{B}}T}\big)+1\big)^{-1}$ gives the probability that an electron is in the quantum state with the energy E. The shift by $q\psi$ in the Gaussian describes the situation that an electric field $-\nabla\psi$ is present in the semiconductor with a weakly spatially varying potential ψ.

Thus, using the variable $\xi = \frac{E-E_L+q\psi}{\sigma_n}$ it follows from (2.2) that

$$\begin{aligned} n &= \frac{N_{n0}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big(-\frac{\xi^2}{2}\Big)\frac{1}{\exp\big(\frac{\sigma_n}{k_{\mathrm{B}}T}\xi - \frac{E_F-E_L+q\psi}{k_{\mathrm{B}}T}\big)+1}\,\mathrm{d}\xi \\ &= \frac{N_{n0}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big(-\frac{\xi^2}{2}\Big)\frac{1}{\exp\big(s_n\xi-\eta_n\big)+1}\,\mathrm{d}\xi \\ &= N_{n0}\mathcal{G}_{s_n}(\eta_n), \qquad \eta_n := \frac{E_F-E_L+q\psi}{k_{\mathrm{B}}T} = \frac{q(\psi-\varphi_n)-E_L}{k_{\mathrm{B}}T}, \quad s_n := \frac{\sigma_n}{k_{\mathrm{B}}T} \end{aligned} \tag{2.3}$$

with the dimensionless quantities s_n and η_n.

Similar to this representation of the electron density by means of the renormalized chemical potential of the electrons, the hole density p is given as function of the renormalized chemical potential of the holes:

$$p = N_{p0}\mathcal{G}_{s_p}(\eta_p), \qquad \eta_p := \frac{E_H - q(\psi - \varphi_p)}{k_B T}, \quad s_p := \frac{\sigma_p}{k_B T},$$

where E_H denotes the HOMO energy.

Next, we collect some properties of the so called Gauss–Fermi statistics $\mathcal{G}_s$ which are useful in the analysis performed in this paper. Since the Fermi function f takes only values between 0 and 1, (2.3) ensures

$$0 < n = n(\eta_n) < \frac{N_{n0}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big(-\frac{\xi^2}{2}\Big)\,\mathrm{d}\xi = N_{n0} \quad \forall \eta_n \in \mathbb{R},$$

such that the carrier density in organic materials remains bounded for all values of η_n. By partial integration we can rewrite

$$\mathcal{G}_s(\eta) = -\frac{1}{\sqrt{2\pi}s} \int_{-\infty}^{\infty} \exp\Big(-\frac{\xi^2}{2}\Big)\xi\, \ln(\exp(-s\xi + \eta) + 1)\,\mathrm{d}\xi.$$

Moreover, the map $\eta \mapsto \mathcal{G}_s(\eta)$ is strictly monotonically increasing, $\mathcal{G}_s$ is differentiable and

$$\mathcal{G}_s'(\eta) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\exp\big(s\xi - \eta\big)}{\big(\exp(s\xi - \eta) + 1\big)^2}\, \exp\Big(-\frac{\xi^2}{2}\Big)\,\mathrm{d}\xi \tag{2.4}$$

$$= -\frac{1}{\sqrt{2\pi}s} \int_{-\infty}^{\infty} \frac{\exp\big(-\frac{\xi^2}{2}\big)\xi\,\mathrm{d}\xi}{\exp(s\xi - \eta) + 1}. \tag{2.5}$$

Note that the fraction in the first integrand takes values only between 0 and 1. Therefore,

$$\mathcal{G}_s'(\eta) \in (0,1), \quad \lim_{\eta\to+\infty} \mathcal{G}_s'(\eta) = \lim_{\eta\to-\infty} \mathcal{G}_s'(\eta) = 0, \quad \mathcal{G}_s'(\eta) = \mathcal{G}_s'(-\eta).$$

Moreover, using $\exp\big(s\xi - \eta\big) < \exp(s\xi - \eta) + 1$ in the expression (2.4) for $\mathcal{G}_s'$, we have

$$\mathcal{G}_s'(\eta) < \mathcal{G}_s(\eta) \quad \forall \eta \in \mathbb{R},\ \forall s \geq 0. \tag{2.6}$$

The properties of the Gauss–Fermi statistics stated in the following lemma are of significant importance for the proof of upper bounds of the carrier densities n and p (strictly less than N_{n0} and N_{p0}, respectively,) of the solutions to the instationary problem (2.1).

LEMMA 2.1. *For all $s > 0$ there are constants $\underline{c}(s)$, $\overline{c}(s) > 0$ such that*

$$\underline{c}(s) \leq \mathrm{e}^{\eta}\,\mathcal{G}_s'(\eta) \leq \overline{c}(s), \quad \mathrm{e}^{\eta}|\mathcal{G}_s''(\eta)| \leq 3\overline{c}(s), \quad \frac{|\mathcal{G}_s''(\eta)|}{\mathcal{G}_s'(\eta)} \leq \frac{3\overline{c}(s)}{\underline{c}(s)} \quad \text{for all } \eta > s. \tag{2.7}$$

Moreover, $\mathcal{G}_s''(\eta) < 0$ for all $\eta \geq 0$.

Proof. According to the expression for $\mathcal{G}_s'(\eta)$ in (2.4) we find for $\eta \geq s$ that

$$\mathrm{e}^{\eta}\,\mathcal{G}_s'(\eta) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\big(-\frac{\xi^2}{2}\big) \frac{\exp\,(s\xi)}{(\exp(s\xi - \eta) + 1)^2}\,\mathrm{d}\xi$$

$$\geq \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} \exp\big(-\frac{\xi^2}{2}\big)\,\mathrm{d}\xi\ \frac{\exp(-s)}{4} =: \underline{c}(s).$$

Moreover, exploiting the inequality

$$\frac{1}{\exp(s\xi-\eta)+1}\le 1 \tag{2.8}$$

we obtain

$$\begin{aligned}
\mathrm{e}^{\eta}\,\mathcal{G}_s'(\eta) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\big(-\frac{\xi^2}{2}\big)\frac{\exp(s\xi)}{(\exp(s\xi-\eta)+1)^2}\,\mathrm{d}\xi \le \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\big(-\frac{\xi^2}{2}\big)\,\exp(s\xi)\,\mathrm{d}\xi\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\big(-\frac{(\xi-s)^2}{2}\big)\,\exp\big(\frac{s^2}{2}\big)\,\mathrm{d}\xi =: \overline{c}(s).
\end{aligned}$$

Additionally, from the expression for $\mathcal{G}_s'(\eta)$ in (2.4) we calculate

$$\begin{aligned}
\mathcal{G}_s''(\eta) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\big(-\frac{\xi^2}{2}\big)\frac{\exp(s\xi-\eta)\big[\exp(s\xi-\eta)-1\big]}{(\exp(s\xi-\eta)+1)^3}\,\mathrm{d}\xi\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\big(-\frac{\xi^2}{2}\big)\exp(s\xi-\eta)\Big[\frac{1}{(\exp(s\xi-\eta)+1)^2}-\frac{2}{(\exp(s\xi-\eta)+1)^3}\Big]\,\mathrm{d}\xi.
\end{aligned}$$

Therefore, (2.8) results in

$$\begin{aligned}
\mathrm{e}^{\eta}\,|\mathcal{G}_s''(\eta)| &\le \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\big(-\frac{\xi^2}{2}\big)\Big[\frac{\exp(s\xi)}{(\exp(s\xi-\eta)+1)^2}+\frac{2\exp(s\xi)}{(\exp(s\xi-\eta)+1)^3}\Big]\,\mathrm{d}\xi\\
&\le \overline{c}(s)+2\overline{c}(s)=3\overline{c}(s),
\end{aligned}$$

such that also the last two assertions in (2.7) follow. Using the expression for $\mathcal{G}_s'(\eta)$ in (2.5), we derive

$$\begin{aligned}
\mathcal{G}_s''(\eta) &= -\frac{1}{\sqrt{2\pi}s}\int_{-\infty}^{\infty}\frac{\exp\big(-\frac{\xi^2}{2}\big)\xi\,\exp(s\xi-\eta)\,\mathrm{d}\xi}{(\exp(s\xi-\eta)+1)^2}\\
&= -\frac{1}{\sqrt{2\pi}s}\int_{0}^{\infty}\xi\exp\big(-\frac{\xi^2}{2}\big)\Big[\frac{\exp(s\xi-\eta)}{(\exp(s\xi-\eta)+1)^2}-\frac{\exp(-s\xi-\eta)}{(\exp(-s\xi-\eta)+1)^2}\Big]\,\mathrm{d}\xi.
\end{aligned} \tag{2.9}$$

For $s>0$, $\xi>0$ and $\eta>0$ we obtain from

$$0<(\mathrm{e}^{s\xi}-1)(\mathrm{e}^{\eta}-1)=\mathrm{e}^{s\xi+\eta}-\mathrm{e}^{\eta}-\mathrm{e}^{s\xi}+1$$

by dividing by e^{η} that $\mathrm{e}^{s\xi-\eta}+1<\mathrm{e}^{-\eta}+\mathrm{e}^{s\xi}$. This ensures the estimate

$$\frac{\exp(s\xi-\eta)}{(\exp(s\xi-\eta)+1)^2}>\frac{\exp(s\xi-\eta)}{(\exp(-\eta)+\exp(s\xi))^2}=\frac{\exp(-s\xi-\eta)}{(\exp(-s\xi-\eta)+1)^2}$$

and the integrand in the second line of (2.9) is positive such that we obtain the property $\mathcal{G}_s''(\eta)<0$ for $\eta>0$. ☐

2.2. Mobility functions. The mobility functions μ_n, μ_p for organic semiconductor materials with Gaussian density of state show a positive feedback with respect to temperature T, density n or p, and with respect to electrical field strength $F=|\nabla\psi|$. In [4] we discussed and summarized the results of [3, 23], and [15] obtained as extension of the Gaussian disorder model for the dependence of the charge carrier mobility. They arise from numerical solutions of the master equation for hopping transport in a disordered energy landscape with a Gaussian density of state to determine these dependencies. Written exemplarily for the electron mobility, [23] ended up in the product form of the mobility

$$\mu_n(T,n,F) = \mu_{n0}(T) \times g_1(n,T) \times g_2(F,T). \tag{2.10}$$

For the further analysis, we suppose as in [4] for the electron and hole mobilities that $\mu_n : \Omega \times (0,\infty) \times [0, \operatorname{ess\,sup} N_{n0}] \times \mathbb{R}_+ \to \mathbb{R}$, $\mu_p : \Omega \times (0,\infty) \times [0, \operatorname{ess\,sup} N_{p0}] \times \mathbb{R}_+ \to \mathbb{R}$ are Caratheodory functions fulfilling

$$\begin{aligned} &0 < \underline{\mu} \le \mu_n(\cdot,T,n,F),\ \mu_p(\cdot,T,p,F) \le \overline{\mu} < \infty \\ &\forall (T,n,p,F) \in [T_a,\infty) \times [0,\operatorname{ess\,sup} N_{n0}] \times [0,\operatorname{ess\,sup} N_{p0}] \times \mathbb{R}_+ \text{ a.e. in } \Omega. \end{aligned} \tag{2.11}$$

2.3. Generation-recombination term. Following the depiction in [5] and in [4], we assume for the generation-recombination term an expression of the form

$$R = r(\cdot,n,p,T)\Big(1 - \exp\frac{q(\varphi_n - \varphi_p)}{k_{\rm B}T}\Big), \quad r(\cdot,n,p,T) = r_0(\cdot,n,p,T)\,np, \tag{2.12}$$

where $r(\cdot,n,p,T) : \Omega \times [0,\operatorname{ess\,sup} N_{n0}] \times [0,\operatorname{ess\,sup} N_{p0}] \times (0,\infty) \to \mathbb{R}$ is a Caratheodory function with $0 \le r_0(\cdot,n,p,T) \le \overline{r}$ for all $(n,p,T) \in [0,\operatorname{ess\,sup} N_{n0}] \times [0,\operatorname{ess\,sup} N_{p0}] \times (0,\infty)$ and a.a. $x \in \Omega$.

In case of Boltzmann statistics, this ansatz is equivalent to the widely used form

$$R(n,p) = C(n,p)(np - n_i^2),$$

where n_i is the intrinsic carrier density. The expression for the rate in (2.12) is compatible with thermodynamic equilibrium. Especially, it reflects the fact, that in equilibrium the quasi Fermi levels of electrons and holes have to coincide.

2.4. Boundary conditions. For the formulation of boundary conditions we decompose $\partial\Omega$ into Ohmic contacts $\Gamma_D = \cup_{i=1}^I \Gamma_{Di}$, a gate contact Γ_G and the semiconductor-insulator interface Γ_N, i.e. Ohmic contacts like semiconductor-metal interfaces are modeled by Dirichlet boundary conditions

$$\psi = \psi_* + V_i, \quad \varphi_n = V_i, \quad \varphi_p = V_i \quad \text{on } \mathbb{R}_+ \times \Gamma_{Di},$$

where V_i denotes the corresponding externally applied contact voltage at Γ_{Di}. The value ψ_* (at the boundary) is defined by the local electroneutrality condition,

$$0 = C - N_{n0}\mathcal{G}_{s_n}\Big(\frac{q\psi_* - E_L}{k_{\rm B}T}\Big) + N_{p0}\mathcal{G}_{s_p}\Big(\frac{E_H - q\psi_*}{k_{\rm B}T}\Big). \tag{2.13}$$

Due to the boundedness of the carrier densities, the solvability of (2.13) gives a restriction to the range of the doping profile. The semiconductor-insulator interface is realized by no-flux boundary conditions

$$\varepsilon_0\varepsilon_r\nabla\psi\cdot\nu = j_n\cdot\nu = j_p\cdot\nu = 0 \quad \text{on } \mathbb{R}_+ \times \Gamma_N,$$

where ν denotes the outer normal vector. Gate contacts are described by Robin boundary conditions for the electrostatic potential ψ and Neumann boundary conditions in the continuity equations

$$\varepsilon_0\varepsilon_r\nabla\psi\cdot\nu + \alpha_{\rm ox}(\psi - V^G) = 0, \quad j_n\cdot\nu = j_p\cdot\nu = 0 \quad \text{on } \mathbb{R}_+ \times \Gamma_G,$$

where $\alpha_{\rm ox} > 0$ and V^G is the applied gate votlage.

3. Analysis of the instationary drift-diffusion model

3.1. Rescaling of the instationary drift-diffusion model. In Section 2, we introduced the instationary drift-diffusion problem (2.1) and discussed the relevant statistical relations, the ansatz for the flux functions, the form of mobility laws and generation-recombination rate for problems in organic electronics in the correct physical quantities. To simplify the notation for the analysis, we now introduce scaled quantities as follows

- The potentials ψ, φ_n, φ_p, V^G and the applied voltage are scaled by $\frac{k_B T}{q}$.
  a
- The band edges $E_{L,H}$ are divided by $k_B T$ and we denote $\zeta_n := -\frac{E_L}{k_B T}$, $\zeta_p := \frac{E_H}{k_B T}$.
- The mobility functions μ_n, μ_p are multiplied by $\frac{k_B T}{q}$.

Dividing the Poisson equation as well as the continuity equations by q and denoting the scaled quantities by the same symbol as the original ones, we obtain in $(0,\infty)\times\Omega$

$$
\begin{aligned}
&-\nabla\cdot(\varepsilon\nabla\psi) = C - n + p, \\
&\frac{\partial n}{\partial t} - \nabla\cdot j_n = -R, \qquad j_n = -n\mu_n\nabla\varphi_n, \quad n = N_{n0}\mathcal{G}_{s_n}\big(\psi-\varphi_n+\zeta_n\big), \\
&\frac{\partial p}{\partial t} + \nabla\cdot j_p = -R, \qquad j_p = -p\mu_p\nabla\varphi_p, \quad p = N_{p0}\mathcal{G}_{s_p}\big(-(\psi-\varphi_p)+\zeta_p\big)
\end{aligned}
\tag{3.1}
$$

with

$$R = R(n,p,\varphi_n,\varphi_p,T) = r(n,p,T)\big(1-\mathrm{e}^{\varphi_n-\varphi_p}\big),$$

and the new coefficients in the Poisson equation and the gate boundary condition are

$$\varepsilon = \frac{\varepsilon_0\varepsilon_r k_B T}{q^2}, \qquad \alpha = \frac{\alpha_{\mathrm{ox}} k_B T}{q^2}.$$

The initial and boundary conditions read as

$$n(0) = n^0, \quad p(0) = p^0 \quad \text{in } \Omega, \tag{3.2}$$

$$
\begin{aligned}
\psi = \psi^D, \quad \varphi_n = \varphi_n^D, \quad \varphi_p = \varphi_p^D \quad &\text{on } (0,\infty)\times\Gamma_D, \\
\varepsilon\nabla\psi\cdot\nu = j_n\cdot\nu = j_p\cdot\nu = 0 \quad &\text{on } (0,\infty)\times\Gamma_N, \\
\varepsilon\nabla\psi\cdot\nu + \alpha(\psi-\psi^G) = 0, \quad j_n\cdot\nu = j_p\cdot\nu = 0 \quad &\text{on } (0,\infty)\times\Gamma_G.
\end{aligned}
\tag{3.3}
$$

REMARK 3.1. Here we consider no flux boundary conditions for j_n and j_p at Γ_N and Γ_G, see (3.3). For the analytical treatment of drift-diffusion systems with inhomogeneous normal fluxes at the boundary, see e.g. [9]. The paper [17] considers a generalized Poisson-Nernst-Planck system with nonlinear electro-chemical reactions at the interface between pores and the solid phases.

3.2. Assumptions on the data. We work with the Lebesgue spaces $L^q(\Omega)$ and the Sobolev spaces $W^{1,q}(\Omega)$, $q \in [1,\infty]$, $H^1(\Omega) = W^{1,2}(\Omega)$. Let $G := \Omega\cup\Gamma_N\cup\Gamma_G$. For $q\in[1,\infty]$ we denote by $W_0^{1,q}(G)$ the closure of the set

$$\big\{v|_\Omega \,:\, v\in C_0^\infty(\mathbb{R}^d),\ \operatorname{supp} v\cap(\overline{G}\setminus G) = \emptyset\big\}$$

in the Sobolev space $W^{1,q}(\Omega)$ equipped with the standard norm of this space. The dual space to $W_0^{1,q'}(G)$, $1/q + 1/q' = 1$ is denoted by $W^{-1,q}(G)$. Moreover, we denote by $y^+ := \sup(0, y)$ and $y^- := \sup(0, -y) \geq 0$ the positive and negative part of a function y, respectively. Note that $y = y^+ - y^-$.

In our estimates, positive constants, which may depend at most on the data of our problem, are denoted by c. In particular, we allow them to change from line to line.

We investigate the instationary drift-diffusion model under the following assumptions:

(A1) $\Omega \in \mathbb{R}^d$ bounded Lipschitz domain, Γ_D, Γ_N, $\Gamma_G \subset \Gamma =: \partial\Omega$ disjoint subsets such that $\overline{\Gamma_D \cup \Gamma_N \cup \Gamma_G} = \Gamma$ and $\operatorname{mes}(\Gamma_D) > 0$.

(A1') $\Omega \in \mathbb{R}^2$, $G := \Omega \cup \Gamma_N \cup \Gamma_G$ is regular in the sense of Gröger ([13]).

(A2) $T = \text{const}$, $N_{i0} = \text{const}$, $\zeta_i = \text{const}$, $\sigma_i = \text{const}$, $i = n, p$.

(A3) $\varepsilon \in L^\infty(\Omega)$, $0 < c \leq \varepsilon$ a.e. in Ω,
ψ^D, φ_n^D, $\varphi_p^D \in W^{1,\infty}(\Omega)$, $\psi^G \in L^\infty(\Gamma_G)$, $\alpha \in L_+^\infty(\Gamma_G)$.

(A4) $\mu_i(\cdot, T, \cdot, \cdot) : \Omega \times [0, N_{i0}] \times \mathbb{R}_+ \to \mathbb{R}$, are Caratheodory functions, $i = n, p$, fulfilling $0 < \underline{\mu} \leq \mu_n(\cdot, T, n, F)$, $\mu_p(\cdot, T, p, F) \leq \overline{\mu} < \infty$ for all $(n, p, F) \in [0, N_{n0}] \times [0, N_{p0}] \times \mathbb{R}_+$ a.e. in Ω.

(A5) $R = r(\cdot, n, p, T)\big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big)$, such that $r(\cdot, n, p, T) = r_0(\cdot, n, p, T)\, n\, p$, where $r_0 : \Omega \times [0, N_{n0}] \times [0, N_{p0}] \times (0, \infty) \to \mathbb{R}$ is a Caratheodory function with $0 \leq r_0(\cdot, n, p, T) \leq \overline{r}\ \forall\, (n, p, T) \in [0, N_{n0}] \times [0, N_{p0}] \times (0, \infty)$ and a.a. $x \in \Omega$.

(A6) n^0, $p^0 \in L^\infty(\Omega)$, $0 < \underline{\gamma} \leq n^0 \leq \overline{\gamma}_n < N_{n0}$, $0 < \underline{\gamma} \leq p^0 \leq \overline{\gamma}_p < N_{p0}$ a.e. in Ω.

In the following we suppress in the writing the spatial position x and the argument T in the mobility functions μ_n, μ_p and in the reaction coefficient r. Moreover, in Section 4 and Section 5 the letter T will denote the endpoint of the time interval $S := [0, T]$.

3.3. Weak formulation. We introduce the following function spaces

$$V_0 := H_0^1(G), \quad V := V_0^3, \quad H := V_0 \times L^2(\Omega) \times L^2(\Omega),$$
$$Z := \big\{v \in H^1(\Omega) \times L^2(\Omega)^2 : (v_i)^- \in L^\infty(\Omega),\ i = n, p\big\},$$
$$U := \big\{u \in V_0^* \times L^2(\Omega) \times L^2(\Omega) : 0 < \operatorname{ess\,inf} u_i,\ u_i < N_{i0},\ i = n, p\big\}.$$

As in [7, 9], we intend to use a weak formulation in the form $u' + A(v) = 0$, $u = E(v)$, $u(0) = u^0$ with the variables $v = (v_0, v_n, v_p) = (\psi, \psi - \varphi_n, \varphi_p - \psi)$, $u = (u_0, u_n, u_p) := (u_0, n, p)$, $u^0 = (u_0^0, u_n^0, u_p^0) := (u_0^0, n^0, p^0)$, where $\langle u_0, w\rangle = \int_\Omega (p - n) w \,\mathrm{d}x$, $\langle u_0^0, w\rangle = \int_\Omega (p^0 - n^0) w \,\mathrm{d}x$ for all $w \in V_0$. We define $e_i : \mathbb{R} \to (0, N_{i0})$, $i = n, p$,

$$e_i(y) := N_{i0}\mathcal{G}_{s_i}(y + \zeta_i), \quad y \in \mathbb{R}. \tag{3.4}$$

Note that the inverse e_i^{-1} is well-defined on $(0, N_{i0})$.

For the weak formulation, we consider the operators $E_0 : v_0^D + V_0 \to V_0^*$, $E : v^D + V \to V^*$, $A : (v^D + V) \cap Z \to V^*$,

$$\langle E_0 v_0, \overline{v}_0\rangle := \int_\Omega \big\{\varepsilon \nabla v_0 \cdot \nabla \overline{v}_0 - C\overline{v}_0\big\} \,\mathrm{d}x + \int_{\Gamma_G} \alpha(v_0 - \psi^G)\overline{v}_0 \,\mathrm{d}\Gamma,$$

$$
\begin{aligned}
E(v) &:= (E_0 v_0, e_n(v_n), e_p(v_p)),\\
\langle A(v), \overline{v}\rangle &:= \int_\Omega \big\{ - n\mu_n(n, |\nabla v_0|)\nabla\varphi_n \cdot \nabla(\overline{v}_n - \overline{v}_0) + p\mu_p(p, |\nabla v_0|)\nabla\varphi_p \cdot \nabla(\overline{v}_p - \overline{v}_0)\big\}\,\mathrm{d}x\\
&\qquad + \int_\Omega r(n,p)\big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big)(\overline{v}_n - \overline{v}_0 + \overline{v}_p + \overline{v}_0)\,\mathrm{d}x\\
&= \int_\Omega u_n\mu_n(u_n, |\nabla v_0|)\nabla(v_n - v_0)\cdot\nabla(\overline{v}_n - \overline{v}_0)\,\mathrm{d}x\\
&\qquad + \int_\Omega u_p\mu_p(u_p, |\nabla v_0|)\nabla(v_p + v_0)\cdot\nabla(\overline{v}_p + \overline{v}_0)\,\mathrm{d}x\\
&\qquad + \int_\Omega r(u_n, u_p)\big(1 - \mathrm{e}^{-v_n - v_p}\big)(\overline{v}_n + \overline{v}_p)\,\mathrm{d}x\\
&= \int_\Omega \big\{ n\mu_n(n, |\nabla\psi|)\nabla\varphi_n\cdot\nabla\overline{\varphi}_n + p\mu_p(p, |\nabla\psi|)\nabla\varphi_p\cdot\nabla\overline{\varphi}_p\big\}\,\mathrm{d}x\\
&\qquad + \int_\Omega r(n,p)\big(\mathrm{e}^{\varphi_n - \varphi_p} - 1\big)(\overline{\varphi}_n - \overline{\varphi}_p)\,\mathrm{d}x \qquad \forall\, \overline{v}_0,\, \overline{v}_n,\, \overline{v}_p \in V_0,
\end{aligned}
$$

where $\overline{\varphi}_n = \overline{v}_0 - \overline{v}_n$, $\overline{\varphi}_p = \overline{v}_p + \overline{v}_0$ and the densities have to be calculated pointwise by $n = u_n = e_n(v_n)$, $p = u_p = e_p(v_p)$.

For the initial state u^0, we denote by v_0^0 the unique solution to $E_0 v_0 = u_0^0$ (E_0 is strongly monotone and Lipschitz continuous). Moreover, let $v_i^0 := e_i^{-1}(u_i^0)$, $i = n, p$, and $v^0 := (v_0^0, v_n^0, v_p^0)$.

The weak formulation of the drift-diffusion system (3.1), (3.2), (3.3) with Gauss–Fermi statistics is the problem

$$
\begin{aligned}
&u' + A(v) = 0, \quad u = E(v) \quad \text{a.e. on } \mathbb{R}_+, \quad u(0) = u^0,\\
&u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, V^*), \quad v - v^D \in L^2_{\mathrm{loc}}(\mathbb{R}_+, V) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, Z).
\end{aligned}
\tag{P}
$$

3.4. Energy estimates for weak solutions. The operator E is a strictly monotone operator with the potential $\Phi : v^D + V \to \mathbb{R}$,

$$
\begin{aligned}
\Phi(v) := &\int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla v_0|^2 - \frac{\varepsilon}{2}|\nabla v_0^D|^2 - C(v_0 - v_0^D) + \sum_{i=n,p}\int_{v_i^D}^{v_i} e_i(y)\,\mathrm{d}y \Big\}\mathrm{d}x\\
&+ \int_{\Gamma_G} \Big\{ \frac{\alpha}{2}(v_0^2 - (v_0^D)^2) - \psi^G(v_0 - v_0^D)\Big\}\,\mathrm{d}\Gamma.
\end{aligned}
\tag{3.5}
$$

The boundedness of e_n, e_p implies $\operatorname{dom}\Phi = V + v^D$. The functional Φ is continuous, strictly convex and Gâteaux differentiable, hence subdifferentiable and $\partial\Phi = E$. The conjugate functional of $\Phi : V^* \to \overline{\mathbb{R}}$, denoted by Ψ, is

$$
\Psi(u) := \Phi^*(u) = \sup_{w\in V}\{\langle u, w\rangle - \Phi(w + v^D)\},
\tag{3.6}
$$

see [1]. The functional Ψ is proper, lower semicontinuous and convex. Additionally, we have $u = E(v) = \partial\Phi(v)$ if and only if $v - v^D \in \partial\Psi(u)$. For a state $u \in V^*$ the quantity $\Psi(u)$ can be interpreted as the free energy of the state u.

By results of convex analysis, the free energy can be calculated for states $u = E(v)$ by

$$
\Psi(u) = \langle E(v), v - v^D\rangle - \Phi(v)
$$

$$= \int_\Omega \frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2 \,\mathrm{d}x + \int_{\Gamma_G} \frac{\alpha}{2}(v_0 - v_0^D)^2 \,\mathrm{d}\Gamma$$
$$+ \sum_{i=n,p} \int_\Omega \frac{N_{i0}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big(\frac{-\xi^2}{2}\Big)\Big\{\frac{v_i - v_i^D}{\exp(s_i\xi - v_i - \zeta_i)+1} - \ln\frac{\exp\{-(s_i\xi - v_i - \zeta_i)\}+1}{\exp\{-(s_i\xi - v_i^D - \zeta_i)\}+1}\Big\}\mathrm{d}\xi\,\mathrm{d}x,$$

where we take advantage from the fact that v_0 is the unique solution to $E_0 v_0 = u_0$. For more details on the free energy functional see the Appendix.

THEOREM 3.1. *Let (A1) – (A6) be fulfilled. If (u, v) is a weak solution to the instationary problem (3.3) then*

$$\Psi(u(t)) \le \Psi(u(0)) + ct \quad \forall\, t > 0.$$

Additionally, if the Dirichlet values are compatible with thermodynamic equilibrium (meaning $\varphi_i^D = const$, $i = n, p$, $v_n^D = -v_p^D$) the free energy $\Psi(u(t))$ is monotonically decreasing.

Proof. Let $t \in \mathbb{R}_+$ be arbitrarily given. We test $u' + A(v) = 0$ by $v - v^D \in L^2(0, t; V)$. Since $u(t) = E(v(t))$ f.a.a. $t \in S$ we obtain $v(t) - v^D \in \partial F(u(t))$ a.e. in S and the Brezis formula (cf. [1, Lemma 3.3]) ensures the chain rule

$$\Psi(u(t)) - \Psi(u(0)) = \int_0^t \langle u'(s), v(s) - v^D\rangle \,\mathrm{d}s = -\int_0^t \langle A(v(s)), v(s) - v^D\rangle \,\mathrm{d}s$$
$$= -\int_0^t \int_\Omega \sum_{i=n,p} \mu_i u_i \nabla\varphi_i \cdot \nabla(\varphi_i - \varphi_i^D) \,\mathrm{d}x\,\mathrm{d}s$$
$$- \int_0^t \int_\Omega r\big(\mathrm{e}^{\varphi_n - \varphi_p} - 1\big)(\varphi_n - \varphi_p - \varphi_n^D + \varphi_p^D) \,\mathrm{d}x\,\mathrm{d}s$$
$$\le \int_0^t \int_\Omega \sum_{i=n,p} u_i(-\underline{\mu}|\nabla(\varphi_i - \varphi_i^D)|^2 + c|\nabla(\varphi_i - \varphi_i^D)||\nabla\varphi_i^D|) \,\mathrm{d}x\,\mathrm{d}s$$
$$+ \int_0^t \int_\Omega c\big(\|v_n^D + v_p^D\|_{L^\infty}\big) \,\mathrm{d}x\,\mathrm{d}s. \tag{3.7}$$

Note that the expression from the generation-recombination term

$$\widetilde{R} := \big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big)(\varphi_n - \varphi_p - \varphi_n^D + \varphi_p^D)$$

is estimated differently for the three different cases

A) $\underline{-\varphi_n^D + \varphi_p^D \ge 0}$:

$$\widetilde{R} \le \big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big)(-\varphi_n^D + \varphi_p^D) \le |-\varphi_n^D + \varphi_p^D| = |v_n^D + v_p^D|$$

B) $\underline{-\varphi_n^D + \varphi_p^D < 0,\ \varphi_n \le \varphi_p}$: $\quad \widetilde{R} \le 0$

C) $\underline{-\varphi_n^D + \varphi_p^D < 0,\ \varphi_n > \varphi_p}$:

$$\widetilde{R} \le \big(1 - \mathrm{e}^{\varphi_n^D - \varphi_p^D}\big)(\varphi_n - \varphi_p - \varphi_n^D + \varphi_p^D)$$
$$\le \big(1 - \mathrm{e}^{\varphi_n^D - \varphi_p^D}\big)(-\varphi_n^D + \varphi_p^D) \le c\Big(\|v_n^D + v_p^D\|_{L^\infty}\Big).$$

In (3.7), we apply Young's inequality and take into account that $\|\nabla\varphi_i^D\|_{L^2} \le c$ and that $u_i \le N_{i0}$ on solutions (since $u(t) = E(v(t))$ f.a.a. t) and obtain $\Psi(u(t)) \le \Psi(u(0)) + ct$

for all $t > 0$. The last assertion for data compatible with thermodynamic equilibrium directly results from (3.7). ∎

Furthermore, the following estimates for the solution to the Poisson equation are available.

LEMMA 3.1. *We assume* (A1) – (A6). *If v_0 is the weak solution to the Poisson equation $E_0 v_0 = u_0$ with right-hand side u_0 then there is a $c > 0$ such that $\|v_0\|_{L^\infty} \le c$. Under the additional assumption* (A1') *(two spatial dimensions, $G = \Omega \cup \Gamma_N \cup \Gamma_G$ regular in the sense of Gröger [13]), there are an exponent $q > 2$ and a constant $c > 0$ such that $\|v_0\|_{W^{1,q}} \le c$.*

If (u, v) is a weak solution to the instationary problem (3.3) *then*

$$\|v_0(t)\|_{L^\infty} \le c, \quad (\textit{under } (\text{A1'}){:}\ \|v_0(t)\|_{W^{1,q}} \le c) \quad \textit{f.a.a. } t \in \mathbb{R}_+.$$

Proof.

(1) Since $E_0 v_0 = u_0$, regularity results for the Poisson equation with L^∞ right-hand side $C - u_n + u_p$ (note that $u_i < N_{i0}$, $i = n, p$) obtained by Moser estimates (see e.g. [4, Lemma 3.1], applicable in the two- and three-dimensional case) give the desired L^∞ estimate for the electrostatic potential.

(2) Under assumption (A1'), by the regularity result of Gröger [13, Theorem 1] we can fix some $q = q(\Omega, \varepsilon) > 2$ such that, if

$$\forall \overline{w} \in V_0 : \int_\Omega \varepsilon \nabla w \cdot \nabla \overline{w} \, \mathrm{d}x = \langle g, \overline{w} \rangle, \quad g \in W^{-1,q}(G), \ w \in V_0$$

then $w \in W_0^{1,q}(G)$ and $\|w\|_{W_0^{1,q}} \le c\|g\|_{W^{-1,q}}$. Here $W^{-1,q}(G)$ means the dual of $W_0^{1,q'}(G)$, where q' denotes the dual exponent to q.

(3) For the instationary problem (P), $\|C - u_n(t) + u_p(t)\|_{L^\infty}$, (in the 2D case with (A1'): $\|C - u_n(t) + u_p(t)\|_{W^{-1,q}}$) is uniformly bounded, therefore we get a uniform bound for $\|v_0(t)\|_{L^\infty}$, (in 2D: $\|v_0(t)\|_{W^{1,q}}$) f.a.a. $t > 0$.

∎

4. Global existence result

In the treatment of the instationary drift-diffusion model in the organic setting, we have to overcome two new essential problems compared to the classical van Roosbroeck system:

(i) The dependence of the mobilities $\mu_{n,p}$ on $|\nabla v_0|$ has to be taken into account and needs new arguments in the existence proof as well as in the lower estimate for the charge carrier densities. On the one hand, in former estimates (see e.g. [7]) the inverse constant mobility was used as one factor in applied test functions for the continuity equations. For constant mobility and constant ε, the treatment of drift terms was realized in this way by substituting the weak formulation of the Poisson equation at this place. On the other hand, known techniques for a uniqueness proof of solutions fail. Moreover, let us mention that even the techniques to prove local-in-time existence of solutions to the van Roosbroeck system presented in [14] do not allow a dependence of the mobility on $|\nabla v_0|$.

(ii) The statistical relation does not satisfy the standard assumption in Gajewski/Gröger [7, (2.3)] (see also [9, (3.5)], [6,10–12] also for the treatment of non-Boltzmann statistics). In particular, we have finite charge carrier densities in the Gauss–Fermi case such that we do not have the property that $\lim_{y\to+\infty} e_i(y) = +\infty$. However, the estimate $e_i(y) \geq e_0 e_i'(y)$ for all $y \in \mathbb{R}$ remains true in the case of Gauss–Fermi statistics which is of importance for the proof of lower bounds for the carrier densities.

The guideline for the existence proof is as follows: To show the existence of a weak solution for any arbitrarily chosen finite time interval $S = [0, T]$, we first discuss a regularized problem $(\mathrm{P_M})$ on the finite time interval S, where the state equations as well as the reaction term are regularized (with parameter M). We ensure the solvability of $(\mathrm{P_M})$ by time discretization, derivation of suitable a priori estimates, and passage to the limit (see Lemma 4.2).

Then, we provide a priori estimates for solutions to $(\mathrm{P_M})$ that are independent of M (see Lemma 4.3, here we use Moser techniques to get positive lower bounds for the carrier densities). Thus a solution to $(\mathrm{P_M})$ is a solution to (P) on S, if M is chosen sufficiently large.

To cover the dependence of the mobility on $|\nabla v_0|$, we restrict our investigations to the spatially two-dimensional case. Here Gröger's regularity result [13] for elliptic equations applied for the gradient of the electrostatic potential in combination with the Gagliardo-Nirenberg inequalities in the two-dimensional setting enable us to establish lower (positive) bounds for the carrier densities (see the proof of Lemma 4.3).

4.1. A regularized problem $(\mathbf{P_M})$. We consider any finite time interval $S := [0, T]$. For

$$M > M^* := \max\Big\{\|e_n^{-1}(u_n^0)\|_{L^\infty}, \|e_p^{-1}(u_p^0)\|_{L^\infty}, \|v_n^D\|_{L^\infty}, \|v_p^D\|_{L^\infty}\Big\}, \tag{4.1}$$

we define the lower cut off function $D_M : \mathbb{R} \to [-M, \infty)$, $D_M(z) := \max\{z, -M\}$ and the regularized statistical relations

$$u_i = e_i(D_M(v_i)) =: e_{Mi}(v_i), \quad i = n, p.$$

For our problem, we regularize the statistical relation and the reaction term (by writing it in terms of densities), and consider regularized operators $E_M : v^D + V \to V^*$, $A_M : U \times (v_0^D + V_0) \times (v^D + V) \to V^*$,

$$\begin{aligned}
E_M(v) &:= (E_0 v_0, e_{Mn}(v_n), e_{Mp}(v_p)),\\
\langle A_M(u, \widetilde{v}_0, v), \overline{v}\rangle &:= \int_\Omega \big\{n\mu_n(n, |\nabla\widetilde{v}_0|)\nabla\varphi_n \cdot \nabla\overline{\varphi}_n + p\mu_p(p, |\nabla\widetilde{v}_0|)\nabla\varphi_p \cdot \nabla\overline{\varphi}_p\big\}\,\mathrm{d}x\\
&\quad + \int_\Omega r_0(n, p)np\big(\exp\big\{-e_n^{-1}(u_n) - e_p^{-1}(u_p)\big\} - 1\big)(\overline{\varphi}_n - \overline{\varphi}_p)\,\mathrm{d}x,
\end{aligned}$$

where $(n, p) = (u_n, u_p)$, $\varphi_n = -v_n + v_0$, $\varphi_p = v_p + v_0$. Note that our regularization of the reaction term differs from the one in [7], its value can be estimated in terms of M since the factor with the exponential is bounded by $\mathrm{e}^{2M} + 1$. We solve the problem

$$u' + A_M(u, v_0, v) = 0,\ u = E_M(v),\ u(0) = u^0,\ v - v^D \in L^2(S, V) \tag{$\mathrm{P_M}$}$$

by time discretization. For any Banach space X and $k \in \mathbb{N}$ we define $h_k := \frac{T}{k}$ and $C_k(S, X)$ as the space of all functions $u : S \to X$ being constant on each of the intervals $((l-1)h_k, lh_k]$, $l = 1, \ldots, k$. Let u^l denote the value of $u \in C_k(S, X)$ on $((l-1)h_k, lh_k]$. Furthermore we define the maps τ_k and Δ_k from $C_k(S, X)$ into itself via

$$(\tau_k u)^l := u^{l-1}, \quad (\Delta_k u)^l := \frac{1}{h_k}(u^l - u^{l-1}), \quad l = 1, \ldots, k,$$

with the given initial value u^0. Additionally, we introduce the continuous, piecewise linear function

$$(K_k u_k)(t) := u^0 + \int_0^t (\Delta_k u_k)(s)\,\mathrm{d}s.$$

The time-discrete analogon of (4.1) now reads

$$\Delta_k u_k + A_M(\tau_k u_k, \tau_k v_{k0}, v_k) = 0,\ u_k = E_M(v_k),\ v_k - v^D \in C_k(S,V) \tag{4.2}$$

or written in more detail

$$\begin{gathered} E_M(v_k^l) + h_k A_M(u_k^{l-1}, v_{k0}^{l-1}, v_k^l) = E_M(v_k^{l-1}), \quad l = 1,\dots,k, \\ u_k^0 = E_M(v_k^0) = u^0. \end{gathered} \tag{4.3}$$

Lemma 4.1. *We assume* (A1) – (A6). *Then for all $k \in \mathbb{N}$ there exists a unique solution (u_k, v_k) to problem* (4.2). *Additionally,*

$$\sup_{k\in\mathbb{N}} \Big\{ \|v_k - v^D\|_{L^2(S,V)} + \|\Delta_k u_k\|_{L^2(S,V^*)} + \|K_k u_k\|_{C(S,H^*)} \Big\} < \infty.$$

Proof.

(1) For $u \in U$ and $w \in V_0 + v_0^D$, the map $v \mapsto \frac{1}{h_k} E_M(v) + A_M(u,w,v)$ is strongly monotone and Lipschitz continuous from $v^D + V$ to V^*. Therefore, for any given $u_k^{l-1} = E_M(v_k^{l-1})$ and v_{k0}^{l-1} there is a unique solution v_k^l to (4.3). Thus, we can compose from the solution for each time step a unique solution to (4.2).

(2) We introduce the regularized functionals $\Phi_M : v^D + V \to \mathbb{R}$, $\Psi_M : V^* \to (-\infty, \infty]$ by

$$\begin{aligned} \Phi_M(v) &:= \int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla v_0|^2 - \frac{\varepsilon}{2}|\nabla v_0^D|^2 - C(v_0 - v_0^D) + \sum_{i=n,p} \int_{v_i^D}^{v_i} e_{Mi}(y)\,\mathrm{d}y \Big\}\,\mathrm{d}x \\ &\quad + \int_{\Gamma_G} \Big\{ \frac{\alpha}{2}(v_0^2 - (v_0^D)^2) - \psi^G(v_0 - v_0^D) \Big\}\,\mathrm{d}\Gamma, \quad v \in v^D + V, \\ \Psi_M(u) &:= \sup_{w\in V} \{ \langle u, w\rangle - \Phi_M(w + v^D) \}, \quad u \in V^*. \end{aligned} \tag{4.4}$$

The functional Φ_M is Fréchet differentiable with derivative $\Phi_M' = E_M$, and the conjugate functional Ψ_M for arguments $u = E_M(v)$ is obtained by

$$\Psi_M(u) = \langle u, v - v^D\rangle - \Phi_M(v) = \big\langle \big(E_0 v_0, e_{Mn}(v_n), e_{Mp}(v_p)\big), v - v^D \big\rangle - \Phi_M(v). \tag{4.5}$$

Moreover, we have $v - v^D \in \partial\Psi_M(u)$ provided that $u = E_M(v)$ for $v \in v^D + V$. Exploiting (4.4) and (4.5), we estimate for $u = E_M(v)$

$$\begin{aligned} \Psi_M(u) &= \int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2 + \sum_{i=n,p} \int_{v_i^D}^{v_i} (u_i - e_{Mi}(y))\,\mathrm{d}y \Big\}\,\mathrm{d}x + \int_{\Gamma_G} \frac{\alpha}{2}(v_0 - v_0^D)^2\,\mathrm{d}\Gamma \\ &\geq c\|v_0 - v_0^D\|_{H^1}^2 + \sum_{i=n,p} \int_\Omega \int_{v_i^D}^{D_M(v_i)} (u_i - e_i(y))\,\mathrm{d}y\,\mathrm{d}x \\ &\geq c\|v_0 - v_0^D\|_{H^1}^2 + \sum_{i=n,p} \int_\Omega \big(u_i - e_i(v_i^D + 1)\big)\,\mathrm{d}x. \end{aligned} \tag{4.6}$$

The estimate in the last line results from separately considering the cases $v_i^D <,> D_M(v_i)$ and $|v_i^D - D_M(v_i)| >,< 1$. Using (4.3), the subdifferential property, and the strong monotonicity of A_M in the last argument, we find for $l = 1, \dots, k$,

$$\begin{aligned}
\Psi_M(u_k^l) - \Psi_M(u^0) &= \sum_{j=1}^{l} \big(\Psi_M(u_k^j) - \Psi_M(u_k^{j-1})\big) \le \sum_{j=1}^{l} \big\langle u_k^j - u_k^{j-1}, v_k^j - v^D \big\rangle \\
&= -h_k \sum_{j=1}^{l} \big\langle A_M(u_k^{j-1}, v_{k0}^{j-1}, v_k^j), v_k^j - v^D \big\rangle \\
&= -h_k \sum_{j=1}^{l} \Big\{ \big\langle A_M(u_k^{j-1}, v_{k0}^{j-1}, v_k^j) - A_M(u_k^{j-1}, v_{k0}^{j-1}, v^D), v_k^j - v^D \big\rangle \\
&\qquad + \big\langle A_M(u_k^{j-1}, v_{k0}^{j-1}, v^D), v_k^j - v^D \big\rangle \Big\} \\
&\le -h_k \sum_{j=1}^{l} \Big\{ \sum_{i=n,p} e_{Mi}(-M)\underline{\mu} \|\nabla(\varphi_{ki}^j - \varphi_i^D)\|_{L^2}^2 + \big\langle A_M(u_k^{j-1}, v_{k0}^{j-1}, v^D), v_k^j - v^D \big\rangle \Big\} \\
&\le -\frac{1}{2} \int_0^{lh_k} \sum_{i=n,p} e_i(-M)\underline{\mu} \|\nabla(\varphi_{ki} - \varphi_i^D)\|_{L^2}^2 \mathrm{d}t + c_M,
\end{aligned} \tag{4.7}$$

where $c_M > 0$ does not depend on k. Here we used that for any test function $w \in L^2(S, V_0)$, we can estimate the reaction term

$$\int_S \int_\Omega r(\tau_k u_k)(\mathrm{e}^{-e_n^{-1}(\tau_k u_{kn}) - e_p^{-1}(\tau_k u_{kp})} - 1) w \,\mathrm{d}x\,\mathrm{d}t \le c\|\mathrm{e}^{2M} + 1\|_{L^2(S,L^2)} \|w\|_{L^2(S,L^2)}. \tag{4.8}$$

As $\Psi_M(u^0) < \infty$, the estimates (4.6), (4.7) guarantee that

$$\sup_{k\in\mathbb{N}} \big\{ \|v_{k0} - v_0^D\|_{L^\infty(S,V_0)} + \|v_k - v^D\|_{L^2(S,V)} \big\} < \infty. \tag{4.9}$$

Since $u_k^l = E_M(v_k^l)$, we now conclude from (4.9) and (4.8) that

$$\sup_{k\in\mathbb{N}} \|A_M(\tau_k u_k, \tau_k v_{k0}, v_k)\|_{L^2(S,V^*)} < \infty, \quad \sup_{k\in\mathbb{N}} \|\Delta_k u_k\|_{L^2(S,V^*)} < \infty.$$

Moreover, from $u_{k0} = E_0 v_{k0}$ and (4.9) we derive $\sup_{k\in\mathbb{N}} \|u_{k0}\|_{L^\infty(S,V_0^*)} < \infty$. Taking into account that $e_i(-M) \le u_{ki} < N_{i0}$, and

$$(K_k u_k)(t) = \Big(\frac{t}{h_k} - l + 1\Big) u_k^l + \Big(l - \frac{t}{h_k}\Big) u_k^{l-1} \quad \text{for } t \in ((l-1)h_k, lh_k]$$

we have $K_k u_k \in C(S, H^*)$ and $\sup_{k\in\mathbb{N}} \|K_k u_k\|_{C(S,H^*)} < \infty$.

∎

Lemma 4.2. *We assume* (A1) – (A6). *Then there exists a solution* (u, v) *to problem* (4.1).

Proof.

(1) Let $\{(u_k, v_k)\}_{k\in\mathbb{N}}$ be a sequence of solutions to the time discretized problems according to Lemma 4.1. Then, we find functions v and u and a non-relabeled subsequence such that

$$v_k - v^D \rightharpoonup v - v^D \text{ in } L^2(S, V), \quad K_k u_k \rightharpoonup u \text{ in } L^2(S, H) \text{ and } H^1(S, V^*). \tag{4.10}$$

(2) Since for $w \in V$ and $t \in S$ the map $z \mapsto \langle z(t), w\rangle$, $z \in H^1(S, V^*)$, gives a continuous linear functional on the space $H^1(S, V^*)$ we obtain from (4.10) that $(K_k u_k)(t) \rightharpoonup u(t)$ in V^* for all $t \in S$. Furthermore, the boundedness of $(K_k u_k)(t)$ in H then ensures $(K_k u_k)(t) \rightharpoonup u(t)$ in H for $t \in S$. From $(K_k u_k)(0) = u^0$, $k \in \mathbb{N}$, we obtain $u(0) = u^0$.

(3) As $\|K_k u_k - u_k\|_{L^2(S,V^*)} \le h_k \|\Delta_k u_k\|_{L^2(S,V^*)} \to 0$ we can find another non-relabeled subsequence such that

$$(K_k u_k - u_k)(t) \to 0 \text{ in } V^*, \text{ and weakly } u_k(t) \rightharpoonup u(t) \text{ in } H, \text{ f.a.a. } t \in S.$$

Since $u_{ki} = e_{Mi}(v_{ki}) < N_{i0}$, e_{Mi} are Lipschitzian, and $\{v_{ki}\}$ are bounded in $L^2(S, H^1)$ we obtain the boundedness of $\{u_{ki}\}$ in $L^2(S, H^1)$, too. By Lebesgue's theorem we additionally ensure that

$$u_{ki} \rightharpoonup u_i \text{ in } L^2(S, L^2(\Omega)), \quad i = n, p. \tag{4.11}$$

We use the inequality (6.40) in [18, p. 529]:

For all $\epsilon > 0$ there is a $L_\epsilon \in \mathbb{N}$ such that

$$\|w\|_{L^2}^2 \le \sum_{j=1}^{L_\epsilon} (w, \psi_j)_{L^2}^2 + \epsilon \|w\|_{H^1}^2 \quad \forall w \in H^1(\Omega) \quad (\{\psi_j\}_{j\in\mathbb{N}} \text{ ON-base in } L^2).$$

We integrate this inequality for $w = u_{ki} - u_{li}$ over S. Using the weak convergence in $L^2(\Omega)$ a.e. in S, the boundedness of $\{u_{ki}(t)\}$ in $L^2(\Omega)$ for $t \in S$, Lebesgue's theorem and the boundedness of $\{u_{ki}\}$ in $L^2(S, H^1(\Omega))$ we verify that $\{u_{ki}\}$ is a Cauchy sequence in $L^2(S, L^2(\Omega))$. And (4.11) leads to the strong convergence

$$u_{ki} \to u_i \text{ in } L^2(S, L^2(\Omega)), \quad i = n, p. \tag{4.12}$$

In connection with $(K_k u_k - u_k)_i \to 0$ in $L^2(S, V_0^*)$ we conclude that $(K_k u_k - u)_i \to 0$ in $L^2(S, V_0^*)$, $i = n, p$.

(4) For any fixed indices k_1 and k_2 of our subsequence and every $w_0 \in V_0$ and $t \in S$ we obtain by partial integration

$$\int_0^t \big\langle \Delta_{k_1} u_{k_1} - \Delta_{k_2} u_{k_2}, (w_0, w_0, -w_0)\big\rangle \, \mathrm{d}s = \big\langle (K_{k_1} u_{k_1} - K_{k_2} u_{k_2})(t), (w_0, w_0, -w_0)\big\rangle = 0.$$

Using $w_0(t) = J_0^{-1}[(K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_0(t)]$, where J_0 is the duality map of V_0, leads to

$$\|(K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_0(t)\|_{V_0^*}^2 = \big\langle (K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_0(t), J_0^{-1}[(K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_0(t)]\big\rangle$$

$$= -\big\langle (K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_n(t) - (K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_p(t), J_0^{-1}[(K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_0(t)]\big\rangle.$$

Integration over S yields

$$\|(K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_0\|_{L^2(S,V_0^*)} \le c \sum_{i=n,p} \|(K_{k_1} u_{k_1} - K_{k_2} u_{k_2})_i\|_{L^2(S,V_0^*)}.$$

Therefore the last convergence result of Step 3 and the weak convergence in (4.10) guarantee the strong convergences $(K_k u_k)_0 \to u_0$ in $L^2(S, V_0^*)$ and $K_k u_k \to u$ in $L^2(S, V^*)$. Together with Step 3, we also have $u_k \to u$ in $L^2(S, H)$, and for a non-relabeled subsequence, $u_k(t) \to u(t)$ in V^* f.a.a. $t \in S$.

(5) Let $\widetilde{S}$ be any subinterval of S and $\widetilde{u} \in V^*$ with $\Psi_M(\widetilde{u}) < \infty$. Using that $v_k - v^D \in \partial\Psi_M(u_k)$ a.e. in S and the lower semicontinuity of Ψ_M we estimate

$$\begin{aligned}\int_{\widetilde{S}} \langle \widetilde{u} - u(t), v(t) - v^D \rangle \,\mathrm{d}t &= \lim_{k\to\infty} \int_{\widetilde{S}} \langle \widetilde{u} - u_k(t), v_k(t) - v^D \rangle \,\mathrm{d}t \\ &\le \limsup_{k\to\infty} \int_{\widetilde{S}} (\Psi_M(\widetilde{u}) - \Psi_M(u_k(t)))\,\mathrm{d}t \\ &\le \int_{\widetilde{S}} (\Psi_M(\widetilde{u}) - \Psi_M(u(t)))\,\mathrm{d}t.\end{aligned}$$

This ensures for a.a. $t \in S$ that $\langle \widetilde{u} - u(t), v(t) - v^D \rangle \le \Psi_M(\widetilde{u}) - \Psi_M(u(t))$ meaning that $v(t) - v^D \in \partial\Psi_M(u(t))$ and $u(t) \in \partial\Phi_M(v(t)) = E_M(v(t))$ for a.a. $t \in S$. By the chain rule [1, Lemma 3.3] we obtain

$$\Psi_M(u(t)) - \Psi_M(u^0) = \int_0^t \langle u'(s), v(s) - v^D \rangle \,\mathrm{d}s \quad \forall\, t \in S. \tag{4.13}$$

(6) Since E_0 is strongly monotone and $u_0(t) = E_0 v_0(t)$, $u_{k0}(t) = E_0 v_{k0}(t)$ a.e. in S we find for the subsequence by testing with $v_{k0} - v_0 \in V_0$ and integration over S

$$c\|v_{k0} - v_0\|^2_{L^2(S,V_0)} \le \int_S \langle E_0 v_{k0} - E_0 v_0, v_{k0} - v_0 \rangle \mathrm{d}t \le \|u_{k0} - u_0\|_{L^2(S,V_0^*)} \|v_{k0} - v_0\|_{L^2(S,V_0)}.$$

Therefore, $c\|v_{k0} - v_0\|_{L^2(S,V_0)} \le \|u_{k0} - u_0\|_{L^2(S,V_0^*)} \to 0$ according to Step 4. In particular we obtain $\nabla v_{k0} \to \nabla v_0$ in $L^2(S, L^2(\Omega))$, which implies with (4.9) also that $\tau_k \nabla v_{k0} \to \nabla v_0$ in $L^2(S, L^2(\Omega))$ and $L^2(S \times \Omega)$. Additionally, from (4.12) we get $\tau_k u_{ki} \to u_i$ in $L^2(S \times \Omega)$, $i = n, p$. For the latter two convergences, we argue as follows: For $w_k \in C_k(S, L^2) \cap L^\infty(S, L^2(\Omega))$ (compare with Lemma 3.1) with $w_k \to w$ in $L^2(S, L^2(\Omega))$, $\|w_k\|_{L^2}$, $\|w\|_{L^2} \le W$ a.e. in S we estimate

$$\begin{aligned}\int_S \|w(t) - (\tau_k w_k)(t)\|^2_{L^2} \,\mathrm{d}t \le & h_k 4W^2 + \int_{h_k}^T \|w(t) - w(t - h_k)\|^2_{L^2} \,\mathrm{d}t \\ &+ \int_{h_k}^T \|w(t - h_k) - w_k(t - h_k)\|^2_{L^2} \,\mathrm{d}t \to 0 \quad \text{for } k \to \infty.\end{aligned}$$

Thus, for a non-relabeled subsequence, $\tau_k \nabla v_{k0} \to \nabla v_0$ and $\tau_k u_{ki} \to u_i$ a.e. in $S \times \Omega$. Using these a.e. convergences and the boundedness of the functions μ_i, the reaction coefficient r as well as of $\tau_k u_{ki}$ and of the exponential term in the reaction rate

$$\left| \mathrm{e}^{-e_n^{-1}(\tau_k u_{kn}) - e_p^{-1}(\tau_k u_{kp})} - 1 \right| \le \mathrm{e}^{2M} + 1$$

we derive by Lebesgue's theorem the convergence

$$A_M(\tau_k u_k, \tau_k v_{k0}, v) \to A_M(u, v_0, v) \quad \text{ in } L^2(S, V^*). \tag{4.14}$$

(7) Since (u_k, v_k) solve (4.2), our convergence results for a subsequence obtained so far ensure (see also Step 2 in the proof of Lemma 4.1)

$$\begin{aligned} 0 &= \lim_{k\to\infty} \int_S \langle \Delta_k u_k + A_M(\tau_k u_k, \tau_k v_{k0}, v_k), v_k - v \rangle \,\mathrm{d}t \\ &= \lim_{k\to\infty} \int_S \Big\{ \langle \Delta_k u_k, v_k - v^D \rangle - \langle u', v - v^D \rangle \end{aligned}$$

$$+ \left\langle A_M(\tau_k u_k, \tau_k v_{k0}, v_k) - A_M(\tau_k u_k, \tau_k v_{k0}, v), v_k - v\right\rangle + \left\langle A_M(\tau_k u_k, \tau_k v_{k0}, v), v_k - v\right\rangle \Big\} \,\mathrm{d}t$$
$$\geq \limsup_{k\to\infty} \Big\{ \Psi_M(u_k^k) - \Psi_M(u^0) + \int_S \Big[\langle u', v^D - v\rangle + \sum_{i=n,p} e_i(-M)\underline{\mu} \|\nabla(\varphi_{ki} - \varphi_i)\|_{L^2}^2 \Big] \,\mathrm{d}t \Big\}.$$

Note that the limit of the last term in the third line is zero because of (4.14) and $v_k - v^D \rightharpoonup v - v^D$ in $L^2(S, V)$. The last term in the last line results from the strong monotonicity of A_M in the last argument. The weak lower continuity of Ψ_M on V^* ensures

$$\limsup_{k\to\infty} \Psi_M(u_k^k) = \limsup_{k\to\infty} \Psi_M(u_k(T)) \geq \Psi_M(u(T)).$$

Therefore, using (4.13), the estimates of Step 7 lead to

$$\varphi_{ki} - \varphi_i \to 0 \text{ in } L^2(S, V_0), \quad i = n, p. \tag{4.15}$$

Since in Step 6 it was already verified that $\|v_{k0} - v_0\|_{L^2(S,V_0)} \to 0$ we also conclude that $\|v_{ki} - v_i\|_{L^2(S,V_0)} \to 0$, $i = n, p$, and finally $\|v_k - v\|_{L^2(S,V)} \to 0$.

(8) For arbitrary $w \in L^2(S, V)$ we estimate

$$\begin{aligned}
&\langle A_M(\tau_k u_k, \tau_k v_{k0}, v_k) - A_M(u, v_0, v), w\rangle \\
&\qquad = \langle A_M(\tau_k u_k, \tau_k v_{k0}, v_k) - A_M(\tau_k u_k, \tau_k v_{k0}, v), w\rangle \\
&\qquad\quad + \langle A_M(\tau_k u_k, \tau_k v_{k0}, v) - A_M(u, v_0, v), w\rangle \\
&\qquad \leq c \sum_{i=n,p} \|\varphi_{ki} - \varphi_i\|_{L^2(S,V_0)} \|w\|_{L^2(S,V)} \\
&\qquad\quad + \|A_M(\tau_k u_k, \tau_k v_{k0}, v) - A_M(u, v_0, v)\|_{L^2(S,V^*)} \|w\|_{L^2(S,V)}.
\end{aligned}$$

Using (4.15) and (4.14) we obtain for the considered subsequence $A_M(\tau_k u_k, \tau_k v_{k0}, v_k) \to A_M(u, v_0, v)$ in $L^2(S, V^*)$. As we know already from Step 1 that $A_M(\tau_k u_k, \tau_k v_{k0}, v_k) = -\Delta_k u_k \rightharpoonup -u'$ in $L^2(S, V^*)$, we verify the identity $u' + A_M(u, v_0, v) = 0$. The relation $u = E_M v$ was already established in Step 5 such that the limit (u, v) is indeed a solution to $(\mathrm{P_M})$ and the proof is complete.

□

4.2. A priori estimate for problem $(\mathbf{P_M})$. Under the assumption (A1'), we use the exponent $q > 2$ from Lemma 3.1 and define related exponents r and r' as well as the quantity κ

$$r := \frac{2q}{q-2}, \quad r' := \frac{2q}{q+2}, \quad \kappa := \Big(\|\nabla v_0\|_{L^\infty(S, L^q(\Omega))} + 1\Big)^{2r}. \tag{4.16}$$

LEMMA 4.3. *We assume* (A1) – (A6), *and* (A1'). *Let $M \geq M^*$ with M^* as in* (4.1). *Then there exists a $c_0 > 0$ depending only on the data (but not on M and T) such that*

$$u_i(t) \geq c_0 \quad \textit{a.e. in } \Omega \quad \forall t \in S,\ i = n, p,$$

for any solution (u, v) to (4.1).

Proof.

(1) Let (u, v) be a solution to $(\mathrm{P_M})$. We set

$$K := \max\Big\{ \max_{i=n,p} \|\ln e_i(v_i^D)\|_{L^\infty}, \max_{i=n,p} \|\big(\ln u_i^0\big)^-\|_{L^\infty} \Big\}.$$

Our choice of K, (A2), (A3), and (A6) guarantee that $\big(\ln u_i + K\big)^-(0) = 0$ and $\big(\ln u_i + K\big)^- \in L^2(S, V_0)$, $i = n, p$. We show the assertion for $i = n$ and use the test function

$$-\alpha\, \mathrm{e}^{\alpha t}\big(0, \frac{z^{\alpha-1}}{u_n}, 0\big) \in L^2(S, V), \quad \alpha \geq 2, \quad z := \big(\ln u_n + K\big)^-.$$

(Analogously this can be done for $i = p$.) Note that due to the definition of the reaction rate, the boundedness of r_0 and the charge carrier density and the sign of the test function

$$R\frac{z^{\alpha-1}}{u_n} = r_0(u_n, u_p)u_n u_p\Big(1 - \exp\big\{-e_n^{-1}(u_n) - e_p^{-1}(u_p)\big\}\Big)\frac{z^{\alpha-1}}{u_n} \leq c z^{\alpha-1}. \tag{4.17}$$

We arrive at

$$\begin{aligned}
&\mathrm{e}^{\alpha t}\|z(t)\|^\alpha_{L^\alpha}\\
&\leq \int_0^t \mathrm{e}^{\alpha s}\alpha \int_\Omega \Big\{\mu_n u_n \nabla(v_n - v_0)\cdot\nabla\Big(\frac{z^{\alpha-1}}{u_n}\Big) + c(z^\alpha + z^{\alpha-1})\Big\}\,\mathrm{d}x\,\mathrm{d}s\\
&\leq \int_0^t \mathrm{e}^{\alpha s}\alpha \int_\Omega \Big\{\mu_n(\nabla v_n - \nabla v_0)\cdot\nabla z\Big((\alpha-1)z^{\alpha-2} + z^{\alpha-1}\Big) + c(z^\alpha + 1)\Big\}\,\mathrm{d}x\,\mathrm{d}s.
\end{aligned} \tag{4.18}$$

With (2.6) it holds that $e_0 e_n'(y) \leq e_n(y)$ for all $y \in \mathbb{R}$ and with $e_0 = 1$ such that

$$\begin{aligned}
\nabla v_n \cdot \nabla z &= -|\nabla v_n|^2 \frac{e_{Mn}'(v_n)\chi_{\mathrm{supp}\ z}}{e_{Mn}(v_n)}\\
&\leq -e_0\Big(|\nabla v_n|\frac{e_{Mn}'(v_n)\chi_{\mathrm{supp}\ z}}{e_{Mn}(v_n)}\Big)^2 = -e_0|\nabla z|^2.
\end{aligned} \tag{4.19}$$

Moreover, we rewrite

$$\begin{aligned}
\alpha(\alpha-1)z^{\alpha-2}|\nabla z|^2 &= \frac{4(\alpha-1)}{\alpha}|\nabla z^{\alpha/2}|^2,\\
\alpha z^{\alpha-1}|\nabla z|^2 &= \frac{4\alpha}{(\alpha+1)^2}|\nabla z^{(\alpha+1)/2}|^2,\\
\alpha\nabla v_0 \cdot \nabla z z^{\alpha-1} &= 2\nabla v_0 \cdot \nabla z^{\alpha/2} z^{\alpha/2}\\
&\leq 2|\nabla v_0|\,|\nabla z^{\alpha/2}|\,|z^{\alpha/2}|,\\
\alpha(\alpha-1)\nabla v_0 \cdot \nabla z z^{\alpha-2} &= 2(\alpha-1)\nabla v_0 \cdot \nabla z^{\alpha/2} z^{\alpha/2-1}\\
&\leq 2(\alpha-1)|\nabla v_0|\,|\nabla z^{\alpha/2}|\,(|z^{\alpha/2}| + 1)
\end{aligned}$$

and continue our estimate (4.18) with suitable $\delta > 0$ and $\widehat{c} > 1$ by

$$\begin{aligned}
&\mathrm{e}^{\alpha t}\|z(t)\|^\alpha_{L^\alpha}\\
&\leq -\int_0^t \mathrm{e}^{\alpha s}\alpha \int_\Omega e_0\mu_n|\nabla z|^2((\alpha-1)z^{\alpha-2} + z^{\alpha-1})\,\mathrm{d}x\,\mathrm{d}s\\
&\quad + \int_0^t \mathrm{e}^{\alpha s}\alpha \int_\Omega \Big\{\mu_n \nabla v_0 \cdot \nabla z\,\Big((\alpha-1)z^{\alpha-2} + z^{\alpha-1}\Big) + c(z^\alpha + 1)\Big\}\,\mathrm{d}x\,\mathrm{d}s
\end{aligned}$$

$$\le \int_0^t \mathrm{e}^{\alpha s}\Big\{ -\delta\|z^{\alpha/2}\|_{H^1}^2 - \frac{\delta}{\alpha}\|z^{(\alpha+1)/2}\|_{H^1}^2 + c\alpha\|\nabla v_0\|_{L^q}(\|z^{\alpha/2}\|_{L^r}+1)\|z^{\alpha/2}\|_{H^1} + c\alpha(\|z^{\alpha/2}\|_{L^2}^2+1)\Big\}\,\mathrm{d}s$$

$$\le \int_0^t \mathrm{e}^{\alpha s}\Big\{ - \frac{\delta}{\alpha}\|z^{(\alpha+1)/2}\|_{H^1}^2 + \widehat{c}\alpha^{2r}\kappa(\|z^{\alpha/2}\|_{L^1}^2+1)\Big\}\,\mathrm{d}s. \tag{4.20}$$

Here we used Hölder's, Gagliardo-Nirenberg's and Young's inequality and the definition of κ in (4.16).

(2) With the estimate for values $\rho \in \mathbb{R}_+$ and the function $z \in V_0$

$$\rho\,\|z\|_{L^1}^2 \le \rho\, c\,\|z\|_{L^{3/2}}^2 = \rho\, c\,\|z^{3/2}\|_{L^1}^{4/3} \le \rho\, c\,\|z^{3/2}\|_{H^1}^{4/3} \le \frac{\delta}{2}\|z^{3/2}\|_{H^1}^2 + c\,\rho^3,$$

we now consider the inequality (4.20) for $\alpha = 2$ and get $\|z(t)\|_{L^2}^2 \le c\kappa^3$ for all $t \in S$. Therefore $\|z(t)\|_{L^1} \le c\|z(t)\|_{L^2} \le c\kappa^{3/2}$ for all $t \in S$.
For arbitrary $\alpha \ge 2$, we exploit (4.20) and omit the first term on the right-hand side to obtain

$$\|z(t)\|_{L^\alpha}^\alpha \le \widehat{c}\alpha^{2r-1}\kappa(\sup_{s\in S}\|z^{\alpha/2}(s)\|_{L^1}^2+1). \tag{4.21}$$

(3) Setting now

$$\omega_m = \sup_{s\in S}\|z(s)\|_{L^{2^m}}^{2^m}+1, \quad m=0,1,2,\dots$$

we find from (4.21) for $\alpha = 2^m$, $m \ge 1$, that $\omega_m \le \widetilde{c}^m\kappa\omega_{m-1}^2$, $\widetilde{c} := \widehat{c}2^{2r}$, and repeated application gives $\omega_m \le (\widetilde{c}\kappa\,\omega_0)^{2^m}$ which means $\|z(t)\|_{L^{2^m}} \le \widetilde{c}\kappa(\sup_{s\in S}\|z(s)\|_{L^1}+1)$, and leads in the limit $m \to \infty$ to

$$\|z(t)\|_{L^\infty} \le \widetilde{c}\kappa(\sup_{s\in S}\|z(s)\|_{L^1}+1) \quad \forall t \in S. \tag{4.22}$$

Together with the uniform bound $\|z(t)\|_{L^1} \le c\|z(t)\|_{L^2} \le c\kappa^{3/2}$ we obtain $\|z(t)\|_{L^\infty} \le c\kappa^{5/2}$ for all $t \in S$. This ensures

$$-\ln u_n(t) \le K + c\kappa^{5/2}, \quad \mathrm{e}^{-K-c\kappa^{5/2}} \le u_n(t) \quad \text{a.e. in } \Omega \quad \forall t \in S.$$

□

4.3. Global solvability of problem (P).

THEOREM 4.1. *We assume* (A1) – (A6), *and* (A1'). *Then, for all* $T > 0$, $S = [0,T]$, *there is a solution to problem*

$$\begin{aligned} &u' + A(v) = 0, \quad u = E(v) \ \text{a.e. on } S, \quad u(0) = u^0, \\ &u \in H^1(S,V^*), \quad v - v^D \in L^2(S,V)\cap L^\infty(S,Z). \end{aligned} \tag{P$_\mathrm{S}$}$$

Proof. For arbitrarily chosen $T > 0$, $S = [0,T]$ the problem (P$_\mathrm{M}$) has a solution, see Lemma 4.2. The a priori estimates for (P$_\mathrm{M}$) in Lemma 4.3 guarantee that for M sufficiently large every solution (u,v) to (P$_\mathrm{M}$) satisfies the equalities $D_M v_i = v_i$, $i = n,p$. Therefore, the reaction terms in $A_M(u,v_0,v)$ and $A(v)$ coincide and we have $E_M(v) = E(v)$, $A_M(u,v_0,v) = A(v)$ and the pair (u,v) is a solution to (P$_\mathrm{S}$), too. □

REMARK 4.1. Due to the dependence of the mobilities on $|\nabla v_0|$ the question of uniqueness of the solution remains still an open question. Other forms of the dependency of the mobilities on the gradients of the quasi Fermi potentials but with included monotonicity properties have been discussed e.g. in [9].

5. Global bounds for solutions to (P)

In the two-dimensional case, global bounds for solutions of the van Roosbroeck system in case of inorganic semiconductors are obtained by the following rules (see e.g. [7,8]). Estimates of the free energy (estimates of $\|u_i \ln u_i\|_{L^1}$ in the Boltzmann case) ensure the start of a Moser iteration for powers of (truncated) charge-carrier densities $(u_i - K)^+$ to obtain global L^∞ bounds for u_i. However, in our case of organic semiconductors the statistical relation does not fulfill $\lim_{y\to+\infty} e_i(y) = +\infty$ and we have $\lim_{y\to+\infty} e_i'(y) = 0$; this technique does not work.

In the case of inorganic semiconductors, with the knowledge of global upper bounds another Moser iteration for $(\ln u_i + K)^-$ guarantees the global positive lower bounds of the densities u_i (see [7,8]). In the case of organic materials we benefit from the fact that $u_i < N_{i0}$ and argue in a similar way to obtain positive lower bounds.

After obtaining these lower bounds we are able to verify suited upper bounds for u_i less than N_{i0} by choosing powers of the function $(\mathrm{e}^{v_i} - K)^+$ for a Moser iteration technique (see Theorem 5.2).

5.1. Global positive lower bounds for solutions to (P).

THEOREM 5.1. *We assume* (A1) – (A6), *and* (A1'). *Then there exists a* $c_0 > 0$ *depending only on the data such that any solution* (u, v) *to* (P) *fulfills*

$$u_i(t) \geq c_0, \quad v_i = e_i^{-1}(u_i) \geq e_i^{-1}(c_0) \quad a.e. \ in\ \Omega \quad \forall t \in \mathbb{R}_+,\ i = n, p.$$

Proof. For any fixed $T > 0$, $S = [0, T]$ the proof of Lemma 4.3 can be done almost in the same way for Problem $(\mathrm{P_S})$ itself. Note that for solutions to (P) we have $u = E(v)$, $v \in L^2(S, H^1(\Omega))$, $(v_i)^- \in L^\infty(S, L^\infty(\Omega))$ and $e_i'(y) \leq c$ such that it is guaranteed that $\frac{[(\ln u_i + K)^-]^{\alpha-1}}{u_i} \in L^2(S, H_0^1)$, $\alpha \geq 2$, is an admissible test function.

In the estimate (4.19) we now argue directly with the original statistical relation e_i instead of e_{Mi}, $i = n, p$. Since the lower bounds for the charge carrier densities established in the proof do not depend on the length T of the time interval S, we obtain the desired global bound. ∎

5.2. Global upper bounds for solutions to (P).

For the derivation of global upper bounds for the densities u_i strictly lower than N_{i0} we verify global finite upper bounds for the potentials v_i, more precisely, for e^{v_i}, $i = n, p$. This is recommendable, since for test functions of the form

$$\frac{\left[(\mathrm{e}^{v_i} - K)^+\right]^{\alpha-1} \mathrm{e}^{v_i}}{e_i'(v_i)} \tag{5.1}$$

in a corresponding Moser iteration, all terms arising from the test of the continuity equation for u_i can be handled. Here the estimates of Lemma 2.1 play an important role.

However, we can not use the function in (5.1) directly since it is not a priori clear that it belongs to $L^2_{\mathrm{loc}}(\mathbb{R}_+, H_0^1)$. We have to approximate it by substituting v_i in (5.1) by $v_L := \min(v_i, L)$ for L large enough and considering the limit $L \to \infty$ in the resulting estimates.

THEOREM 5.2. *We assume* (A1) – (A6), *and* (A1'). *Then there exists a* $c_* < 1$ *depending only on the data such that any solution* (u, v) *to* (P) *satisfies*

$$u_i(t) \leq c_* N_{i0} \quad a.e. \ in\ \Omega \quad \forall t \in \mathbb{R}_+,\ i = n, p.$$

Proof.

(1) Let (u, v) be a solution to (P). We set

$$K := \max\Big\{ \max_{i=n,p} \mathrm{e}^{\|v_i^D\|_{L^\infty}}, \max_{i=n,p} \mathrm{e}^{\|e_i^{-1}(u_i^0)\|_{L^\infty}}, \max_{i=n,p} \mathrm{e}^{s_i-\zeta_i} \Big\}.$$

Lemma 2.1 ensures for $v_i \geq s_i - \zeta_i$ the inequalities

$$\begin{aligned} \frac{\mathrm{e}^{\zeta_i}}{\overline{c}(s_i)N_{i0}} &\leq \frac{1}{\mathrm{e}^{v_i}e_i'(v_i)} = \frac{\mathrm{e}^{\zeta_i}}{\mathrm{e}^{v_i+\zeta_i}N_{i0}\mathcal{G}_{s_i}'(v_i+\zeta_i)} \leq \frac{\mathrm{e}^{\zeta_i}}{\underline{c}(s_i)N_{i0}}, \\ \frac{|e_i''(v_i)|}{e_i'(v_i)} &= \frac{|\mathcal{G}_{s_i}''(v_i+\zeta_i)|}{\mathcal{G}_{s_i}'(v_i+\zeta_i)} \leq \frac{3\overline{c}(s_i)}{\underline{c}(s_i)}, \quad e_i''(v_i) < 0, \quad i = n, p. \end{aligned} \tag{5.2}$$

We show the assertion of the theorem for $i = n$ (analogously this can be done for $i = p$).

(2) Let

$$L > \ln K > 0, \quad v_L := \min(v_i, L), \quad \widetilde{L} := e_n(L), \quad u_{\widetilde{L}} := \min(u_n, \widetilde{L}).$$

We intend to use the test function

$$\alpha\, \mathrm{e}^{\alpha t}(0, F_L(v_n), 0) := \alpha\, \mathrm{e}^{\alpha t}\Big(0, \frac{z_L^{\alpha-1}\mathrm{e}^{v_L}}{e_n'(v_L)}, 0\Big), \quad \alpha \geq 2, \quad z_L := \big(\mathrm{e}^{v_L} - K\big)^+. \tag{5.3}$$

Since $e_n'(y) > 0\ \forall\, y$ and $\mathcal{G}_s''(\eta) < 0$ for all $\eta \geq 0$, we obtain $e_n'(v_L) \geq c(L) > 0$ for $v_n \geq \ln K$. Moreover, $\mathrm{e}^{v_L} < \widetilde{c}(L)$. (5.2) ensures an upper bound for $|e_n''(v_L)|$. Thus we find an estimate for

$$\begin{aligned} \nabla F_L(v_n) = \Big\{ &\frac{(\alpha-1)[(\mathrm{e}^{v_L} - K)^+]^{\alpha-2}\mathrm{e}^{2v_L}}{e_n'(v_L)} + \frac{[(\mathrm{e}^{v_L} - K)^+]^{\alpha-1}\mathrm{e}^{v_L}}{e_n'(v_L)} \\ &- \frac{[(\mathrm{e}^{v_L} - K)^+]^{\alpha-1}\mathrm{e}^{v_L}e_n''(v_L)}{(e_n'(v_L))^2} \Big\} \nabla v_n\ \chi_{\{x:\ln K \leq v_n \leq L\}} \end{aligned}$$

such that $F_L(v_n) \in L^2_{\mathrm{loc}}(\mathbb{R}_+, H^1)$. Moreover, our choice of K guarantees that $z_L(0) = 0$ and $z_L = 0$ on Γ_D. Thus, $F_L(v_n) \in L^2_{\mathrm{loc}}(\mathbb{R}_+, H^1_0)$, and (5.3) is an admissible test function.

Next, we rewrite

$$F_L(v_n) = \frac{[(\mathrm{e}^{e_n^{-1}(u_{\widetilde{L}})} - K)^+]^{\alpha-1}\mathrm{e}^{e_n^{-1}(u_{\widetilde{L}})}}{e_n'(e_n^{-1}(u_{\widetilde{L}}))} =: \widetilde{u}_{\widetilde{L}}$$

and obtain

$$\int_0^t \alpha\mathrm{e}^{\alpha s}\langle u_n', \widetilde{u}_{\widetilde{L}}\rangle\, \mathrm{d}s = \int_\Omega \big(\mathrm{e}^{\alpha t}g(u_n(t)) - g(u_n^0)\big)\, \mathrm{d}x - \int_0^t \int_\Omega \alpha\mathrm{e}^{\alpha s}g(u_n(s))\, \mathrm{d}x\, \mathrm{d}s, \tag{5.4}$$

where

$$g(y) := \int_0^y \frac{[(\mathrm{e}^{e_n^{-1}(\min(\tau,\widetilde{L}))} - K)^+]^{\alpha-1}\mathrm{e}^{e_n^{-1}(\min(\tau,\widetilde{L}))}}{e_n'(e_n^{-1}(\min(\tau,\widetilde{L})))}\, \mathrm{d}\tau.$$

The validity of (5.4) is clear for smooth $u_n \in H^1_{\rm loc}(\mathbb{R}_+, H)$. For general u_n the validity of this relation is obtained via approximation by smooth functions and passing to the limit. Note that due to the choice of K we have $g(u_n^0) = 0$. Additionally, we have that

$$g(u_n) \geq g(\min(u_n, \widetilde{L})) = g(u_{\widetilde{L}}) = \int_0^{\min(u_n,\widetilde{L})} \frac{[(\mathrm{e}^{e_n^{-1}(\min(\tau,\widetilde{L}))} - K)^+]^{\alpha-1} \mathrm{e}^{e_n^{-1}(\min(\tau,\widetilde{L}))}}{e_n'(e_n^{-1}(\min(\tau,\widetilde{L})))}\,\mathrm{d}\tau$$
$$= [(\mathrm{e}^{e_n^{-1}(\min(u_n,\widetilde{L}))} - K)^+]^\alpha = [(\mathrm{e}^{\min(v_n,L)} - K)^+]^\alpha = [(\mathrm{e}^{v_L} - K)^+]^\alpha = z_L^\alpha.$$

Moreover, using (5.2), $g(u_n)$ can be estimated from above by

$$g(u_n) = g(u_{\widetilde{L}}) + g(u_n) - g(u_{\widetilde{L}}) \leq g(u_{\widetilde{L}}) + (u_n - \widetilde{L})^+ \frac{[(\mathrm{e}^{e_n^{-1}(u_{\widetilde{L}})} - K)^+]^{\alpha-1} \mathrm{e}^{e_n^{-1}(u_{\widetilde{L}})}}{e_n'(e_n^{-1}(u_{\widetilde{L}}))}$$
$$\leq z_L^\alpha + N_{n0} \frac{[(\mathrm{e}^{v_L} - K)^+]^{\alpha-1} \mathrm{e}^{v_L} \mathrm{e}^{v_L}}{e_n'(v_L)\,\mathrm{e}^{v_L}} \leq z_L^\alpha + c z_L^{\alpha-1}(z_L + K)^2 \leq c(z_L^{\alpha+1} + 1).$$

(3) Note that due to the form of the reaction rate, the boundedness of r_0 and of the charge carrier densities by N_{i0} and the lower bounds for v_i, $i = n, p$, from Theorem 5.1 and (5.2) we arrive at the estimate

$$-R \frac{z_L^{\alpha-1} \mathrm{e}^{v_L}}{e_n'(v_L)} = r_0(n,p) np \Big(\mathrm{e}^{-v_n - v_p} - 1\Big) \frac{z_L^{\alpha-1} \mathrm{e}^{v_L}}{e_n'(v_L)}$$
$$\leq c \frac{z_L^{\alpha-1} \mathrm{e}^{v_L} \mathrm{e}^{v_L}}{\mathrm{e}^{v_L} e_n'(v_L)} \leq c z_L^{\alpha-1}(z_L + K)^2 \leq c(z_L^{\alpha+1} + 1). \tag{5.5}$$

(4) Using the test function (5.3) and the relation (5.4), the estimates for the function g, and (5.5) it follows that

$$\mathrm{e}^{\alpha t} \|z_L(t)\|_{L^\alpha}^\alpha$$
$$\leq \int_0^t \mathrm{e}^{\alpha s} \alpha \int_\Omega \Big\{ -\mu_n u_n \nabla(v_n - v_0) \cdot \nabla\Big(\frac{z_L^{\alpha-1} \mathrm{e}^{v_L}}{e_n'(v_L)}\Big) + c(z_L^{\alpha+1} + 1)\Big\}\,\mathrm{d}x\,\mathrm{d}s$$
$$= \int_0^t \mathrm{e}^{\alpha s} \int_\Omega \Big\{ -\mu_n u_n \Big(I_1 + I_2 + I_3 + I_4 + I_5 + I_6\Big) + c\alpha(z_L^{\alpha+1} + 1)\Big\}\,\mathrm{d}x\,\mathrm{d}s, \tag{5.6}$$

where the terms I_i, $i = 1, \ldots, 6$, are defined and estimated separately. We use the properties $\nabla v_n \cdot \nabla z_L = |\nabla z_L|^2 \mathrm{e}^{-v_L}$, $z_L < \mathrm{e}^{v_L}$, $\nabla v_n \cdot \nabla v_L = |\nabla v_L|^2$ as well as the estimates in (5.2) such that

$$I_1 := \alpha(\alpha-1) \nabla v_n \cdot \nabla z_L\, z_L^{\alpha-2} \frac{\mathrm{e}^{v_L}}{e_n'(v_L)} \geq \alpha(\alpha-1) |\nabla z_L|^2 z_L^{\alpha-2} \frac{z_L}{\mathrm{e}^{v_L} e_n'(v_L)}$$
$$= \alpha(\alpha-1) |\nabla z_L|^2 z_L^{\alpha-1} \frac{1}{\mathrm{e}^{v_L} e_n'(v_L)} = \frac{4\alpha(\alpha-1)}{(\alpha+1)^2} \frac{|\nabla z_L^{(\alpha+1)/2}|^2}{\mathrm{e}^{v_L} e_n'(v_L)}$$
$$\geq \frac{8}{9} \frac{\mathrm{e}^{\zeta_n}}{\bar{c}(s_n) N_{n0}} |\nabla z_L^{(\alpha+1)/2}|^2,$$

$$I_2 := -\alpha \nabla v_n \cdot \nabla v_L\, z_L^{\alpha-1} \frac{\mathrm{e}^{v_L} e_n''(v_L)}{(e_n'(v_L))^2} \geq 0, \qquad I_3 := \alpha |\nabla v_L|^2 z_L^{\alpha-1} \frac{\mathrm{e}^{v_L}}{e_n'(v_L)} \geq 0.$$

Moreover, for the term I_4 we have the estimate

$$\begin{aligned}
I_4 &:= \alpha(\alpha-1)\nabla v_0\cdot\nabla z_L\, z_L^{\alpha-2}\frac{\mathrm{e}^{v_L}}{e_n'(v_L)} = \alpha(\alpha-1)\nabla v_0\cdot\nabla z_L\, z_L^{\frac{\alpha-1}{2}} z_L^{\frac{\alpha-3}{2}}\frac{\mathrm{e}^{v_L}}{e_n'(v_L)}\\
&= \frac{2\alpha(\alpha-1)}{\alpha+1}\nabla v_0\cdot\nabla(z_L^{\frac{\alpha+1}{2}})z_L^{\frac{\alpha-3}{2}}\frac{\mathrm{e}^{v_L}\mathrm{e}^{v_L}}{\mathrm{e}^{v_L}e_n'(v_L)},\\
|I_4| &\le c\alpha|\nabla v_0||\nabla z_L^{\frac{\alpha+1}{2}}|\big(|z_L^{\frac{\alpha+1}{2}}|+1\big)\frac{1}{\mathrm{e}^{v_L}e_n'(v_L)} \le c\alpha|\nabla v_0||\nabla z_L^{\frac{\alpha+1}{2}}|\big(|z_L^{\frac{\alpha+1}{2}}|+1\big).
\end{aligned}$$

Finally, for I_5 and I_6, we compute that

$$\begin{aligned}
I_5 &:= -\alpha\nabla v_0\cdot\nabla v_L\, z_L^{\alpha-1}\frac{\mathrm{e}^{v_L}e_n''(v_L)}{(e_n'(v_L))^2} = -\alpha\nabla v_0\cdot\nabla z_L z_L^{\frac{\alpha-1}{2}} z_L^{\frac{\alpha-1}{2}}\frac{\mathrm{e}^{v_L}}{\mathrm{e}^{v_L}e_n'(v_L)}\frac{e_n''(v_L)}{e_n'(v_L)},\\
|I_5| &\le c|\nabla v_0||\nabla z_L^{(\alpha+1)/2}|\big(|z_L^{\frac{\alpha+1}{2}}|+1\big)\frac{1}{\mathrm{e}^{v_L}e_n'(v_L)}\frac{|e_n''(v_L)|}{e_n'(v_L)}\\
&\le c|\nabla v_0||\nabla z_L^{(\alpha+1)/2}|\big(|z_L^{\frac{\alpha+1}{2}}|+1\big),\\
I_6 &:= \alpha\nabla v_0\cdot\nabla v_L\, z_L^{\alpha-1}\frac{\mathrm{e}^{v_L}}{e_n'(v_L)} = \alpha\nabla v_0\cdot\nabla z_L z_L^{\frac{\alpha-1}{2}} z_L^{\frac{\alpha-1}{2}}\frac{\mathrm{e}^{v_L}}{\mathrm{e}^{v_L}e_n'(v_L)},\\
|I_6| &\le c|\nabla v_0||\nabla z_L^{(\alpha+1)/2}|\big(|z_L^{\frac{\alpha+1}{2}}|+1\big)\frac{1}{\mathrm{e}^{v_L}e_n'(v_L)} \le c|\nabla v_0||\nabla z_L^{(\alpha+1)/2}|\big(|z_L^{\frac{\alpha+1}{2}}|+1\big).
\end{aligned}$$

The estimates for I_i, $i=1,\dots,6$, $\mathrm{mes}(\Gamma_D)>0$, (A4), (A5), (5.6) and the global positive lower estimates of the charge carrier densities from Theorem 5.1 ensure with a suitable $\delta>0$ that

$$\begin{aligned}
\mathrm{e}^{\alpha t}\|z_L(t)\|_{L^\alpha}^\alpha &\le \int_0^t \mathrm{e}^{\alpha s}\Big\{-\delta\|z_L^{\frac{\alpha+1}{2}}\|_{H^1}^2 + c\alpha(\|z_L^{\frac{\alpha+1}{2}}\|_{L^2}^2+1)\\
&\qquad + c\alpha\|\nabla v_0\|_{L^q}(\|z_L^{\frac{\alpha+1}{2}}\|_{L^r}+1)\|z_L^{\frac{\alpha+1}{2}}\|_{H^1}\Big\}\,\mathrm{d}s\\
&\le \int_0^t \mathrm{e}^{\alpha s}\Big\{-\frac{\delta}{2}\|z_L^{\frac{\alpha+1}{2}}\|_{H^1}^2 + \widehat{c}\alpha^{2r}\kappa(\|z_L^{\frac{\alpha+1}{2}}\|_{L^1}^2+1)\Big\}\,\mathrm{d}s, \qquad (5.7)
\end{aligned}$$

where we used the quantities q, r and κ from Lemma 3.1 and (4.16). As in the estimate (4.21) in the proof of Lemma 4.3, we applied Hölder's, Gagliardo-Nirenberg's and Young's inequality, but now for the function $z_L^{\frac{\alpha+1}{2}}$ instead of $z_L^{\frac{\alpha}{2}}$.

(5) Next, we estimate

$$\begin{aligned}
\|z_L^{\frac{\alpha+1}{2}}\|_{L^1}^2 &= \Big(\int_\Omega z_L^{\frac{\alpha+1}{2}}\,\mathrm{d}x\Big)^{\frac{4}{\alpha+1}} \le \Big(\|z_L^{\frac{\alpha}{4}}\|_{L^2}\|z_L^{\frac{\alpha+2}{4}}\|_{L^2}\Big)^{\frac{4}{\alpha+1}}\\
&= \Big(\|z_L^{\frac{\alpha}{2}}\|_{L^1}^{\frac12}\,\|z_L^{\frac{\alpha+1}{2}}\|_{L^{\frac{\alpha+2}{\alpha+1}}}^{\frac{\alpha+2}{2(\alpha+1)}}\Big)^{\frac{4}{\alpha+1}}\\
&= \|z_L^{\frac{\alpha}{2}}\|_{L^1}^{\frac{2}{\alpha+1}}\,\|z_L^{\frac{\alpha+1}{2}}\|_{L^{\frac{\alpha+2}{\alpha+1}}}^{\frac{2(\alpha+2)}{(\alpha+1)^2}} \le \widetilde{c}\|z_L^{\frac{\alpha}{2}}\|_{L^1}^{\frac{2}{\alpha+1}}\,\|z_L^{\frac{\alpha+1}{2}}\|_{H^1}^{\frac{2(\alpha+2)}{(\alpha+1)^2}}\\
&\le \widetilde{c}\Big(\frac{4\delta\widehat{c}\alpha^{2r}\kappa}{4\delta\widehat{c}\alpha^{2r}\kappa}\Big)^{\frac{\alpha+2}{(\alpha+1)^2}}\|z_L^{\frac{\alpha}{2}}\|_{L^1}^{\frac{2}{\alpha+1}}\,\|z_L^{\frac{\alpha+1}{2}}\|_{H^1}^{\frac{2(\alpha+2)}{(\alpha+1)^2}}\\
&\le \frac{\delta}{4}\frac{1}{\widehat{c}\alpha^{2r}\kappa}\|z_L^{\frac{\alpha+1}{2}}\|_{H^1}^2 + \widetilde{c}^{\frac{(\alpha+1)^2}{\alpha^2+\alpha-1}}\Big(\frac{4\widehat{c}\alpha^{2r}\kappa}{\delta}\Big)^{\frac{\alpha+2}{\alpha^2+\alpha-1}}\|z_L^{\frac{\alpha}{2}}\|_{L^1}^{\frac{2(\alpha+1)}{\alpha^2+\alpha-1}}\\
&\le \frac{\delta}{4}\frac{1}{\widehat{c}\alpha^{2r}\kappa}\|z_L^{\frac{\alpha+1}{2}}\|_{H^1}^2 + \widetilde{c}^{\frac{(\alpha+1)^2}{\alpha^2+\alpha-1}}\Big(\frac{4\widehat{c}\alpha^{2r}\kappa}{\delta}\Big)^{\frac{\alpha+2}{\alpha^2+\alpha-1}}(\|z_L^{\frac{\alpha}{2}}\|_{L^1}^2+1)
\end{aligned}$$

which leads together with (5.7) and a suitable $c_\delta > 1$ to

$$\begin{aligned}&\mathrm{e}^{\alpha t}\|z_L(t)\|^\alpha_{L^\alpha}\\ &\le \int_0^t \mathrm{e}^{\alpha s}\Big\{ -\frac{\delta}{4}\|z_L^{\frac{\alpha+1}{2}}\|^2_{H^1} + \widetilde{c}^{\frac{(\alpha+1)^2}{\alpha^2+\alpha-1}}\Big(\frac{4}{\delta}\Big)^{\frac{\alpha+2}{\alpha^2+\alpha-1}}\Big(\widehat{c}\alpha^{2r}\kappa\Big)^{1+\frac{(\alpha+1)^2}{\alpha^2+\alpha-1}}(\|z_L^{\frac{\alpha}{2}}\|^2_{L^1}+1)\Big\}\,\mathrm{d}s\\ &\le \int_0^t \mathrm{e}^{\alpha s}\Big\{ -\frac{\delta}{4}\|z_L^{\frac{\alpha+1}{2}}\|^2_{H^1} + c_\delta\alpha^{6r}(\|z_L^{\frac{\alpha}{2}}\|^2_{L^1}+1)\Big\}\,\mathrm{d}s. \qquad (5.8)\end{aligned}$$

(6) We find for values $\rho \in \mathbb{R}_+$

$$\rho\,\|z_L\|^2_{L^1} \le \rho\, c\,\|z_L\|^2_{L^{3/2}} = \rho\, c\,\|z_L^{3/2}\|^{4/3}_{L^1} \le \rho\, c\,\|z_L^{3/2}\|^{4/3}_{H^1} \le \frac{\delta}{2}\|z_L^{3/2}\|^2_{H^1} + c\,\rho^3.$$

Inserting this in estimate (5.8) for $\alpha = 2$ we establish that $\|z_L(t)\|_{L^2} \le c$ for all $t \in \mathbb{R}_+$ and therefore also $\sup_{t\in\mathbb{R}_+}\|z_L(t)\|_{L^1} \le c$.
For arbitrary $\alpha \ge 2$, it results from (5.8) that

$$\|z_L(t)\|^\alpha_{L^\alpha} \le c_\delta\alpha^{6r-1}\big(\sup_{s\in S}\|z_L^{\frac{\alpha}{2}}(s)\|^2_{L^1}+1\big). \qquad (5.9)$$

(7) Setting now

$$\omega_m = \sup_{s\in\mathbb{R}_+}\|z_L(s)\|^{2^m}_{L^{2^m}} + 1, \quad m = 0,1,2,\dots$$

we find from (5.9) for $\alpha = 2^m$, $m \ge 1$, and $\overline{c} := c_\delta\, 2^{6r}$ that $\omega_m \le \overline{c}^m\omega^2_{m-1}$ and repeated application gives $\omega_m \le (\overline{c}\,\omega_0)^{2^m}$ which means $\|z_L(t)\|_{L^{2^m}} \le \overline{c}\,(\sup_{s\in\mathbb{R}_+}\|z_L(s)\|_{L^1}+1)$, and leads in the limit $m \to \infty$ to

$$\|z_L(t)\|_{L^\infty} \le \overline{c}\,(\sup_{s\in\mathbb{R}_+}\|z_L(s)\|_{L^1}+1) \quad \forall t\in\mathbb{R}_+. \qquad (5.10)$$

With the uniform estimate for $\sup_{t\in\mathbb{R}_+}\|z_L(t)\|_{L^1}$, (5.10) ensures that $\|z_L(t)\|_{L^\infty} \le c_\infty$ for all $t \in \mathbb{R}_+$.

(8) The constant c_∞ does not depend on the choice of L. Therefore we can pass to the limit $L \to \infty$ in this estimate and derive $\|\big(\mathrm{e}^{v_n} - K\big)^+(t)\|_{L^\infty} \le c_\infty$ and

$$\mathrm{e}^{v_n(t)} \le K + c_\infty, \quad v_n(t) \le \ln(K+c_\infty), \quad u_n(t) \le e_n(\ln(K+c_\infty)) < N_{n0} \quad \forall t\in\mathbb{R}_+.$$

□

Remark 5.1. Using the global positive lower bounds for the charge carrier densities of solutions to (P) established in Theorem 5.1 and the energy estimates performed in (3.7) in the proof of Theorem 3.1, we obtain, under the assumptions (A1) – (A6), and (A1'), the estimates $\|\varphi_i\|_{L^2(S,H^1)} \le c(S)$, $i = n,p$. Together with the $W^{1,q}$ estimate for v_0 from Lemma 3.1 and the relation of φ_i and v_i estimates of the form $\|v_i\|_{L^2(S,H^1)} \le c(S)$, $i = n,p$, with a constant $c(S)$ also depending on the length of the time interval $S = [0,T]$ are ensured. Furthermore, together with the global upper bounds for v_n, v_p this leads to the estimates for the whole vectors

$$\|A(v)\|_{L^2(S,V^*)},\ \|u'\|_{L^2(S,V^*)} \le c(S).$$

Appendix. Properties of the free energy functional. We collect important properties of the free energy functional in the case of Gauss–Fermi statistics. First, note that

$$\begin{aligned}\frac{1}{N_{i0}}\int_{v_i^D}^{v_i} e_i(y)\,\mathrm{d}y = &\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big(-\frac{\xi^2}{2}\Big)\\ &\times\Big\{\ln[\exp\{-(s_i\xi - v_i - \zeta_i)\}+1] - \ln[\exp\{-(s_i\xi - v_i^D - \zeta_i)\}+1]\Big\}\mathrm{d}\xi\\ =&\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big(-\frac{\xi^2}{2}\Big)\Big\{\ln\frac{\exp\{-(s_i\xi - v_i-\zeta_i)\}+1}{\exp\{-(s_i\xi - v_i^D-\zeta_i)\}+1}\Big\}\,\mathrm{d}\xi\\ =&\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big(-\frac{\xi^2}{2}\Big)\Big\{v_i - v_i^D + \ln\frac{\exp\{-(s_i\xi-\zeta_i)\}+\exp\{-v_i\}}{\exp\{-(s_i\xi-\zeta_i)\}+\exp\{-v_i^D\}}\Big\}\,\mathrm{d}\xi.\end{aligned}\tag{6.1}$$

Here we used the relation

$$\ln\frac{\mathrm{e}^{a+b_1}+1}{\mathrm{e}^{a+b_2}+1} = \ln\frac{\mathrm{e}^{b_1}(\mathrm{e}^{a}+\mathrm{e}^{-b_1})}{\mathrm{e}^{b_2}(\mathrm{e}^{a}+\mathrm{e}^{-b_2})} = b_1 - b_2 + \ln\frac{\mathrm{e}^{a}+\mathrm{e}^{-b_1}}{\mathrm{e}^{a}+\mathrm{e}^{-b_2}}.\tag{6.2}$$

Second, for $u\in L^2(\Omega)^3$ with $u_i<0$ or $u_i>N_{i0}$ on a set $\mathcal{M}$ of positive measure for $i=n$ or $i=p$ it holds true that $\Psi(u)=+\infty$. (For this we argue as follows: Let, e.g., $u_n<0$ on a set $\mathcal{M}$. We take a subset $\mathcal{M}_0\subset\mathcal{M}$ of positive measure with $\mathcal{M}_0\cap\Gamma_D=\emptyset$ and choose $w=(0,w_n,0)\in V$ such that $w_n<0$ a.e. on $\mathcal{M}_0$, $w_n=0$ a.e. on $\Omega\setminus\mathcal{M}_0$. We define sequences $\{w^l\}_{l\in\mathbb{N}}$, $\{v^l\}_{l\in\mathbb{N}}$, with $w^l:=lw\in V$, $v^l:=w^l+v^D$. Then by (6.1), and $v_n^l<v_n^D$ on $\mathcal{M}_0$ we find $\Phi(v^l)<0$. Additionally, by construction $\langle u,w^l\rangle\to\infty$ as $l\to\infty$. Thus (3.6) ensures $\Psi(u)=+\infty$. Similar arguments can be used for $u_p<0$ on a set $\mathcal{M}$.

Let now $u_n>0$ a.e. in Ω and $u_n>N_{n0}$ on a set $\mathcal{M}$. We again use a corresponding subset $\mathcal{M}_0$ and take $w=(0,w_n,0)\in V$ such that $w_n>0$ on a.e. $\mathcal{M}_0$, $w_n=0$ a.e. on $\Omega\setminus\mathcal{M}_0$. We define sequences $\{w^l\}_{l\in\mathbb{N}}$, $\{v^l\}_{l\in\mathbb{N}}$, with $w^l:=lw\in V$, $v^l:=w^l+v^D$ and calculate

$$\begin{aligned}&\langle u,w^l\rangle-\Phi(v^l)\\ &=\int_{\mathcal{M}_0}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big(-\frac{\xi^2}{2}\Big)\Big\{u_nw_n^l - N_{n0}\Big\{\ln\frac{\exp\{-(s_n\xi-v_n^l-\zeta_i)\}+1}{\exp\{-(s_n\xi-v_n^D-\zeta_i)\}+1}\Big\}\Big\}\,\mathrm{d}\xi\,\mathrm{d}x\\ &\ge\int_{\mathcal{M}_0}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big(-\frac{\xi^2}{2}\Big)(u_n-N_{n0})lw_n\,\mathrm{d}\xi\,\mathrm{d}x\\ &\ge\int_{\mathcal{M}_0}(u_n-N_{n0})lw_n\,\mathrm{d}x\to+\infty\quad\text{as } l\to\infty\end{aligned}$$

and again obtain $\Psi(u)=+\infty$. In the last chain of estimates we used (6.2) where the last term is negative for $b_1>b_2$.

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